24th NATIONAL SEMINAR ON CRYSTAL GROWTH AND APPLICATIONS (XXIV NSCGA - 2020)

3-5, February - 2020

Organized By

Department of Physics
Periyar University
(NAAC A Grade – State University – NIRF Rank 68)
Salem - 636 011

In Association With

Indian Association of Crystal Growth (IACG)

National Advisory committee

Dr. Anbalagan. G, University of Madras, Chennai

Dr. Arivanandhan. M, Anna University, Chennai

Dr. Arun Kumar. R, PSG Technology, Coimbatore

Dr. Athimoolam. S, Anna University, Nagercoil Campus

Dr. Balachandar. S, AKSH Optifiber Pvt. Ltd., Rajasthan

Dr. Balakumar. S, University of Madras, Chennai

Dr. Bamzai. K. K, University of Jammu, Jammu

Dr. Binay Kumar, University of Delhi, New Delhi

Dr. Bhagavannarayana. G, VSM Institutions, Andhra Pradesh

Dr. Brahadeeswaran. S, BIT-Anna University, Trichy

Dr. Byrappa. K, Mangalore University, Karnataka

Dr. Chauhan. A.K, BARC, Mumbai

Dr. Das. S.K, KIIT University, Odisha

Dr. Deshpande, M.P, Sardar Patel University, Gujarat.

Dr. Elangovan. T , Periyar University, Salem

Dr. Gadkari. S. C, BARC, Mumbai

Dr. Gadkari. D. B, Mithibai College, Mumbai

Dr. Ganeshamoorthy. S, IGCAR, Kalpakkam

Dr. Ganesan. S, Indian Institute of Science (IISc), Bangalore

Dr. Ganesha. R. University of Mysore, Mysuru

Dr. Gopalakrishnan. N, NIT, Trichy

Dr. Bhat. H.L, IISc, Bangalore.

Dr. Gunasekaran. K. University of Madras, Chennai

Dr. Indranil Bhaumik, LMDDD, RRCAT, Indore

Dr. Jeganathan. K, BARD, Trichy

Dr. Jayavel. R, Anna University, Chennai

Dr. Jerome Das. S, Loyola College, Chennai

Dr. Kalainathan. S, VIT University, Vellore

Dr. Karnal. A. K, LMDDD, RRCAT, Indore

Dr. Karunagaran. N, SRM University, Chennai

Dr. Mani. V.N, DRDO, C-MET, Hyderabad

Dr. Maadeswaran. P, Periyar University, Salem

Dr. Madhusoodanan. U, IGCAR, Kalpakkam

Dr. Magesh. M, Saveetha University, Chenna

Dr. Mahadevan. C. K, PSNCET, Tirunelveli

Dr. Madhavan. J, Loyola College, Chennai

Dr. Meenakshi Sundaram. S. P, Annamalai University

Dr. Mihir J. Joshi, Saurashtra University, Gujarat

Dr. Moovendaran. K, Institute of Physics, Taiwan

Dr. Moorthy Babu. S, Anna University, Chennai

Dr. Mohan Kumar. R, Presidency College, Chennai

Dr. Mohit Tyagi, BARC, Mumbai

Dr. Murugakoothan. P, Pachaiyappa's College, Chennai

Dr. Natarajan. S, Madurai Kamaraj University, Madurai

Dr. Natarajan. V, RIC-DRDO, Chennai

Dr. Narayana Kalkura. S, Anna University, Chennai

Dr. Pari. S, National College, Trichy

Dr. Ravi. G, Alagappa University, Karaikudi

Dr. Rai. R.N, Banaras Hindu University, Varanasi

Dr. Radha Perumal Ramasamy, Anna University, Chennai

Dr. Rajan Babu. D, VIT University, Vellore

Dr. Rajesh. N. P, SSN Institutions, Chennai

Dr. Rajesh. P, SSN Institutions, Chennai

Dr. Rajni Kant, University of Jammu, Jammu

Dr. Ramachandra Raja. C, GAC, Kumbakonam

Dr. Ramachandra Rao. K, Govt. College, Rajamundry

Dr. Ramesh Babu. R, Bharathidasan University, Trichy

Dr. Raj. V, Periyar University, Salem

Dr. Ravichandran. A. T, National College, Trichy

Dr. Rewatkar. K, Dr. Ambedker College, Nagpur

Dr. Robert. R, Government College, Krishnagiri.

Dr. Sahaya Jude Dhas. S, Tagore Engg. College, Chennai

Dr. Sangeetha. K, Sastra University, Thanjavur

Dr. Sangeetha, BARC, Mumbai

Dr. Sankaranarayanan. K, Alagappa University Karaikudi

Dr. Sethuraman. K, Madurai Kamaraj University, Madurai

Dr. Selvarajan. P, Aditanar College, Tiruchendur

Dr. Shanthi. S, Anna University, Chennai

Dr. Shashwati Sen, BARC, Mumbai

Dr. Sivakumar. R, Alagappa University, Karaikudi

Dr. Srinivasan. K, Bharathiyar University, Coimbatore

Dr. Stella Marry. S, St. Peters University, Chennai

Dr. Suja Elizabeth, Indian Institute of Science, Bangalore

Dr. Sunil Verma, LMDDD, RRCAT, Indore

Dr. Suresh. K, Bharathiar University, Coimbatore

Dr. Tanusree Kar, IACS, Kolkatta

Dr. Thamizhavel. A, TIFR, Mumbai

Dr. Thangappan. R, Periyar University, Salem

Prof. Velmurugan. D, University of Madras, Chennai

Dr. Vijayan. N, NPL, New Delhi

Dr. Vinitha. G, VIT University, Chennai

ORGANIZING COMMITTEE

Chief Patron
Prof.P.Kolandaivel, Vice-Chancellor, Periyar University, Salem

Patron
Prof.K.Thangavel, Registrar(i/c), Periyar University, Salem

Co-Patron
Prof. V. Krishnakumar, Dean, Periyar University, Salem

Chief Chairman
Prof. P. Ramasamy, President, Indian Association for Crystal Growth (IACG).

Chairman
Prof. P. Kumaradhas, Head of the Department, Dept. of Physics, Periyar University, Salem

Convener and Organizing Secretary
Dr. J. Kalyana Sundar, Department of Physics, Periyar University, Salem

Joint Organizing Secretaries

Dr. Muthu Senthil Pandian, SSN Institutions, Chennai (IACG)
Dr. M. Srinivasan, SSN Institutions, Chennai (IACG)

Local Organizing Committee Members

Dr. E.K. Girija, Dept. of Physics, Periyar University, Salem
Dr. T. Pazhanivel, Dept. of Physics, Periyar University, Salem
Dr. R. Ramesh, Dept. of Physics, Periyar University, Salem
Dr. M. Selvapandiyan, Periyar University (PG Ext.), Dharmapuri
Dr. S. A. Martin Britto Dhas, Sacred Heart College, Tirupattur (IACG)

PERIYAR UNIVERSITY

NAAC Reaccredited 'A' Grade - State University

Salem - 636 011, Tamil Nadu, India

Professor P. Kolandaivel

Vice Chancellor

Date: 29-01-2020

MESSAGE

I am happy to that the Department of Physics, Periyar University, Salem is Organizing the **"XXIV National Seminar on Crystal Growth and Applications (XXIV NSCGA - 2020)"** to be held during 3-5, February 2020.

Wonderful to know that a large number of researchers and eminent scientists from all over India are participating in related topics of crystal growth and applications. The seminar particularly encourage the interaction of research scholars and budding scientists with more established scientific community in such way that it would be golden opportunity to present and to discuss the systematic investigation of structural, morphological and optical properties of crystal which would enable the progressive path to the state of the art work. I believe that these experts would enlighten the participants to understand and interpret the application oriented details of their research materials in a meaningful way and to open the floodgates of possible emerging areas in the advanced areas of technologically versatile fields.

I congratulate the Department of Physics, the convener of this seminar Dr.J. Kalyana Sundar and organizing committee members of **XXIV NSCGA – 2020** for their dedicated work in making this event a great success. Several distinguished scientists are attending this seminar and I am sure all the delegates will be benefited by the deliberation in the seminar.

Best Wishes and Good luck.

P. Kolandaivel

[P. Kolandaivel]

PERIYAR UNIVERSITY VICE CHANCELLOR OFFICE SALEM-636 011

Telephone 0427-2345161 (O) | Res 0427 - 2345464 | Fax 0427-2345565 (O) | E-mail vcperiyar@gmail.com | Website www.periyaruniversity.ac.in

Prof.P. RAMASAMY
President

Indian Association for Crystal Growth (IACG)

Office: Dean (Research)
SSN College of Engineering
Chennai-603110, Tamilnadu, INDIA
Telephone : +91-9283105760
Fax : +91-044-27475166
Email: ramasamyp@ssn.edu.in

Prof. P. RAMASAMY
(Former Vice Chancellor, Alagappa University, Karaikudi
Founder Director, Crystal Growth Centre, Anna University, Chennai)
Director, SSN Research Centre, SSN Institutions, Chennai

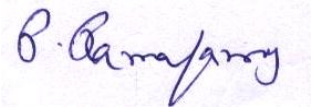
MESSAGE

I am happy that the Department of Physics, Periyar University, Salem is organizing the **"XXIV National Seminar on Crystal Growth and Applications (XXIV NSCGA-2020)"** during 3-5 February 2020. The seminar would involve active participation and healthy discussion among hundreds of researchers, including pioneers in the field of Crystal Growth. I am sure the eminent resource persons with their wide experience in Crystal Growth will be able to provide a new impetus to the budding researchers. I am confident that this would give them a good platform for exchange of ideas.

To be a successful lifetime researcher one must ensure, all the time, an updated knowledge of the current developments in one's own chosen field. This necessitates, among other things, participation in serious Scientific Conferences. Physical participation in conferences creates lasting interests, impressions and new bonds of friendship and networking which potentially are stronger and are likely to last longer. I understand that there are 35 invited Lectures and 250 Contributed Papers. Though organizing a seminar of this nature is a huge task the rich experience of the organizers will certainly ensure successful conduct of the programme.

I congratulate the Convener of this seminar **Dr. J. Kalyana Sundar**, Co-Conveners **Dr. Muthu Senthil Pandian** and **Dr. M. Srinivasan** and organizing committee of XXIV NSCGA-2020 for their dedicated work in making this event a great success. Several distinguished scientists are attending this conference and I am sure all the delegates will be benefited by the deliberations in the conference. I wish the XXIV NSCGA-2020 a grand success.

I am delighted to acknowledge the solid support extended by the Vice-Chancellor **Prof.P.Kolandaivel** and the Dean **Prof. V. Krishna Kumar** to the organizers of this important national event of Crystal Growth community of our country.



P.RAMASAMY

Dr. J. Kalyana Sundar
Convener (NSCGA-2020)
Department of Physics
Periyar University
Salem - 636 011

MESSAGE

The crystals are omnipresent and play a fundamental role in our daily lives. Crystallography has enabled us to learn to manipulate the properties of crystals and use them to our benefit, this being in large part one of the pillars upon which science and technology have contributed to building the welfare state. Today our world would be inconceivable without the technology that crystals enable and provide for example, the piezoelectric effect of some crystals allows us to build devices like the sonar and ultrasounds, etc. The "National Seminar on Crystal Growth and Applications (NSCGA-2020)" provides a platform to exchange the new ideas about crystal growth and applications among the Scientists, Technologists and Researchers all over the Country. Narrow focusing of this seminar is, on crystal growth, covering the fields from theory and experiment to applications of crystals in recent technology. This seminar is being organized by Department of Physics, Periyar University in association with the Indian Crystal Growth Association. The University is reaccredited by the NAAC with "A" grade in 2015. The University bagged 68th rank among Indian Universities by MHRD NIRF 2019. Department of Physics focus on the research areas include Crystal growth, X-ray Crystallography, Biomaterials, Nanotechnology, Solar energy and Thin films.

In this seminar, more than forty scientists delivering invited lectures. Around two hundred recent researches on crystals done by the young researchers are being discussed. It is expected totally 350 members are being participated. Hope, this seminar will be more helpful for the young scientists to grow the knowledge and opportunity to deliver the new ideas about crystals research. I express my deep sense of thanks to honorable Vice Chancellor, Dr .P. Kolandaivel to encourage and support to contact the seminar. In addition, I also thank all those who are helping and working for the good way of seminar.

Thanks to all!

Dr. J. Kalyana Sundar

Index

Invited Talk

Abstract No.	Title	Author's Name	Page No.
IT-01	Experimental and theoretical investigation on indigenously developed DS furnace for growing mc-Si ingot for PV applications	Dr. M. Srinivasan & Dr. P. Ramasamy*	1
IT-02	Techniques for investigating the kinetics of crystal growth process, measuring device relevant properties and establishing correlation with the defects structure of Laser and detector crystals	Dr. Sunil Verma	2
IT-03	Modeling of Strained Si-Ge Heteroepitaxy: From Quantum Dots to Quantum Dot Molecules	Monika Dhankhar and Dr. Madhav Ranganathan*	3
IT-04	Growth and Property Studies of Relaxor Ferroelectric and Multiferroic Single Crystals for Sensor and Transducer Applications	Dr. R. Jayavel	4
IT-05	Challenges in evaluation of some new organic-inorganic indigenously grown nonlinear crystals for efficient Terahertz generation and its Defense Applications	Prof. A.K Chaudhary	4
IT-06	Unveiling properties of Bis (potassium hydrogen l-malate).malic acid nonlinear optical single crystal	Dr. P. Murugakoothan	5
IT-07	Crystal Growth of Silicon Carbide: a purposive wide bandgap material	Dr.R.Radhakrishnan Sumathi	7
IT-08	Development of 4-methylbenzylamine based semiorganic crystals for laser applications	Dr. C. Ramachandra Raja	7
IT-09	Structural, Optical, Thermal, Magnetic and Electrical properties of L – Alanine and 8-Hydroxyquinoline added L-Alanine crystals	Dr.M.Selvapandiyan* , N.Suresh	7
IT-10	Structural Aspects of Bioactive Materials towards their In-vitro Biomineralization and Biocompatibility for Various Biomedical Applications	Dr.S. Balakumar* and S. Chitra	8
IT-11	A whiff of crystallography Bikshandarkoil	Dr.R. Srinivasan	9
IT-12	Alkali halide and sulphate crystals for dosimetry applications	Dr.U.Madhusoodanan	10
IT-13	Crystal Growth and Characterization of Technologically Advanced Materials	Dr.R. Dhanasekaran	10
IT-14	Piezoelectric Nanocrystals for Energy Harvesting Applications	Nidhi Sinha, Dr. Binay Kumar*	11
IT-15	Influence Of Different Dopants/Surfactants On The Magnetic And Gas Sensing Properties Of Cofe2o4 Nanoparticles/Thin Films	Dr.R. Ramesh Babu	12
IT-16	Development of device quality 4-Nitrophenol derivative nonlinear optical single crystals and fabrications of type-I and type-II SHG elements	Dr. Muthu Senthil Pandian*, P. Ramasamy	13
IT-17	Synthesis of hierarchical architecture of chalcopyrite CuInS2 microspheres and Flake-like Al doped ZnO	Dr. K. Sethuraman	14

	thin films for efficient solar cell applications		
IT-18	Template induced nucleation of desired polymorhs of food and pharmaceutical materials	Dr. K. Srinivasan	15
IT-19	Microtube-Czochralski growth of novel organic crystals for NLO applications	Dr. M Arivanandhan	16
IT-20	Effect of CNTs and graphene upon chitosan-gold gels	Dr. R. Radha Perumal	17
IT-21	Quantum Chemical and Spectroscopic Study on Some Anti-Influenza Drugs with ADMET Predictions and Molecular Docking Studies	Dr. M.Prasath	17
IT-22	Nucleation Kinetics, Growth, Structural, Optical, Laser Damage Threshold And Dielectric Studies of Dicarboxylic Acid Based Single Crystals	Dr. C. Senthilkumar	18
IT-23	Low temperature Synthesis and surface modification of biopolymer-ceramic composites	Dr. S. Narayana Kalkura	19
IT-24	Enhancement of the growth rate of the Crystal in TG-SR Method	Dr. K.Sankaranarayanan	21
IT-25	Investigations on the gray tracking effects of potassium titanyl phosphate single crystals for electro-optic applications	Dr. Rajesh Narayana Perumal*, Dr.P. Ramasamy	22
IT-26	Laser Shock Peening Employed Materials Science Tetrahedron Approach on Ferrous and Non-Ferrous Metal Alloys	Dr. Kalainathan Sivaperuman* S. Prabhakaran	23
IT-27	Characterization of some organic NLO crystals grown by solution method P.Selvarajan	Dr. P.Selvarajan	24
IT-28	Growth of 1, 3, 5 - Triphenylbenzene Scintillator Single Crystal by Modified Vertical Bridgman Method and its characterization for Scintillation Application	Dr. P.Selvarajan	25
IT-29	Synthesis, Growth and Physical characterization of AgIn0.5Ga0.5S2 single crystal for Mid-IR applications	Dr. P. Rajesh*, M. Manikandan, Dr. P. Ramasamy	26
IT-30	Unidirectional Growth and Quantum Chemical Studies On NLO Active L-Alanine and L-Histidine Single Crystals	Dr. Robert R	26
IT-31	Assessment of Sustainability of Molecular and Structural Properties of Crystals by Shock Waves	Dr.S.A.Martin Britto Dhas	27
IT-32	Growth and characterization of Semi-organic and Organic Single Crystals for Nonlinear optical Applications	Dr. A.Senthil*, and Dr. P. Ramasamy	28
IT-33	Modeling and Simulation of mc-Silicon Crystal Growth Process: Investigation of Transport Effects in Melt and Crystal Phases	Dr. M. Srinivasan* & Dr.P. Ramasamy	29
IT-34	Single crystals: Potential candidate for reference material for technological applications	Dr. Anuj Krishna	30
IT-35	Characterization of surface treated Cd0.9Zn0.1Te Single Crystals	Dr. S.Ganesamoorthy	30

IT-36	Studies on integration of Piezo thin films on Si substrates for realizing MEMS devices	Dr. E. Varadarajan and Dr. V.Natarajan	31
IT-37	Hydrothermal Synthesis of Glutamic acid Cobalt based Mesoporous Microspheres with a large Size and High Porosity	A.Sakthi, M.Annalakshmi	32
IT-38	Ab initio prediction of the High energetic and biological molecules – A validation study	Dr. P. Srinivasan and A. David stephen	32

Best Thesis Presentation

Abstract No.	Title	Author's Name	Page No.
BT-01	Growth and Characterization of Some Amino Acid Doped ADP Crystal	Dr. Joshi Jaydeep Hitendrakumar	33
BT-02	Synthesis, Characterization and Structure-NLO property relationship of certain organic single crystals	Jesby George	34
BT-03	Growth and Characterization of 4–Dimethylamino–N–Methyl–4–Stilbazolium Tosylate (DAST) Crystal for Photonic Applications	M. Manivannan S.A. Martin Britto Dhas and M. Jose	35
BT-04	Structural, spectral and optical analysis of some 4-methylbenzylamine based crystals	Aarthi. R and Ramachandra Raja. C	36
BT-05	Synthesis, Structural Elucidation and Pharmaceutical Activities of Heterocyclic Based Salts And Co-Crystals	Dr.R.Mekala	37
BT-06	Crystal Growth of Some Correlated Metal Oxides Using the Optical Floating-Zone Technique	Rabindranath Bag and Surjeet Singh	38
BT-07	Growth, Spectral, Thermal And Other Properties of Some Single Crystals For Optical Applications	D.Shanthi	40
BT-08	Crystal Growth And Characterization Of 4-Nitrophenol Derivative Single Crystals For Nonlinear Optical Applications	P. Karuppasamy,*1 Muthu SenthilPandian1, P. Ramasamy1	41
BT-09	Synthesis, Growth And Physico-Chemical Investigations On Pyridine Based Single Crystals For Nonlinear Optical (Nlo) Applications	V. Sivasubramani, Muthu Senthil Pandian* P. Ramasamy	42

Oral Presentation

Abstract No.	Title	Author's Name	Page No.
OP-01	Nonlinear optical and antibacterial activities of Zn/Cu/Al 2 O 4 nanoparticles prepared by microwave-assisted combustion method	A. Lakshmanana, P. Surendrana, S. SakthyPriyaa, K. Balakrishnana, Tejaswi Ashok Hegdeb, G. Vinithab, G. Ramalingamc, P. Rameshkumara,	44
OP-02	Fluorescent carbon quantum dots from orange waste peels for nonlinear optical applications	P. Surendran, A. Lakshmanan, S. Sakthy priya1, K. Balakrishnan, G. Vinitha, G. Ramalingam, P. Rameshkumar*	44
OP-03	Studies on growth and characterization of nonlinear optical L-tartaric acid–nicotinamide single crystal	P. Rameshkumar, P. Surendran, S.Sakthy Priya, A. Lakshmanan S.Pushpalatha	45
OP-04	Modification of Optical Properties of Ammonium Dihydrogen Phosphate Crystal by Employing Shock Waves	A.Sivakumar and S.A. Martin Britto Dhas Sathiyadhas	46
OP-05	Development and Certification of Bharatiya Nirdeshak Dravaya (α-Alumina): Standard used for the calibration of Powder X-ray diffractometer	Ravinder Kumar N. Vijayan, Naghma Khan R. P. Pant2	47
OP-06	Growth of Potassium Acid Phthalate (KAP) single crystal by conventional slow evaporation solution technique (SEST) and Sankaranarayanan-Ramasamy (SR) unidirectional method: A comparative Investigation	Manju Kumari, N.Vijayan, Debabrata Nayak,and R.P.Pant	47
OP-07	Growth of Ethyl P-hydroxybenzoate single crystal by Solution and Vertical Bridgeman technique	Debabrata Nayak, N. Vijayan, Manju Kumari, Nikhilesh Kumar Dilwaliya, R.P.Pant	48
OP-08	Growth and Second order NLO Characterization of tetrakis-thiourea nickel sulphate crystals (TTNS) by slow evaporation method	U. Rajesh Kannan, G. Narayanasamy, P. Selvarajan, M. Malathi	49
OP-09	Supersaturation dependent nucleation control of paracetamol polymorphs through swift cooling process	S. Kavipriya and K. Srinivasan	49
OP-10	Nucleation, growth morphology and characterization of Methyl-p-Hydroxybenzoate (p-MHB) single crystals in selected solvents	V.Manikandan,M. Kowsalya and K.Srinivasan	50
OP-11	Control of oiling-out phenomena and nucleation of stable polymorph of vanillin through vapor	S. Supriya, S. Sushmitha and K. Srinivasan	51

	diffusion crystallization process at selected solvent environments		
OP-12	Crystallization of DL-Methionine polymorphs in the presence of structurally compatible additives	M. Suresh and K. Srinivasan	51
OP-13	Growth of non-linear optical γ glycine single crystals from aqueous solution in the presence of potassium carbonate and their characterization	T. Anitha and K.Srinivasan	52
OP-14	Crystal structure and thermal kinetic approach on benzylideneaniline derivative:p-nitrobenzylidene-p-phenylamineaniline	N. Sivakumar, G. Anbalagan and R. Jayavel	52
OP-15	Solvatochromic effects on the properties of Sodium Acid phthalate crystals	C. Ramalakshmi @ sathya, K. Sangeetha1	53
OP-16	Bulk Crystal Growth, Optical, Raman, Thermal and Third Order NLO Properties of 2-[4-(Diethylamino)benzylidene]malononitrile (DEBM) Single Crystals	S. Ananda, S. Kalainathana, Elisabetta Landinib, R. R. Sumathib	54
OP-17	Linear and nonlinear optical properties of mercury cadmium bromide thiocyanate (MCBT) crystal for laser applications	S.M. Ravi Kumar, S. Sivaraja and G.J. Shanmuga Sundar	55
OP-18	Synthesis, Structure and Electrical Characterization of TlBiSe2 Crystal for Thermoelectric Application	K. Aravinth, P. Ramasamy	55
OP-19	Investigations on 4-methyl benzophenone (4MB) single crystal grown by Czochralski method and its characterization	V. Mohankumar, K. Ramachandran, M. Senthil Pandian and P. Ramasamy	56
OP-20	Synthesis and structural evaluation of silicon nanowires by PECVD using Indium catalyst	Nafis Ahmed, P. Ramasamy andP. Balaji Bhargav	57
OP-21	Comparative study of Experimental results of various Crystals grown by Slow Evaporation method and Sankaranarayanan–Ramasamy (SR) method.	Pankaj D.Ghodke, Dr.S.S.Hussaini, Dr.M.D.Shirsat.	57
OP-22	Synthesis and characterization of a Nonlinear Optical Property of Urea Nickel Ammonium Sulfate (UNAS)	G. Sathishkumar, R. Oviya and M.Lenin	58
OP-23	Crystal structure and Computational evaluation of a novel intermediate salt of N-cyclohexyl-N-(cyclohexylcarbamoyl)-4-(trifluoromethyl)benzamide as potential Potassium channel blocker in Epileptic paroxysmal seizures	Natchimuthu V, Srinivas Bandaru, Anuraj Nayarisseri, Ravi S	59
OP-24	OFZ Growth of Y2Ti2O7 Single Crystal and its Characterization	M. Suganya, P. Vijayakumar, Amirdha Sher Gill1, R. Ramaseshan and S. Ganesamoorthy	60
OP-25	Effects of 1,2-dichloroethane on the optical, thermal, mechanical and NLO behaviors of ADP crystals	M. Saravanan	60
OP-26	Experimental study of parametric dependency of ZnO nanorods based vibration sensor	Iyappan Gunasekaran1 ,Govindaraj Rajamanickam2,	61

		Ramasamy Perumalsamy2, Kiruthika Ramany3, Radha Shankararajan3	
OP-27	Temperature dependent photoluminescence of 4-Methoxybenzylammonium chloride (4-MBACl)	E. Anu Ranjani1, K. Sangeetha1,*	62
OP-28	Enhanced nonlinear polarizabilityof Cu doped L-tartaric acid single crystals	S. Rajkumar1 and K. Sangeetha1,*	63
OP-29	Effect of Molybdenum Shield on Non-metallic Impurities in mc-silicon Grown by Directional Solidification Process	M. Avinash Kumar, M. Srinivasan*, P. Ramasamy	64
OP-30	Electrical impedance analysis and optical analysis of Chalcone (BMP) crystal grown by VASR method.	N. Madhavan, S.A. Martin Britto Dhas*	64
OP-31	Rare-earth ions integrated silica nanocrystals derived from rice husk via microwave-assisted combustion method for bioimaging applications	T. Saravanan, G. Suresh Kumar	65
OP-32	Investigation on the impact of xylenol orange dye on the growth and properties of unidirectional grown KDP crystals for photonic applications	Saranraj1, S. Sahaya Jude Dhas2, M. Jose1, S. A. Martin Britto Dhas*1	66
OP-33	Investigations On L-Valine) Dopped Imidazolinium L-Tartrate Single Crystal	P. Dhivya1, R. Arun Kumar2	67
OP-34	CVD grown graphene on commercial and electroplated Cu substrates- analysis & suitability	Balaji Ca), Ganesh Kumar, P. Balaji Bhargav, Arokiyadoss R, Nafis Ahmed	67
OP-35	Physicochemical and quantum chemical calculations of new bis (2-amino-6-methylpyridinium pyrimidinetrioate) tetrahydrate organic single crystal for nonlinear applications	R. Kaliammal, G. Parvathy, K. Velsankar, G. Maheswaran, S.Sudhahar	68
OP-36	Crystal growth and characterization of 3,4-diamino benzopheone: A novel benzophenone derivative for NLO applications	S. Usharani1, J.Judes1, V. Natarajan2*, M. Arivanandhan3, P. Anandan4	69
OP-37	Bio-Supramolecular gel metal organic framework and its transformation to metal complexes by controlled pH	Sasikala Vadivel and Kalyana Sundar Jeyaperumal *	69
OP-38	Growth and Low frequency Raman study of meta nitro aniline crystals	S. Boomadevi*1, S.K.Pandiyan2, M. Kaliwoda3, R.R.Sumathi3 and D.Sastikumar1	70
OP-39	Growth and characterization of pure and L-lysine doped sulphamic acid single crystals	J. Arumugam 1, 2, 3, M. Selvapandiyan2*	71
OP-40	Structural, Optical and Electrical Properties of Benzo [e] Indolium based D-π-A chromophore Single Crystal	P. Eniya, R. Anbarasan and J. Kalyana Sundar	72

Poster Presentation

Abstract No.	Title	Author's Name	Page No.
PP-01	Advancement and promising depictions of NLO organic crystal 4-nitrophenol 8-hydroxyquinoline (4n8Q) for electronic applications	Mrs.J. Vidhyakannan R. Padmavathi	73
PP-02	Structure Property Correlation of a Series of Halogenated Schiff Base Crystals and Understanding Molecular Basis Through Nanoindentation	C. Ragaverthini. Soumyajit Ghosh	73
PP-03	Design of Mechanically Flexible Fluorescent Molecular Crystals	Nipun. P Soumyajit Ghosh	74
PP-04	Microwave combustion synthesis of tin oxide decorated silica nanostructure using rice husk template for supercapacitor applications	R. Vijayan G. Suresh Kumar N. Surumbarkuzhali S. Prabhu R. Ramesh	75
PP-05	A new non-linear optical material and mechanical studies for pure and sarcosine doped L-tartaric acid of single crystal by Slow Evaporation Method	S. Aron Rabi A.T. Ravichandran	76
PP-06	Investigations on structural, electrical, third order nonlinear optical and antibacterial activity of Benzimidazolium maleate single crystal	S. Sakthy Priya K. Balakrishnan P. Surendran A. Lakshmanan S. Pushpalatha G. Vinitha P. Rameshkumar	76
PP-07	Effect of precursor concentration of calcination Temperature dependent investigation on the properties of the La2O3 nanoparticles: Photocatalytic application	S.Karthikeyan M.Selvapandiyan	77
PP-08	Growth And Comparative Studies Of Third Order NLO Organic Crystals: Beta Alanine (Ba) And Beta-Alaninium Maleate (Bam)	D.Shanthi P. Selvarajan S. Perumal	78
PP-09	Investigation on Growth, Structural and Optical studies of Potassium Sulphamate single crystal –A Material for Non-Linear Optical application	Ravinder Kumar N. Vijayan Naghma Khan	79
PP-10	Growth, and analysis of Optical and Mechanical properties of L-Asparagine Monohydrate Single Crystal for Non Linear Optical Applications	Naghma Khan N. Vijayan Ravinder Kumar	79
PP-11	Hirshfeld surface analysis of a chalcone derivative	Lohith T. N. Akhileshwari P Sirdhar M. A	80
PP-12	Growth and characterization of nicotinium tartrate single crystal: An efficient organic nonlinear optical material	S.Pushpalatha S.Sakthy Priya K. Balakrishnan A. Lakshmanan P. Surendran P. Rameshkumar	81
PP-13	Synthesis, Growth, Structural and Hirshfeld Surface	C. S. Juliet Brintha	82

	Analysis of the NLO 3-Nitroanilinium chloride Single Crystals.	S. E. Joema	
PP-14	Computational studies of intermolecular interactions in a chalcone derivative	Akhileshwari P Sridhar M. A	82
PP-15	Investigations On Semi Organic Nonlinear Optical Single Crystal: L-Tyrosine Hydrobromide (LTHB)	D.Abila Darling S.E.Joema	83
PP-16	Synthesis and Characterization of ZnSe nanoparticles by Co-precipitation method	V. Beena Dr. S. L Rayar Dr. S. Ajitha	84
PP-17	Structural, growth, optical and mechanical properties of Potassium 4-methyl benzene sulfonate single crystal	C.Amirthakumar B. Valarmathi R. Mohan Kumar	85
PP-18	Growth And Studies On Sodium Selenite Doped Tgs Single Crystals	N.Thangaraj C.Gnana Sambandam N. Joseph John	86
PP-19	Studies on bioactive single crystal 2,4,6-Triaminopyrimidinium Nitrobenzoate	M. Tamil Elakkiya K. Anitha	86
PP-20	Synthesis and properties of MgO nanoparticles doped with strontium ions	A.Suba P.Selvarajan J.Jebaraj Devadasan	87
PP-21	Growth, spectral, second and third order NLO properties of L-histidine tartaric acid crystals	S.Sudharthini P. Selvarajan C.Gnana Sambandam	88
PP-22	Green Synthesis And Studies Of Aluminium Nitride (Aln) Nanoparticles	M.Malathi P.Selvarajan U.Rajesh Kannan	89
PP-23	XRD, Optical , NLO and thermal properties of mono-urea oxalic acid crystals doped with zinc sulfate	T. Manju P. Selvarajan U.Rajesh Kannan	89
PP-24	Studies of L-lysine acetic acid crystals by grown by solution method	C. Anbulakshmi Selvarajan S.Selvaraj	90
PP-25	Investigation on undoped and zinc sulfate doped magnesium iodate crystals	P.Geneva Sequirea Roche A.Lesly Fathima P. Selvarajan	91
PP-26	Growth of defect free non-linear optical 4-aminobenzophenone (ABP) single crystals from pure and mixed solvents	A.Mythili K. Srinivasan	92
PP-27	Synthesis and Crystal Growth of Acetylsalicylic Acid from Aqueous Solution	M. Ramya S. Supriya K. Srinivasan	92
PP-28	Structural, Hirshfeld surface studies and computation of interaction energies of a compound 2-Chloro-3-(1'-napthyl)-5,5-dimethyl-2-cyclohexenone	N R Sreenatha A S Jeevan Chakravarthy B Suchithra B N Lakshminarayana S Hariprasad D P Ganesha	93
PP-29	Synthesis of Organic Dye and Its characteristics for Dye Sensitized Solar Cell (DSSC) Applications	Dr. S. Kotteswaran Ramasamy Perumalsamy	95
PP-30	Temperature dependent dielectric study of	S.Swathi	95

	Graphene-Chitosan-Cotton Green Fabrics	Radha Perumal Ramasamy Vinod K. Aswal Miriam H. Rafailovich	
PP-31	Structural, Hirshfeld surface studies and computation of interaction energies of a compound 4-Amino-N– (3-Chloropyrazin-2-yl)benzene- 1-Sulfonamide.	D P Ganesha N R Sreenatha B N Lakshminarayana C R Gnanendra S Madan Kumar	96
PP-32	Linear magnetoresistance in Bi1.5Sb0.5Te1.7Se1.3 topological insulator single crystals	Gopi G Anandha Babu G	98
PP-33	Spin-glass behavoiur in nanocrystalline ZnFe2O4 spinel ferrite	S.Thilagavathi Praveen Shanker N C.Venkateswaran	98
PP-34	Geometrical Parameters, Atomic charges and electrostatic properties of dodecahydro-2H,2'H-2,2'-bi(cyclopenta) [b] thiphene by AIM Theory	S.Palanisamy P. Srinivasan K. Selvaraju	99
PP-35	Fabrication of Stable DSSC Using Hydrothermally Synthesized TiO2 Nanostructures based photoanode	R. Govindaraj P. Ramasamy	100
PP-36	Growth and Characterization of 4-Aminopyridinium 4-Nitrophenolate 4-Nitrophenol (4AP4N) Single Crystal for Nonlinear Optical (NLO) Applications	T. KAMALESH P. Karuppasamy Muthu Senthil Pandian P. Ramasamy Sunil Verma A. K. Karnal	102
PP-37	Structure and Hirshfeld computation study of N-(2-Aminophenyl)-2-(4-bromophenoxy) acetamide	Chandana S N Fares Hezam Al-Ostoot Yasser Hussein Eissa Mohammed	103
PP-38	Growth and characterization of 4-Nitrobenzaldehyde – Phenylhydrazone Single Crystal	R. Gnanadeepam A. senthil	105
PP-39	Growth of 1, 3, 5-Triphenylbenzene Single-crystal by modified Vertical Bridgman method and its Characterization for optical and Scintillation application	M.Manikandan P. Rajesh P. Ramasamy	105
PP-40	Structure Assembly And The Biological Behaviour Of 2-Amino-4, 6-Dimethyl Pyrimidine With Gallic Acid And Pimelic Acid	R.Mekala R.Mathammal	106
PP-41	Growth and characterization studies of L-cysteine hydrochloride monohydrate single crystal for Nonlinear Optical applications	Sudha Yadav Mukesh Jewariya Girija Moona N. Vijayan Manju Kumari Debabrata Nayak Rina Sharma	106
PP-42	Study on Third Order Nonlinear behaviour of Bulk Iminodiacetic acid Single crystal for Optical limiting Application	Debabrata Nayak N. Vijayan Manju Kumari R.P. Pant	107
PP-43	Studies on Synthesis, Growth and characterization	Manju Kumari	108

	of Nonlinear Optical Single Crystal: Sodium Acid Phthalate	N.Vijayan Debabrata Nayak R.P.Pant	
PP-44	Structural, optical, thermal, and SHG studies on new organic NLO Co-crystal: 4-Pyridone succinic acid	M. Subha K. Anitha	108
PP-45	Recovering Resources from the End-of-Life PV Modules	Nagarajan S G Srinivasan M Ramasamy P	109
PP-46	Growth And Characterization Of Pure And Cerium Doped KDP Crystals Grown By Gel Medium	Vinu Barathi M T.Asaithambi	110
PP-47	Enhancing the SHG effect of Zinc Chloride doped DAST single crystal: A new potential material for nonlinear optical device applications	T. Sivakumar Jeyaperumal Kalyana Sundar	110
PP-48	Synthesis, growth and characterization of semi-organic single crystal: p-Toluidinium nitrate for nonlinear optical application	Suresh Shanmugam C. Amirthakumar B. Valarmathi R. Mohan Kumar	111
PP-49	Effects of 2-amino-4,6-dimethoxypyrimidine on PVDF/KI/I2 based solid polymer electrolytes for dye sensitized solar cell application	Kannadhasan S Senthil Pandian Muthu Ramasamy Perumalsamy	112
PP-50	Crystal Growth and Optical Properties of Lithium Sodium Acid Phthalate (LiNaP) Single Crystal	Elavarasi C.Senthilkumar M.Srinivasan	112
PP-51	Modified Hot-Zone DS System to enhance the mc-Si ingot quality	Aravindan Gurusamy, Srinivasan M Ramasamy P	113
PP-52	Optimization of thermal properties by using different heat exchanger blocks in directional solidification furnace and experimental verification	Kesavan V Nagarajan S.G Srinivasan M Ramasamy P	114
PP-53	Studies on the synthesis and characterization of semiorganic Lithium bis(2-methyllactato) borate monohydrate crystal	G.Gokila C.Ramachandra Raja	115
PP-54	Synthesis, Growth and Spectral characterization of halogen substituted Schiff base materials.	Dr. S. Leela Afrin Banu U.Poomalai	115
PP-55	Growth of sodium selenite doped Potassium Dihydrogen Phosphate single crystals by SR method and its Characterization	K.Usha N.Joseph John	116
PP-56	Preparation and Characterization of Undoped and Samarium doped SnO2 thinfilms by Spray Pyrolysis method	K.Radhidevi G.Selvan M.Karunakaran K.Kasirajan G.Rajeshkanna	117
PP-57	VSM Studies On Some Undoped And Doped Single Crystals	Ayarine G. Dhas N. Joseph John	117
PP-58	Synthesis, crystal growth and characterization of an organic nonlinear Material: L- Alanine Mandelic acid single Crystal	V. Sudarvizhi M. Sathish T. Balakrishnan	118
PP-59	Experimental Investigations on Bromoanilinium malonate	P. Yogheshwari M. Tamil Elakkiya S. Suresh Kumar	118

		K. Anitha	
PP-60	Exploring the Effect of π-spacers on D-D-π-A Based Triphenylamine Dyes for Dye Sensitized Solar Cell Applications – Computational Approach	P. Pounraj M. Senthil Pandian P. Ramasamy	119
PP-61	Synthesis and Characterization of Disc-Shaped Thiophene Based Zn-Porphyrin for Organic Solar Cells Application	M. Muthu P. Pounraj N. Santhosh M. Senthil Pandian P. Ramasamy	120
PP-62	Organic methyl 4-aminobenzoate (MAB) single crystal grown by Bridgman- Stockbarger method: A potential candidate for optical applications	Mr. K. Ramachandran A.Raja Muthu Senthil Pandian P. Ramasamy	120
PP-63	Photophysical-chemical properties of ethylenediamine ditartrate xirganomet acentric single crystal for nonlinear optical application	K.Sudhakar, P. Murugakoothan	121
PP-64	Enhancement in ferroelectric, pyroelectric and photoluminescence properties in Lithium Lactate doped TGS crystals	P. G. Praveen Ayarine G. Dhas N. Joseph John	121
PP-65	Growth and characterization of organometallic Calcium Lactate added L-Asparagine cadmium chloride single crystal by slow evaporation technique	R. Rakesh Ayarine G. Dhas Joseph John N	122
PP-66	Structural and Electrical Properties of (1-x)Bi ½ Na ½ TiO 3 –xBaTiO3 single crystals across the morphotropic phase boundary by TSSG method	M. William Carry Muthu Senthil Pandian P. Ramasamy	123
PP-67	Effects of ZnO substitution on dielectric properties of CaCu3Ti4O12 ceramics by a solid-state reaction method	M. Chinnathambi R. Robert	123
PP-68	Highly efficient visible light photocatalytic activity and inherent property of pure & polymer capped SnO2 nanoparticles by chemical precipitation method.	A.Sabarinathan R.Robert	124
PP-69	Role of Coupling Divalent Metal Ion of Tin on Structural and Magnetic Properties of NiFe2O4Nanoparticles	V.Mowlika C.S.Naveen A.R.Phani R.Robert	124
PP-70	Growth and characterization of sodium nitrate doped L-Histidine hydrochloride monohydrate single crystals	Sweatha L Robert R	125
PP-71	Structural, Optical and Thermal Properties of Hg2+ Doped	Silviya M Robert R	125
PP-72	Growth and characterization of DSTMS Crystal for nonlinear optical applications	D.Bharath S.Kalainathan D.Anbuselvi	126
PP-73	Studies on growth and characterization of nonlinear optical L-tartaric acid–nicotinamide single crystal	Dr. P. Rameshkumar P. Surendran128 S.Sakthy Priya A. Lakshmanan S.Pushpalatha	127
PP-74	Crystal Structure and Hirshfeld Surfaces Analysis of Biologically Important Piperidine Derivative	P.Periyannan M.Beemarao	128

		K.Ravichandran	
PP-75	Crystal Structure and HOMO – LUMO Analysis of Pyran Derivative	M.Beemarao P.Periyannan K.Ravichandran	129
PP-76	Synthesis, Growth and Characterization of 2-Amino-5-Nitropyridine 4-Chlorobenzoic Acid (1:1): A New Organic Single Crystal for Third-Order Nonlinear Optical (NLO) Applications	V.Sivasubramani Muthu Senthil Pandian P. Ramasamy	130
PP-77	Growth difficulties and growth of crack free Eu2+ activated KSr2I5 scintillator single crystal by vertical Bridgman-Stockbarger technique for radiation detection applications	A. Raja P. Ramasamy	131
PP-78	Growth difficulties and growth of crack free Eu2+ activated KSr2I5 scintillator single crystal by vertical Bridgman-Stockbarger technique for radiation detection applications	Arumugam Raja* and P. Ramasamy	132
PP-79	Temperature-dependent index of refraction, type I and type II phase-matching angle of monoclinic imidazolium L-tartrate single crystal	S. CHINNASAMI Rajesh Paulraj Rajeev Bhatt Indranil Bhaumik P. Ramasamy A. K. Karnal	133
PP-80	Growth Of High Quality Organic 2ap4n Single Crystal By Sr, Rsr, Rt-Sr And Point Seed Rotation Methods: Fabrication Of Type-I And Type-Ii Phase Matching Elements For Nlo Applications	P. Karuppasamy T. Kamalesh Muthu Senthil Pandian P. Ramasamy Sunil Verma	134
PP-81	Synthesis and characterization of Silver nanowires for optoelectronic applications	Mathew K Francis P. Balaji Bhargav Nafis Ahmed Balaji C	135
PP-82	Growth and characterization of bisglycine cobalt dichloride xiirganomet semiorganic single crystal	P. REVATHI M. Sathish T. Balakrishnan	136
PP-83	Synthesis and characterization of CZTS Thin Films by SILAR method for Solar Cells application	Ganesh Kumar K Balaji Bhargav P	136
PP-84	Crystal Growth of Indium Monoselenide for Photovoltaic Applications	Teena Mathew Bibin John A G Kunjomana1	137
PP-85	Microstructural Characteristics and Mechanical Properties of Melt Grown SnTe Crystals	A G Kunjomana Bibin John Teena Mathew Athira Rose Chittilappilly	138
PP-86	Crystal growth, structure, mechanical, thermal, spectral and optical properties of xiirganometallic of L – Proline Strontium Bromide Tetrahydrate single crystal for nonlinear optical applications	M. Thairiyaraja S. Sathiskumar	139
PP-87	Influence of Si3N4 Coating Thickness on Multi Crystalline Silicon Ingot: Oxygen Impurities	G. ANBU G.Aravindan M. Srinivasan P. Ramasamy	140
PP-88	Studies on growth and optical behaviour of L-	Nikhilesh Kumar	140

	Ornithine Monohydrochloride Single crystal for nonlinear applications	Dilwaliya N. Vijayan M. A. Shah Debabrata Nayak Manju	
PP-89	Crystal growth, structural, piezoelectric, photoluminescence and HOMO-LUMO mechanism of guanidinium tetrafluoroborate single crystal	Nandhini.S P. Murugakoothan	141
PP-90	Compact discussions on the structural, morphological and optical properties of thiophenol capped cadmium sulphide (CdS) quantum dots	S. Muniyappan P. Murugakoothan	142
PP-91	Electronic, Nonlinear Optical and Optical limiting properties of 2- Amino-3-(1H-imidazole-4-yl) Propanoic Tetrafluoroborate (2A3PT) Single Crystal	M.Madhangi P. Murugakoothan	142
PP-92	Growth, Structure, Vibrational, Optical characterization of Imidazolium Glycine NLO Single Crystal	S. Ranjith Priyan R. Fathima Beebei	143
PP-93	Growth & Structure of Inorganic Pottasium Penta Borate Tetra Hydrate (PPBTH) NLO Single Crystal	C. Bavatharani G. Suguna G.Vanmathi R. Fathima Beebei	144
PP-94	Effect of Cd/Ni inclusion on structural and magnetic properties of strontium hexaferrite	T.Jayakumar C.Ramachandra Raja	145
PP-95	Effects of Rb and Cs dopants on the structural and optical properties of potassium pentaborate crystal	A.N.Vigneshwaran C. Ramachandra Raja	145
PP-96	Effect of Annealing on Directionally Solidified Multi – Crystalline Silicon Ingot for Solar Cell Applications	S. Sanmugavel	146
PP-97	Anatase TiO2 Nanospheres Synthesized Via Sol-Gel Process with High Light Scattering Effect for Dye-Sensitized Solar Cell Application	N. Santhosh K.R. Acchutharaman R. Isaac Daniel M. Senthil Pandian P. Ramasamy	147
PP-98	Investigation of Structural and Magnetic Phase Behaviour of Nickel Oxide Nano Particles under Shock Wave Recovery Experiment	A. Rita A.Sivakumar S.A.Martin Britto Dhas	147
PP-99	One step method to synthesize flower-like hydroxyapatite architecture using mussel shell bio-waste as a calcium source	S. Mowniga*, G. Suresh Kumar*	148
PP-100	Synthesis and characterization of hydroxyapatite nanocrystals for the developments of biological probes	R. Kirubakaran M. Dhanasekar G. Suresh Kumar	149
PP-101	Morphology and size controlled synthesis of zinc oxide nanocrystals and their optical properties	S. Surendhar G. Suresh Kumar	149
PP-102	Study of Seed Layer Effect on ZnO Nanorods Growth on SiO2 / Si by Hydrothermal Method	ManojkumarChellamuthu, Subramanian Senthilkumar,SivamKalaiyarasi	150
PP-103	Effect of Additives on Characterizations and Photocatalytic Activity of BiPO4-ZnO Nanocomposite Prepared via Wet chemical synthesis method	Prabhakaran Selvaraj Subramanian Senthilkumar	150

PP-104	Effect Of Temperature On The Mechanical, Optical, Electrical And Magnetic Properties Of Nano Hydroxyapatite Biomedical Applications	Nikela Ramasamy Subramanian Senthilkumar	151
PP-105	Eco-friendly Synthesis and characterization of Nanostructured SnO2 Thin films using Citrus aurantifolia peel extract by Spin coating Method	Megala Devarasan , Subramanian Senthilkumar, Sivam Kalaiyarasi	152
PP-106	Preparation and Characterization of Ni Added ZnO Thin film by Sol-Gel Spin Coating Techniques	Saranya Natarajan Subramanian Senthilkumar Sivam Kalaiyarasi	152
PP-107	Phytosynthesis and Characterization of TiO2 Nanoparticles using Diospyros ebenum leaf extract and their Antibacterial and Photocatalytic Degradation of Crystal Violet	M.C.Satheesh Subramanian Senthilkumar	153
PP-108	Green synthesis of CeO2- TiO2 compound using Cleome chelidonii leaf extract for excellent photocatalytic activity	Rangasamy Mayilsamy Subramanian Senthilkumar	153
PP-109	Effective photocatalytic performance of CdS/TiO2 nanocomposites synthesized under hydrothermal process	B. GomathiThanga Keerthana P. Murugakoothan	154
PP-110	Crystal Growth and Optical Properties of Lithium Sodium Acid Phthalate (LiNaP) Single Crystal	C. Elavarasia S. Mugundanb C.Senthilkumarc M.Srinivasand	154
PP-111	Effects Of Amino Acids Doped With Kcl Crystal By Slow Evaporation Techniques	T.R.K. Priyadarzini S. Sharmila Ruth Ebenezar R. Daphine	155
PP-112	An investigation on optical, mechanical and thermal properties of nickel sulphate hexahydrate single crystal – a UV band pass filter	J. Thirupathy S.A. Martin Britto Dhas	156
PP-113	Growth, Structural and Optoelectronic Properties of γ-glycine Single Crystals Using Nickel Chloride as an Additive	V.Vijayalakshmi P.Dhanasekaran N.M.Ganesan1	157
PP-114	Synthesis And Characterization Of Glycine Magnesium Chloride	K. Karthika P. Srinivasan	157
PP-115	Growth and Characterization of Histidine Phosphite Single Crystals	M. Arivumathi C. Shobana S. Shanmuga Sundari	158
PP-116	Synthesis And Characterization Of Copper Sulphate Doped Clum Leaves Extract	R. Revathil P. Manikandan1 V. Vinayagamoorthy1	159
PP-117	Role Of Sn On Structural And Optical Properties Of ZnO Chunk Shaped Nanostructures	S.S. Kanmani1 K.R.N. Jaya Prasanth V. Gowthambabu	159
PP-118	Effect Of Mg Doping On Structural And Optical Properties Of ZnO Chunk Shaped Nanostructures	V. Gowthambabu S.S. Kanmani1	160
PP-119	Growth, Characterization And Nucleation Kinetics Of L-Glutamine Based Non Linear Optical Crystals	Jebaraj P.G Sivashankar.V Helina.B	161

		Anuradha.G.Vb	
PP-120	Selective Review Of Recent Researches On The Growth And Characterization Of Technologically Significant Crystals By S-R Method	Jebaraj.P.G Sivashankar.V Helina.B AnuradhaG.V	161
PP-121	Investigation on dielectric and mechanical properties of guanidinium p-toluenesulfonate single crystal	Paavai. Eraa P. Murugakoothana	162
PP-122	Growth, Experimental And Theoretical Investigations On Piperazinium Bis (5-Chloro-2-Hydroxybenzoate) Nonlinear Optical Material	G. Parvathy R. Kaliammal G. Maheshwaran K. Velsankar S. Sudhahar	163
PP-123	Investigation Of Piperazinium Phthalate Single Crystal With Its Mechanical, Thermal, Structural And Morphological Properties For Non-Linear Optics	G. Maheshwaran K. Velsankar G. Parvathy R. Kaliammal S. Sudhahar	163
PP-124	Dual approach on experimental and theoretical investigation of new single crystal from amino acid family	Radhakrishnan Anbarasan Palaniyasan Eniya Jeyaperumal Kalyana Sundar	164
PP-125	Molecular structure and Electron deisnty analysis of high energetic 2,4,6-Trinitropyridine N-oxide molecule via Quantum chemical calculations	L. Sathya B. Gnanavel A. David Stephen P. Srinivasan	164
PP-126	Crystal structure, DFT and Hirshfeld surface analysis of N-Acetyl-t-3-Isopropyl-r-2,c-6-diphenylpiperidine (AIDP)	P.Periyannan M.Beemaraoa K.Ravichandrana	165
PP-127	Synthesis and Characterization of Zn1-xYbxO nanocrystals for thermoelectric applications	T.M.V.Murugu Thiruvalluvan V.Natarajan P.Anandan M.Arivanandhan R.Jayavel	166
PP-128	Preparation and characterization of BixCo3-xO4 nanocrystals for thermoelectric applications	S. Alagar Nedunchezhian D.Sidharth N. Yalini Devi R.Rajkumar G.Anbalagan M. Arivanandhan R. Jayavel	166
PP-129	Structure Determination And Spectroscopic Analysis Of A New Active Nlo Azo Derivative	P.Sangeetha	167
PP-130	Hardness And Dielectric Behaviour Of Lithium Sulfate Monohydrate Sodium Iodide Crystal	Preetha P Chellammal R Anithalakshmi M	167
PP-131	Thermal Characteristics Of Sodium Iodide Doped Lithium Sulfate Monohydrate Single Crystal	Saranya N Anithalakshmi M	168
PP-132	Growth And Characterization Of L-Alanine Cadmium Iodide Crystal For Nonlinear	S.Thangavel R.Ashokkumar	168

	Optical Applications.		
PP-133	Growth And Optical Properties Of Pure And Metal Ions Doped Sodium D-Isoascorbate Monohydrate Single Crystals	R. Sathyaranayanan M. Selvapandiyan	169
PP-134	Preparation of 3D flower-like CuO/Co3O4/rGO heterostructure and high performance asymmetric hybrid supercapacitor	S. Prabhu P. Maadeswaran S. Sohila R. Ramesh	170
PP-135	A theoretical interpretation and screening of perylene based metal-free organic dye sensitizers withdifferent lengths and functional groups of acceptors for DSSC's	D. Nicksonsebastin M. Prasath	170
PP-136	Quantum mechanical, Spectroscopic and Molecular docking studies of Doxofylline by Density Functional Method	N. Mani M.Prasath	171
PP-137	Structure and intermolecular interactions of some benzodiazepine derivative molecules with GABA-A receptor: A molecular docking and quantum chemical	M. Ramaraj M. Prasath	172
PP-138	Spectroscopic investigation (FTIR,FT-Raman), (RS)-N,N-bis(2-chloroethyl)-1,3,2 oxazaphosphinan -2-amine2-oxide an anti-cancer drug by HOMO-LUMO, ADMET and molecular docking evaluation	M.Govindammal M.Prasath	172
PP-139	Vibrational, electronic spectral analysis and molecular docking evaluation of Isowighteone as Neuraminidase inhibitor against influenza diseases using DFT simulations	B. Sathya M. Prasath	173
PP-140	Fabrication of MoO3/Ag2S hybridized with graphitic-C3N4 for effective catalyst under visible-light exposed photocatalytic activity	Shanmugam Vignesh Jeyaperumal Kalyana Sundar	174
PP-141	Structural, spectroscopic, magnetic behaviour and DFT investigations of L-tyrosinato nickel (II) coordination polymer	G. Gayathri, V. Sasikala and J. Kalyana sundar	175
PP-142	Growth and characterization of sodium penta fluoro antimonate crystal	Dr. C.BESKY JOB	175
PP-143	Observation of Intermediate Band in $CuGaS_2$ thin films via Fe doping by using Chemical Spray Pyrolysis Technique	S. Suba Viveka and K. Sethuraman	176

Crystal Display

Abstract No.	Title	Author's Name	Page No.
CD-01	4-Nitrophenol derivative single crystals	T. Kamalesh and P. Karuppasamy	177

Invited Talk

IT-1

Experimental and theoretical investigation on indigenously developed DS furnace for growing mc-Si ingot for PV applications

M. Srinivasan & P. Ramasamy

SSN Research centre, SSN College of Engineering, Chennai-603110.
Email: *ramasamyp@ssn.edu.in*

The majority of PV solar cells is fabricated from bulk silicon crystals, which may be either single-crystalline or multi-crystalline. Market share of mono- and multi-crystalline silicon (mc-Si) is more than 90% at present and will be so in the foreseeable future. Multi-crystalline silicon is an important material with advantages of low-production cost and high conversion efficiency of solar cells. It has a market share of more than 60% among all photovoltaic materials. Directional solidification (DS) method has become the leading technique for producing mc-Si. Indian solar cell industries import silicon cells and convert them into solar modules. Today 98% of the silicon cells imported into country are mc-silicon cells. No serious research activities have been done on the mc-Si crystal growth modelling as well as experiments in Indian laboratories. We took efforts to start the modelling activities on silicon growth eight years ago in SSN Research centre, and experimental activity four years ago with the support of MNRE, Government of India. Modelling and experimental mc-Si growth lab are established well in SSN RC. Several Ph.D. scholars and scientists are currently working in the field of mc-Si growth process and are getting good results. The growth of mc-silicon in the directional solidification system involves complex nonlinear transport phenomena of heat and mass transfer. This work focuses on simulation and optimization of directional solidification silicon growth process and build a fundamental baseline process for understanding of DS process using Solar Grade Silicon (SoG-Si) as feedstock and resulting in a baseline solar cell efficiency of 16% with an average lifetime of >3μs. The segregation and precipitation of the impurities in the mc–Si has serious problems, which affect the performance of the solar cells. They can be controlled by simulating the growth process using numerical methods. The stress and dislocation density are main factors which are reduced using various modification in DS furnace and optimizing the control parameters. We have installed indigenously manufactured machines for brick making, wafering and polishing of grown mc-Si ingot. And, we have done the characterizations for those wafers produced from various parts of grown mc-Si ingot.

****

IT-2

Techniques for investigating the kinetics of crystal growth process, measuring device relevant properties and establishing correlation with the defects structure of Laser and detector crystals

Dr. Sunil Verma[ab]

[a]Scientific Officer (G)
Laser & Functional Materials Division
Raja Ramanna Centre for Advanced Technology
Indore – 452013, Madhya Pradesh

[b]Associate Professor (Phys. & Engg.)
Homi Bhabha National Institute
ARC Training School Complex, Anushakti Nagar
Mumbai – 400 095, Maharashtra
Email: *sverma@rrcat.gov.in, sverma1118@gmail.com*

Crystals are driving the current photonics revolution. Material scientists need to have detailed understanding of how crystals grow, whereas device engineers need crystals of adequate size and quality for the end applications. Since crystal growth process is a non-equilibrium process, therefore different type of defects get incorporated in the crystal during growth. The crystal growth rate and its defect structure are a function of the time-dependent spatial distribution of the temperature, convection and concentration fields during the growth process. Therefore, it is important to map these processes and understand their influence on the growing crystal. The first half of the presentation discusses the principle and results obtained by application of multi-modal optical techniques such as laser shadowgraphy, birefringence interferometry, Michelson interferometry, Mach-Zehnder interferometry and dual-wavelength interferometry for online and in-situ investigations of the crystal growth process. After growth, the crystals have to be cut along specific directions and then polished, to obtain the elements for use in the desired devices. However, before deploying a crystal element in a particular device, it is necessary to assess its quality and measure the device relevant properties. The second half of the presentation discusses various techniques for these measurements, such as interferometric techniques for investigating the refractive index homogeneity and birefringence of the crystal, UV-Vis-NIR spectrophotometric studies, dislocation etch pit density using optical microscopy, optical data storage properties of photorefractive crystals using two-wave coupling, damage threshold measurements, 3rd order NLO properties using Z-scan, and photoconductivity as a function of temperature and wavelength. Finally, establishing a correlation between the defects structure of the crystal and its optical properties is essential, as it has implications for the desired device applications. This is achieved by imaging the defects structure of the crystal using X-ray topography, the crystalline perfection is assessed using HRXRD and the metallic impurity distribution is obtained using X-ray fluorescence. Salient results obtained using above techniques will be presented.

****

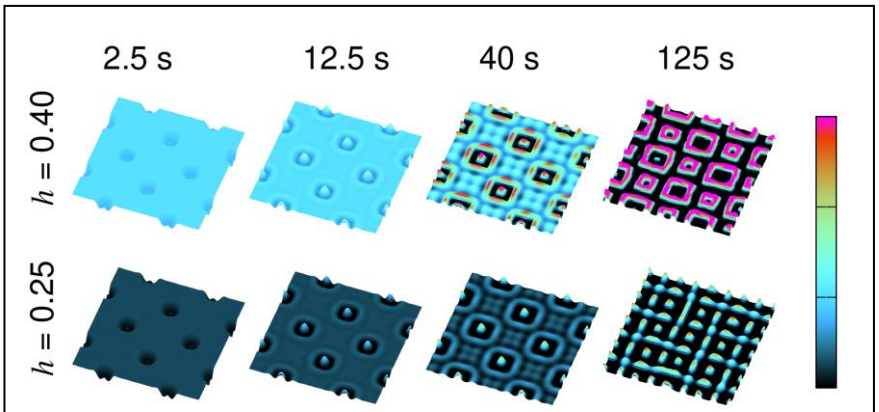
IT-3

Modeling of Strained Si-Ge Heteroepitaxy: From Quantum Dots to Quantum Dot Molecules

Monika Dhankhar and Madhav Ranganathan*

Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India
Email: *dmonika@iitk.ac.in*

Heteroepitaxy of SiGe/Si(001) has been of interest over the past several decades because of its importance in the microelectronics industry. Thin films of SiGe on Si(001) are characterized by Stranski-Krastanov growth and show the spontaneous formation of nanostructures such as nanowires, ridges, quantum dots etc[1,2]. The use of pre-patterned substrates results both in ordering of quantum dots and in the formation of novel nanostructures referred to as quantum dot molecules (QDMs). The QDMs consist of a symmetric assembly of four quantum dots around a central pit. This represents a particularly interesting morphology and a possible alternate route towards strain relief from the usual quantum dots. In this talk, we will show the theoretical models used to describe these phenomena and their numerical implementation [3,4]. This framework based on continuum mechanics and incorporates both surface energy anisotropy and elastic strain. An advanced numerical technique developed in our group is used to solve the problem and calculate the evolution of the system. Our results show how the experimentally relevant parameters such as temperature, growth flux and film thickness can be used to control the formation of variety of nanostructures[5,6].



Time evolution of Si-Ge films on patterned substrates of different thickness showing

References:

1. J.L. Gray, R. Hull and J. A. Floro, App. Phys. Lett. 81, 2445 (2002).
2. J. L. Gray et al, Phys. Rev. B 72 , 155323 (2005).
3. G.K. Dixit and M. Ranganathan, J. Phys. Condens. Matter 29, 375001 (2017).
4. G.K. Dixit and M. Ranganathan, Nanotechnology, 29, 365305 (2018).
5. M. Dhankhar and M. Ranganathan, J. Cryst. Growth, accepted.
6. G.K. Dixit, M. Dhankhar and M. Ranganathan, Phys. Chem. Chem. Phys., under review.

****

IT-4

Growth and Property Studies of Relaxor Ferroelectric and Multiferroic Single Crystals for Sensor and Transducer Applications

R. Jayavel

Crystal Growth Centre, Anna University, Chennai-600 025.
E-mail: *rjvel@annauniv.edu*

Relaxor ferroelectric and multiferroic single crystals find wide-spread applications in advanced technology. Relaxor ferroelectric materials like PMN-PT and PZN-PT are closely related to the morphotropic phase boundary (MPB) effects. The formation of macro-domain states, resulting from the substitution of Ti^{4+} ions in the B-site of the perovskite structure facilitates their use in ultrasonics and underwater communication systems. Hence growth of these single crystals at morphotropic phase boundary is an important task. In this study, single crystals of relaxor ferroelectric materials namely, PZN-PT, PYN-PT and PSN-PT were grown by flux method. The structural, optical, electrical and mechanical properties have been systematically studied. The Raman spectra of the grown crystals indicate the existence of local structural distortion, which are different from that of the cubic structure. The growth parameters have been optimized in order to improve the performance of the crystals for device applications. New multiferroic crystals like MnSb2S4 have also been grown by Bridgman technique. The results will be discussed in detail.

****

IT-5

Challenges in evaluation of some new organic-inorganic indigenously grown nonlinear crystals for efficient Terahertz generation and its Defense Applications

Prof. A.K Chaudhary

Advanced Center of Research in High Energy Materials (ACRHEM), University of Hyderabad, Hyderabad-500046(India)
Email: *akcsp@uohyd.ernet.in, akcphys@gmail.com*

Terahertz range of E-M spectra falls between 0.1 - 10 x 10^{12} Hz frequency range which bridges the gap between the microwave and Far-infrared regions. It has several unique properties such as high reflective to metals, transmission through non-polar, non-metallic materials and high absorption in water. In this lecture I will discuss some of the critical challenges related to evaluation of linear and nonlinear optical properties of some newly indigenously grown organic crystals such as DAST, BNA, 2A5NPDP , OH1 etc. with respect to commercially available semiconductor crystals like ZnTe, CdTe and GaSe etc... In addition to irregular shape, the non-availability of proper transmission/ absorption, damage threshold data along with Sellmeier equations possess a major challenge to find the suitability of these new organic materials as a source of frequency generation between UV-Vis-NIR extended up to THz range. We employ different types of linear and nonlinear optical techniques based on Spectrophotometer to tunable wavelength between 780-1200 nm ranges obtained from 50 fs and 140 fs pulses Ti: sapphire lasers

at 1 kHz and 80 MHz repetition rate obtained from Ti: sapphire amplifier and oscillator amplifier. Linear optical techniques help us to select the proper wavelength and Refractive index of the organic materials while femtoseconds laser help us to ascertain the Refractive index, absorption coefficients, coherence length in THz domain. These data are finally used to measure the efficiency of the generated THz signal. I shall also discuss the role of surface roughness to reflection coefficients and optical impedance, conductivities of these materials

Finally, generated THz radiation is used for recording of finger print spectra of Explosive and other organic molecules at room and high temperatures. We have also detected explosives mixed in soil.

****

IT-6

Unveiling properties of Bis (potassium hydrogen l-malate).malic acid nonlinear optical single crystal

P. Murugakoothan

Dept. of Physics, C. Kandaswami Naidu College for Men, Chennai – 600 102
E-mail: *murugakoothan03@yahoo.co.in*

The fast-developing fields, such as photonics and opto-electronics are mainly centred on semi-organic nonlinear optical (NLO) materials because they are broadly used for second harmonic generation and in other optical applications. Bis (potassium hydrogen l-malate).malic acid (PMM), a semi-organic nonlinear optical material was synthesized and crystal was grown from aqueous solution by slow evaporation solution growth technique. The lattice parameters and space group were confirmed by single crystal X-ray diffraction study. Powder X-ray diffraction study revealed the crystalline nature of the title material. Optical transmittance study showed that the grown crystal has good transparency in the entire visible region. The lower cut-off wavelength of the grown crystal was found to be at 210 nm.The luminescent property of the title crystal was investigated through photoluminescence spectroscopy. The CIE 1931 color chromaticity diagram was drawn to examine the suitability of the title crystal for blue laser applications. Second harmonic generation efficiency was found using Kurtz-Perry powder technique. Thermal analyses revealed that the crystal is stable up to 230°C. The mechanical strength of the crystal was assessed by Vickers microhardness tester. The dielectric behaviour and its parameters were established through dielectric study.

****

IT-7

Crystal Growth of Silicon Carbide: a purposive wide bandgap material

R. Radhakrishnan Sumathi

Materials Science and Crystallography Institute, Ludwig-Maximilians-University (LMU), D-80333 Munich, Germany
Email: *sum66@hotmail.com*

Relatively a new class of compound semiconductor materials known as wide bandgap semiconductors (at least a bandgap energy > 3eV) usually made up of carbides, nitrides or oxides and their corresponding devices fabricated, do have exorbitantly useful characteristics in numerous civilian systems and components, due to their utilization even in extreme-environment-use conditions. Among carbides, silicon carbide (SiC) is a material exceptional for high-temperature, high-frequency, and high-power device operations. SiC also possesses superior electronic, thermal and mechanical properties, which make it suitable for a variety of applications such as junction field effect transistors, switching devices, light emitting diodes and radiation detectors. However, growth technology of this SiC material is not matured sufficiently as compared to silicon (Si). In SiC growth, there are still some basic problems to be resolved that limit the full commercial utilization of this material. These problems are related to crystal size and both, macroscopic and microscopic defects. It is well known that defects degrade the performance of the electronic devices and greatly diminish their reliability.

For the growth of any material, it is preferable to use a simple technique with high growth rate. Unfortunately, SiC does not form a stoichiometric liquid phase and furthermore, Si has a low solubility of carbon and consequently the growth rate is very low. So, growing SiC from solution is not an appropriate method. The seeded sublimation growth is the most promising technique for growing SiC single crystals. Methods like standard Lely method, Acheson processes, physical vapour transport (PVT) for high growth rate, hot wall chemical vapour deposition to grow crystals with low screw dislocation (SDs) density will be reviewed. Another specialty of this material is that there exists more than 200 polytypes. One of the main challenges of growing SiC is controlling even the major polytypes (6H, 4H). SDs have been reported to act as step sources that help maintain polytypes and commercially viable growth rates. The factors affecting the nature of the grown polytypes will be presented. Other growth issues like the restriction of SDs, the presence of polytype inclusions and reduction of micropipe defects could be deliberated. Yet another interesting aspect of SiC is that it could take the forms in both hexagonal and zinc blende (cubic) structure. 3C-SiC single crystal growth, in which elimination of twin boundaries is a difficult task, might also be discussed. Potentiality of such 3C-SiC wafers are promising and are in demand that could pave the way to future high-performance electronics.

****

IT-8

Development of 4-methylbenzylamine based semiorganic crystals for laser applications

C. Ramachandra Raja

Government Arts College (Autonomous), Kumbakonam-612 002, Tamilnadu.
Email: *crrajaphy@gmail.com*

Nonlinear optical crystals play a vital role in generating coherent radiation at new frequencies that are not available with conventional laser sources. Organic crystals carry excellent nonlinear optical properties, but they cannot withstand laser beam impact due to its low thermal and physical stability. Inorganic crystals exhibit good physical and thermal stability but they possess low nonlinear efficiency. To strike a balance between organic and inorganic crystals, the semiorganic crystals were emerged and still attempts have been made by several groups throughout the world to find efficient semiorganic crystals for laser applications. Amino acid based semiorganic crystals are considered to be promising nominees for NLO applications. Also, semiorganic crystals developed from combining amines as organic part and halogen based inorganic part gives rise to the supramolecular structure with hydrogen bonds. These structures results in good physical, mechanical and nonlinear optical properties. In this work, halogen based inorganic part and 4-methylbenzylamine were reacted and new crystals were developed through slow solvent evaporation technique. Their structures were solved and reported. The structure property relationship of the grown crystals were analyzed through Single crystal X-ray diffraction, Powder X-ray diffraction, UV-Vis-NIR spectroscopy, Fourier transform infrared spectroscopy, Fourier transform Raman spectroscopy, Thermogravimetric analysis, Differential thermal analysis, Nuclear magnetic resonance spectroscopy, second harmonic generation test and Z-scan technique. The results will be presented.

****

IT-9

Structural, Optical, Thermal, Magnetic and Electrical properties of L – Alanine and 8-Hydroxyquinoline added L-Alanine crystals

M. Selvapandiyan[a*] , N. Suresha

[a]Department of Physics, Periyar University PG Extension Center, Dharmapuri- 636701, Tamil Nadu, India
Email:*mselvapandiyan@rediffmail.com*

Nonlinear optical L- Alanine (LA) and 8-Hydroxyquinoline added L- Alanine (HQLA) was synthesized and grown from low temperature solution growth method especially from slow evaporation technique at ambient temperature. Lattice parameters of the grown materials are a= 6.013Å b = 12.35 Å c= 5.782 Å and angle $\alpha=\beta=\Upsilon=90^{o}$ with space group $P2_12_12_1$ which reveals that the crystal posses orthorhombic structure in nature. The cut off wavelength of LA and HQLA is about 242.1nm and 236.6nm, respectively. The high intense emission peak at 419.2 nm is attributed to both LA and HQLA crystals originating from the excitonic transition between the conduction and valence band. The pure and HQ doped LA sample was endowed stable upto

193.5˚C and 200.16˚C, respectively. Dark current has higher efficiency while comparing to photo current which falls in photo negativity. Low dielectric loss with higher the frequency for the grown crystal enables that the crystal possess good optical quality with lesser defects which is the suitable property for NLO applications.

Keywords: Crystal growth; Structural; Photoluminescence; Dielectric; Powder XRD; TGA/DTA

****

IT-10

Structural Aspects of Bioactive Materials towards their *In-vitro* Biomineralization and Biocompatibility for Various Biomedical Applications

S. Balakumar and S. Chitra

National Centre for Nanoscience and Nanotechnology
University of Madras' Guindy Campus,
Email: *balasuga@yahoo.com*

Biocompatible glass materials evolved to develop superior bioactivity than existing bio ceramics. Bioglass composed of silica, calcium, sodium and phosphate sources to form matrix. Currently this material consumes special research focuses due to their tremendous biocompatibility, osteo-conductivity and osteo-inductive properties. Still the research is need to be focusses on the structural characteristics of bioactive materials. Because cell integration with materials is mainly owing to their crystal structure, morphology and porosity at the site of interaction. Ionic release, resorption and degradation properties primarily influence the compatibility and proliferation of cells at physiological environment. Hence, our main aim is to focus on different crystalline phases of bioactive materials and their role towards mineralization and biocompatibility properties. Therefore, we developed 45S5 bioglass, 53S bioglass, 80S bioglass and also varied the fabrication parameters to attain appropriate crystalline phases of the bioactive materials. Besides, prepared single crystalline structures of $Na_2Ca_2Si_3O_9$ (combeite) and $Na_2Ca_4(PO_4)_2SiO_4$ (silicorhenanite) mineral phases to attain substantial apatite precipitations at biological environment. In the current study, we investigated the structural properties with respect to Nano-fabrication processes towards rapid mineralization and acceptable biocompatibility. Investigated the bioactive materials with various calcium, phosphate and sodium precursor, also varied the nano-synthesis as well sintering parameters to engineer the network to attain prompt mineralization. XRD, Raman and FT-IR results of developed bioactive ceramics denotes the structural modification by various parameters. Morphological information's reveled the surfaces and appetences of engineered bioactive materials. Biocompatibility with erythrocytes and osteoblast like cell lines exhibits the biocompatibility properties. Still we provide attention on the crystal structure of bioactive glass to develop better apatite growth at biological environment.

****

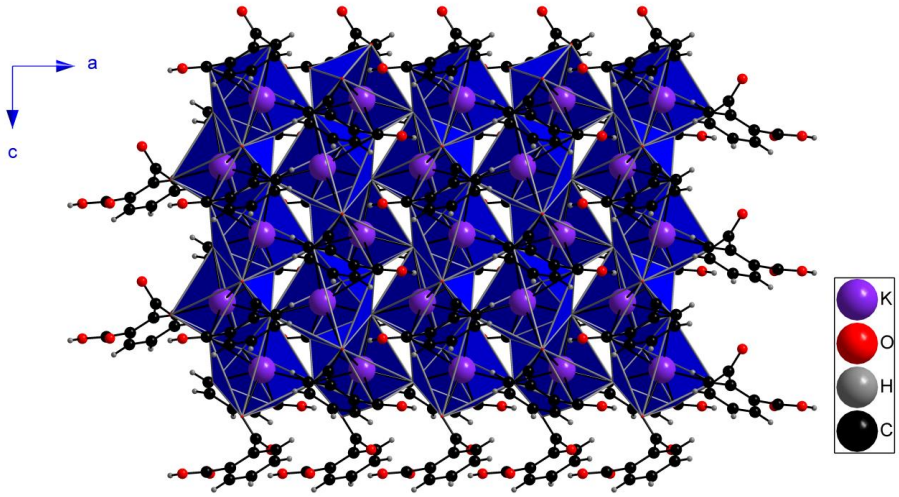
IT-11

A whiff of crystallography

Bikshandarkoil R. Srinivasan

School of Chemical Sciences, Goa University, Goa 403206, India
Email: *srini@unigoa.ac.in*

Study of growth, structure characterization and properties of new crystalline materials is a topical area of research. The discovery of X-rays by Röntgen in 1895 followed by the advent of X-ray crystallography has made it possible to understand the arrangement of atoms in crystalline materials. Rapid advances in X-ray instrumentation in the last three to four decades have been responsible for a facile determination of difficult structures including large proteins. The ready availability of X-ray diffractometers in many institutions has not only enabled easy compound characterization but also given rise to the development of new areas of study like coordination polymers, metal-organic frameworks (MOF) materials etc. In this talk I intend to make a journey in time scale to highlight the development of studies of crystals. The usefulness of X-ray methods for an understanding of different structure types will be explained by taking examples from the literature and our own work. In addition to describing the importance and classification of space groups, it will be demonstrated as to how one can build a structure like the one below from the information in a CIF file.



****

IT-12

Alkali halide and sulphate crystals for dosimetry applications

U. Madhusoodanan

Luminescence Programme, Indira Gandhi Centre for Atomic Research, Kalpakkam 603 102.
Email: *ums@igcar.gov.in*

Thermo luminescence dosimetry is widely used for personal as well as environmental radiation monitoring applications all over the world. But, using this technique measurement of very low radiation doses is a very challenging work, due to the interference of infra red signals arising from the heater strips with luminescence signal. Hence the read out is carried out using optically stimulated luminescence where the signal is obtained using LED as an excitation source. But growing crystals for such applications like α – Alumina doped with carbon and mixed fluorides with rare earths are very complicated. Hence simple crystals like Lithium sulphate with double dopants and Alkali halides with rare earth co-dopants have been grown and tested for their use in practical dosimetry applications. Lithium sulphate doped with divalent metal ions and Potassium Chloride with rare earths Cerium and Europium was found to be good materials for OSL applications.

****

IT-13

Crystal Growth and Characterization of Technologically Advanced Materials

R. Dhanasekaran

Crystal Growth Centre, Anna University, Chennai – 600 025.
Email: *r.rdcgc@yahoo.com*

Single crystal growth and characterization of technologically important materials used for accousto-optic, SONAR, scintillator applications will be presented in detail. Relaxor ferroelectrics are a special class of ferroelectric materials, which typically have a perovskite or tungsten bronze structure type and distinctive material properties such as a broad maximum of the dielectric permittivity as a function of temperature, strong frequency dispersion of the dielectric constant, and the existence of polar regions at temperature well above this maximum. The largest group of relaxor ferroelectrics is found in the family of complex lead based perovskites having the general formula $Pb(B', B'')O_3$, where B' is a low-valence cation, such as Mg^{2+}, Ni^{2+}, Sc^{3+}, Fe^{3+} and Zn^{2+} and B'' is a high valence cation, such as Nb^{5+}, Ta^{5+} and W^{6+}. PZN and PT are relaxor and normal ferroelectrics with rhombohedral and tetragonal symmetry at room temperature, respectively. Growth of PZNT (91/9) single crystals at morphotropic phase boundary has been carried out by flux and flux Bridgman methods. Effects of multinucleation on morphology and effect of PbO evaporation on crystal growth are discussed. The grown crystals were cut along (0 0 1) direction and crystals were poled at the rate of 1 kV/mm. The slow scan X-ray diffraction results of the oriented crystals show a structural phase transition on poling. The phase transition has been studied with slow scan X-ray diffraction pattern for powdered $Pb(Zn_{1/3}Nb_{2/3})O_3$–$PbTiO_3$ (PZN–PT) crystal and (0 0 1) oriented single crystal which shows the existence of stressed phases and trapped phases in both cases. Further the grown PZN–PT single crystals have been subjected to compositional

studies. Electrical characterizations such as hysteresis measurement, strain measurement and piezoelectric measurement were carried out and the results are discussed in detail. Lead-free piezoelectric single crystals of $Na_{1/2}Bi_{1/2}TiO_3$–$BaTiO_3$ (NBT–BT) have been grown by flux and zone melting techniques. Growth was carried out by employing two flux systems: (a) Bi_2O_3 and (b) Bi_2O_3 and Na_2CO_3 fluxes. In order to avoid the serious problem of composition variations suffered in flux growth technique, metal strip heated zone melting (MSHZM) technique was employed for the growth of NBT–BT crystals. Inductively coupled plasma (ICP) analysis was carried out for the grown crystals and the composition variations in the crystals obtained from flux and MSHZM techniques were analyzed. Results reveal that the composition variations suffered in the flux-grown crystals have been avoided by adopting the zone melting technique. Ferroelectric single crystal Ce doped NBT-BT have been grown by flux technique. It is found that the addition of Ce plays a significant role in improving the ferroelectric properties of NBT-BT crystals.. In order to study the role of oxygen vacancies on the dielectric/ferroelectric properties, some of the crystal samples oriented along (0 0 1) and (1 0 0) planes were subjected to oxygen and nitrogen annealing processes to create different concentrations of oxygen vacancies in the samples. Dielectric and its loss measurements were carried out to analyze the role of oxygen vacancies and their corresponding dielectric behavior on NBT–BT crystals. Electron energy loss spectrum (EELS) has revealed that increasing oxygen vacancies has reduced oxidation states of Ti. X-ray rocking curve analysis has confirmed the degradation in the structural quality also on increasing the oxygen vacancies. The results are discussed in detail.

****

IT-14

Piezoelectric Nanocrystals for Energy Harvesting Applications

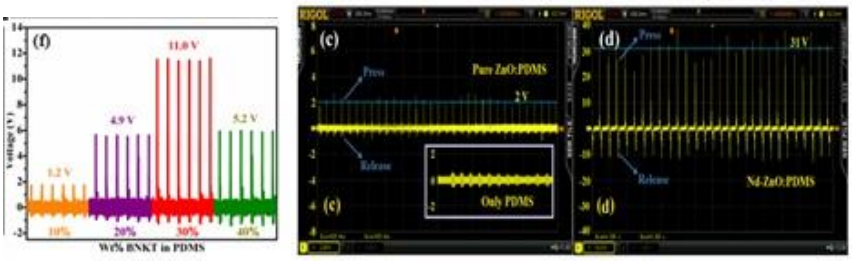
Nidhi Sinha[1,2], Binay Kumar[1]

[1]Crystal Lab, Department of Physics & Astrophysics,
[2]Department of Electronics, SGTB Khalsa College,
University of Delhi, Delhi-7
Email: *b3kumar69@gmail.com; nidhisinha5@yahoo.co.in*

Sustainable self-powered Piezoelectric NanoGenerators (NGs) are future alternate energy source to harvest energy directly from local environment like finger tapping, walking, breathing, etc [1]. Versatile ZnO exhibits interesting ferroelectric, piezoelectric, optical, etc. properties when doped with various rare earth elements (e.g. Cr, Eu, Gd, Y, Nd, etc.) [2]. As a result of doping, enhanced piezoelectrical charge coefficient were achieved in different ZnO structure, synthesized by wet chemical route, showing different morphology for improved performance of piezoelectrical devices. Similarly, some other high performance piezoelectrical nano/microsystems, including lead based perovskite BNKT and (KNN-BNZ) were synthesized by high temperature solid state reaction followed by ball milling [3,4]. These nanoparticles were characterized for structural (XRD), morphological (FESEM/HRTEM), dielectric, ferroelectric, piezoelectric and optical (PL, Raman, UV-Vis), etc properties.

These high performance piezoelectric nanocrystals were used, both as direct nanostructure as well as in the form of thick flexible composite tapes. For this, thick tape of piezoelectricnano-crystals / PDMS on ITO/PET substrate were fabricated by spin coating. The generation of electrical energy by simple finger tapping and using force simulater was studied. Applied force

and its frequency were varied in the range of 0.3 N- 20N and 5 Hz – 100 Hz, respectively. High voltage output in the range of 0.5 – 50 V were obtained. It has been demonstrated that the synthesized piezoelectric nanocrystals can be used for energy harvesting.



Reference

1. Y-doped ZnO nanosheets: Gigantic piezoelectric response for an ultrasensitive flexible piezoelectric nanogenerator, Ceramics International 44 (2018) 8582
2. A review on piezo-/ferro-electric properties of morphologically diverse ZnO nanostructures, JALCOM 816 (2020) 152491
3. Lead-free 0.95(K0.6Na0.4)NbO3-0.05(Bi0.5Na0.5)ZrO3 ceramic for high temperature dielectric, ferroelectric and piezoelectric applications, JALCOM 818 (2020) 152874
4. Flexible lead-free piezo-/ferroelectric Bi0.5(Na0.6K0.4)0.5TiO3 ceramic incorporated PDMS polymer composites for energy harvesting application, Journal of Materials Science: Materials in Electronics, 30 (2019) 6157

****

IT-15

Influence of Different Dopants/Surfactants on The Magnetic And Gas Sensing Properties Of $Cofe_2o_4$ Nanoparticles/Thin Films

R. Ramesh Babu

Crystal Growth and Thin Film Laboratory, Department of Physics,
Bharathidasan University, Tiruchirappalli-620 024.
Email: *rampap2k@yahoo.co.in*

Cobalt ferrite ($CoFe_2O_4$) is one of the versatile magnetic materials belong to the spinel ferrites family. Owing to their special characteristics such as strong magnetocrystalline anisotropy, high coercivity at room temperature, moderate saturation magnetization, high Curie temperature and high chemical and thermal stabilities, $CoFe_2O_4$ magnetic materials can have a wide range of practical and potential applications in many present day technologies like microwave device, high frequency device, permanent magnets, magnetic data storage, magnetic resonance imaging, magnetic drug delivery and gas sensing applications. Generally, the addition of small amount of impurity leads to an effective modification on the electrical, magnetic and gas sensing properties of host material. In AB_2O_4 ($CoFe_2O_4$) system, the change in cation distribution affects the physical properties and also the addition of different valence states leads to various tetrahedral (A) and octahedral (B) sites distribution. Moreover, the addition of surfactants in the synthesis process of ferrite magnetic nanoparticles helps to control the particle growth, and agglomeration between the magnetic nanoparticles due to its steric hindrance and stabilization properties. In the present study, the influence of metal dopants and surfactants on the physical and magnetic properties of $CoFe_2O_4$

nanoparticles is investigated. In addition, the role of metal ions substitution on the physicochemical and gas sensing properties of spray deposited $CoFe_2O_4$ thin films is also investigated. The obtained results will be discussed in detail.

References:

1.M. Vadivel, R. Ramesh Babu, K. Sethuraman, K. Ramamurthi, M. Arivanandhan, Journal of Magnetism and Magnetic Materials, 362 (2014) 122-129.
2.M. Vadivel, R. Ramesh Babu, M. Arivanandhan, K. Ramamurthi, Y. Hayakawa, RSC Advances, 5 (2015) 27060-27068.
3.M. Vadivel, R. Ramesh Babu, K. Ramamurthi, M. Arivanandhan, Ceramics International, 42 (2016) 19320-19328.
4.M. Vadivel, R. Ramesh Babu, K. Ramamurthi, M. Arivanandhan, Journal of Physics and Chemistry of Solids, 102 (2017) 1.
5.M. Vadivel, R Ramesh Babu,, K. Ramamurthi, M. Arivanandhan (2017), Nano-Structures & Nano-Objects, 11, 112–123. (0.632)
6.M Vadivel, R Ramesh Babu, P Selvakumar, M Arivanandhan, K Ramamurthi,(2017), Springer Proceedings in Physics book series (SPPHY- Recent Trends in Materials Science and Applications, 189, 179-193.

****

IT-16

Development of device quality 4-Nitrophenol derivative nonlinear optical single crystals and fabrications of type-I and type-II SHG elements

Muthu Senthil Pandian*, P. Ramasamy

SSN Research Centre, SSN Institutions, Chennai-603110, Tamil Nadu
****Email:*** *senthilpandianm@ssn.edu.in*

Gravity driven concentration gradient is used in the uniaxially solution-crystallization method of Sankaranarayanan-Ramasamy (SR). TGS, GPI, KAP, SSDH, DGZCD, DGBCM, benzophenone and many more crystals have been successfully grown by SR method. Longest benzophenone crystal having dimension of 1350 mm length and 55 mm diameter was grown for the first time in solution growth by SR method. Starting with a thin plate as seed a large size crystal can be grown. The physical properties and crystalline perfection of the SR method grown crystal is normally superior to the conventional method grown crystals. The quality of the SR method grown crystals has been improved by several modifications made in SR method. The impurity segregation cannot be avoided in the existing SR method. So we planned to introduce the RSR method for growing good quality, unidirectional single crystals. The effect of rotation on unidirectional crystal growth method (Rotational Sankaranarayanan - Ramasamy (RSR)) has been proposed for the first time. The organic nonlinear optical 2-Aminopyridinium 4-nitrophenolate 4-nitrophenol (2APNP) crystals have been grown by (i) conventional slow evaporation, (ii) Sankaranarayanan-Ramasamy (SR) method and Rotational SR (RSR) method. The grown 2APNP crystals were subjected to various studies like HRXRD, laser damage threshold, chemical etching, Vickers microhardness, birefringence, UV-Vis NIR, dielectrics and piezoelectrics. The Rotational Sankaranarayanan-Ramasamy (RSR) method grown crystals show excellent optical, mechanical, dielectric and piezoelectric behavior and higher laser damage threshold capability compared to the conventional and normal SR method grown crystals. HRXRD and etching studies showed that the

quality of the RSR method grown crystal is better than conventional and normal SR method grown crystal. The Rotational Sankaranarayanan-Ramasamy (RSR) method can be used to grow single crystals along a specific crystallographic direction such as the phase matching direction in nonlinear optical (NLO) crystals. The unidirectional crystal growth method is ideally suited for crystal growth along this direction to obtain large size crystals required for obtaining SHG elements with minimum wastage. In addition, the unidirectional solution crystallization usually occurs at around room temperature; much lower thermal stress is expected in these crystals over those grown at high temperatures. Successful development of this unidirectional method will provide the technology to produce crystals at a yield close to 100% and easy scaling-up process.

2AP4N crystals grown by (a) Conventional method, (b) SR method and (c) RSR method

References:

1. X. Luo, S. Pan, X. Fan, J. Wang and G. Liu, *J. Cryst. Growth*, **2009**, **311,** 3517-3521.
2. P. Karuppasamy, Muthu Senthil Pandian, P. Ramasamy, Sunil Verma, *Opt. Mater.* **2018**, 79, 152-171.

****

IT-17

Synthesis of hierarchical architecture of chalcopyrite $CuInS_2$ microspheres and Flake-like Al doped ZnO thin films for efficient solar cell applications

K. Sethuraman

School of Physics, Madurai Kamaraj University, Madurai – 625 021.
Email: *sethuraman_33@yahoo.com*

First, the nano-flakes self-assembled porous (NFSAP) - $CuInS_2$ (CIS) microspheres have been optimized on CIS seed layer by controlling the synthetic strategy. Later, Cd and V were incorporated as foreign impurity ions into the NFSAP - CIS microspheres. The pristine and doped CIS microspheres films result in a body-centered-tetragonal crystal structure that was confirmed from the XRD and SAED patterns. The electron microscopic images clearly depict the formation of a solid and an elongated NFSAP - CIS microsphere under Cd and V doping, respectively. The change in the morphological structure was attributed to the suppression and expansion of the laterally orientated crystallographic plane. Cd and V doped CIS microspheres films have superior photoelectric response compared to the pristine CIS films. The controlled laterally orientated crystallographic plane in CIS microspheres by doping induces the modification in the surface morphological structure that results in improved electrical and photo-physical properties. The results of this study provide a framework for fabricating an optimized CIS absorber layer in photovoltaic devices.

ZnO thin film with flake-like surface morphology has been optimized by Al doping via the home-built chemical spray pyrolysis technique at substrate temperature 250 °C. Then, its performance as an anti-reflecting as well as highly transparent and conducting window layer in $CuInS_2$ based solid-state solar cell is explored here. All the films exhibit good optical transmittance nearly ~90-95% in the visible energy region. Further, the 2 wt% Al-doped ZnO film shows low reflection loss in the same region. The good electrical parameters i.e., high conductivity (0.26 mho cm^{-1}) and low resistivity (3.8 Ω cm) are found in the 2 wt% Al-doped ZnO film. Eventually, 2 wt% Al-doped ZnO flake-like morphology film used as a window layer in $CuInS_2$ based solid-state solar cell shows a pronounced photocurrent density result in higher power conversion efficiency (PCE), 2.20% is obtained. This efficiency is superior to all others and 53% higher than that of pristine ZnO window layer based photovolt.

****

IT-18

Template induced nucleation of desired polymorhs of food and pharmaceutical materials

Dr. K. Srinivasan

Department of Physics, Bharathiar University, Coimbatore-641 046
Email: *nivas_5@yahoo.com*

Nucleation control and separation of desired polymorphic forms is a daunting task in the food and pharmaceutical industries since it influences every aspect of the solid state properties. The variations in the physical properties of a solid, such as crystal habit, solubility, hardness, color, optical properties, melting point or chemical reactivity play an essential part in the formulation of the solid and in the application of the formulated product. It also leads to dramatic effects in biological activity between two forms of the same food and drug product. Hence control of polymorphism is an important factor in maintaining high product quality and reproducibility in food and pharmaceutical industry and is also a key issue in several scientific, technological and industrial fields. There are several indentifed methods available to separate the polymorphic forms among them template-induced heterogenous nucleation method plays a vital role in the separtion of polymorphs. Efforts were taken to separate the rare and desired polymorphic forms of two multipotent substances paracetamol and vanillin using the soluble, insoluble polymers and metal, non-metal templates respectively. Successfully separated polymorphs were characterized and the results will be presented.

****

IT-19

Microtube-Czochralski growth of novel organic crystals for NLO applications

M. Arivanandhan

Centre for Nanoscience and Technology, Anna University, Chennai 600025, India
Email: *arivucz@gmail.com*

Organic crystals are promising for various optical applications such as optical filter, optical windows and nonlinear optics (NLO) based frequency converters. The NLO materials are playing an important role in generating the green and blue lasers by second harmonic generation (SHG) of low frequency laser radiations. Moreover, the development of NLO crystals has increased the hope of obtaining tunable laser radiations with high power in the deep ultraviolet regions as well [1]. Organic NLO crystals have received huge attention because of their high NLO performance and fast response compared to the inorganic crystal. However, bulk growth of high quality single crystals of organic materials is a challenging task as they have low thermal stability with poor mechanical strength. Czochralski (CZ) pulling technique is one of the well-established promising techniques to grow bulk unidirectional crystals. However, to grow unidirectional bulk crystals, a pre-grown high quality seed crystals are required. Obtaining a high quality seed crystals is difficult for the organic materials. Microtube-Czochralski (µT-CZ) is a novel growth method to grow bulk crystals without the need of pre-grown seed crystals [1, 2]. A series of benzophenone derivatives have been grown by solution growth and their physicochemical properties have been investigated [3-5]. Recently, the µT-CZ technique has been effectively utilized to grow various kinds of organic NLO materials and studied their physicochemical properties. The seeding temperature (T_s), microtube diameter, rotation rate, length of microtube underneath the melt surface (l_{ums}) are the critical parameters in the µT-CZ growth process. For every material, one has to optimize the each parameter for successful growth of bulk crystals. µT-CZ growth of various organic crystals will be discussed in detail.

References:

1.K.Sankaranarayanan, P.Ramasamy, J. Cryst. Growth, 193 (1998) 252-256.
2.M Arivanandhan et al., Opt Mater, 2005, *27*, 1864-1868.
3.V. Natarajan, M. Omprakash, M. Arivanandhan, Y. Hayakawa, Mat. Chem. Phys. 141 (2013) 160.
4.V. Natarajan, S. Usharani, M. Arivanandhan, P. Anandan, Y. Hayakawa, Spectrochim. Acta A, 145 (2015) 329.
5.S.Usharani, J.Judes, V.Natarajan, M.Arivanandhan, P.Anandan, Dmitry A.Vorontsov, Mikhail O.Marychev, Opt Mater, 100 (2020) 109603.

****

IT-20

Effect of CNTs and graphene upon chitosan-gold gels

R. Radha Perumal

Department of Applied Science and Technology, Anna University, ACT Campus, Chennai, Tamil Nadu, India – 600 025.
E-mail: *perumalramasamy@annauniv.edu*

In this research the effect of addition of carbonaceous materials such as graphene and CNTs in chitosan – gold gels is presented. Chitosan gold gels where formed by adding appropriate amounts of $HAuCl_4$ to chitosan solution. Chitosan is an abundantly available biopolymer and has several advantages such as being environmentally friendly and having excellent film forming capacity. 1 wt % chitosan solution with 1.5% acetic acid was made as stock solution. To this solution different amounts of HAuCl4 was added to obtain gels. These gels collapse in time. To these solutions (before forming gels) conducting carbonaceous materials (CNTs and graphene) was added. It is observed that the concentration of CNT and graphene affect the rheological and electrical properties of the gels. The mechanism of modification in the mechanical and electrical characteristics of the gels is explained based on the reduction of Au (III) on CNTs and graphene. This research could benefit use of gels in batteries.

****

IT-21

Quantum Chemical and Spectroscopic Study on Some Anti-Influenza Drugs with ADMET Predictions and Molecular Docking Studies

M. Prasath

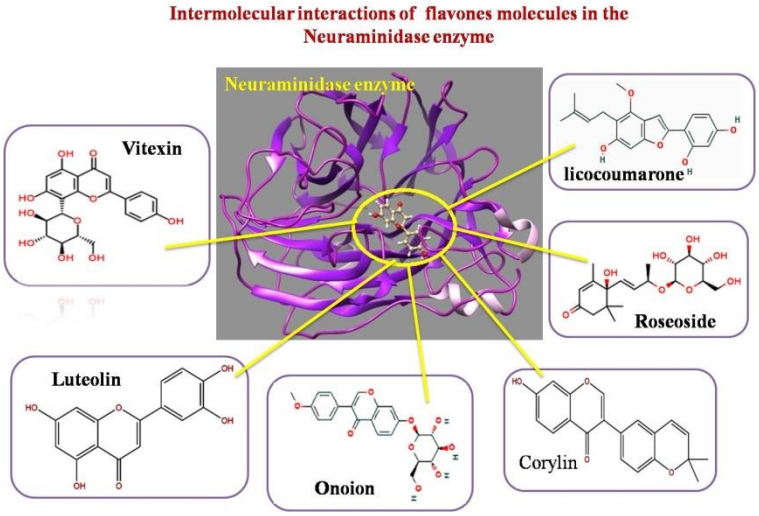
Department of Physics, Periyar University PG Extension Centre, Dharmapuri – 636701
E-mail id: *sanprasath2006@gmail.com*

Influenza A virus is a rapidly contagious virus, causing acute to chronic respiratory disease in humans, and it has been responsible for several global outbreaks. The virus is also a zoonotic pathogen infecting swine, avian, horse, and other species. The swine have been recognized as a primary influenza virus mixing vessel because they are susceptible to infection by both human and avian influenza viruses, facilitating re-assortment among different influenza virus strains. The neuraminidase (NA) enzyme of influenza A virus is a potential target to develop antiviral drugs. NA is an enzyme; it cleaves sialic acid groups from glycoproteins, which is required for flu viral infection replication. So far, three neuraminidase inhibitors have been approved for the treatment of flu infection, namely, zanamivir, oseltamivir and peramivir. In recent years the researchers are developing plant derivative drugs for treating influenza virus.

In the present context, the plant derivative drugs like Luteolin, Vitexin, Ononin, Corylin, Licocoumarone and Roseoside are taken for further calculations. The structure of the molecules was optimized and their values are compared with docked values. The experimental data of FT–IR, FT–Raman vibrational frequencies and UV-Vis spectra was recorded and their values are good agreement with computational results. The molecular orbital contributions were studied by using

the total (TDOS), partial (PDOS), and overlap population (OPDOS) density of states. The molecules obeys the properties of Lipinski's rule of five, hence the molecules exhibit good bioactive score. A molecular docking analysis of molecules was carried out with neuraminidase enzyme. The docking result shows the lowest binding affinity and inhibition constant of the molecule present in the active site, which is considered to be a better inhibitor.

The HOMO-LUMO reveals the good kinetic stability and less toxicity of the molecules in active site. The dipole moment is an important molecular parameter to study the orientation of the dipole vector and intermolecular interactions of the molecule such as dipole-dipole interactions of non-bonded type. The natural bond orbitals, Fukui functions and molecular electrostatic potential (MEP) shows the chemical selectivity and reactivity site of the molecules. The above mentioned calculations are executed for molecules such as Luteolin, Vitexin, Ononin, Corylin, Licocoumarone and Roseoside. The results for all molecules are compared with each other and shows which one is better candidate for influenza A virus.



****

IT-22

Nucleation Kinetics, Growth, Structural, Optical, Laser Damage Threshold and Dielectric Studies of Dicarboxylic Acid Based Single Crystals

Senthilkumar Chandran[a*], Rajesh Paulraj[b], P.Ramasamy[b]

[a]Department of Physics, Government Arts College, Hosur, Tamilnadu- 635109
[b]Department of Physics, SSN College of Engineering, Kalavakkam, Tamilnadu
Email: *senthilkumarchandran89@gmail.com*

As per the current and futuristic need of advanced technology and optical industries the optical materials are demanded in the form of single crystals for broad applications such as laser technology, electronics, photonics, frequency conversion and so on. Single crystals of materials which are having good crystalline perfection, optical transmittance, piezoelectricity, dielectric, mechanical and thermal properties have been required because of their broad applications. Considerable progress and impressive achievements have been got in bulk crystal growth during the last six decades. Since recent years the semi-organic crystals have been attracted due to their

interesting physical and chemical properties. In this view, the present thesis deals with nucleation kinetics, crystal growth, physical and chemical properties of dicarboxylic acid based semi-organic single crystal

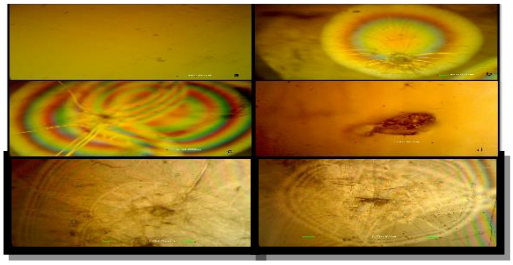


***Figure 1*:** Laser damage site

Keywords: Crystal Growth, Nucleation kinetics, Optical properties, Dielectric

****

IT-23

Low temperature Synthesis and surface modification of biopolymer-ceramic composites

Dr. S. Narayana Kalkura

Crystal Growth Centre, Anna University, Chennai, India -60025
E-mail: *kalkura@yahoo.com/kalkurasn@annauniv.edu*

Common degradable and non-degradable implant materials can be divided into synthetically produced metals and metal alloys, ceramics, polymers, and composites or modified natural materials. Whereas non-resorbable materials like steel or titanium alloys are commonly used for prosthetic devices. Resorbable bone substitute materials are mainly investigated for their feasibility in bone replacement therapies. Whether or not a material is biodegradable, its surface properties will influence the initial cellular events at the cell-material interface. Study of finding a substitution for the bone parts and repairing seriously damaged portions of the human body is a challenging area of multidisciplinary research.

The nano-scale changes in surface like grain size distribution, charge distribution is known to influence the biological performance of the biomaterial. Further, the porosities produced would help in the flow body fluids, bone tissue growth coupled with good biocompatibility. Hydroxyapatite (HAp, $Ca_{10}(PO_4)_6(OH)_2$), a bioceramic is the main constituent of the bones and teeth of vertebrates as well as almost all hard tissues of humans.. It has been widely used to reconstruct or substitute spoiled bone tissues. It has poor mechanical strength that limits its application in the load bearing areas and its low reactivity, leads to slow integration with bone. When applied as coating on metallic surfaces the dissolution rate in the body environment is high that results in the disappearance of the coating at an early stage after implantation. Conventional high temperature sintering of HAp may reduce its reactivity and also result in the conversion to its α-phase and calcium oxide, which is undesirable as it increases the dissolution rate in vivo. To tolerate the corrosive environment of the human body and to control the dissolution rate, surface

modifications of the implant materials is being employed. The ion beam irradiation or implantation enables modification of the chemistry of the bioceramics in a reproducible way so as to optimize the bone response to the implant and improve biointeraction.

Synthesis of polymer composites by various techniques will be discussed. The method of preparation of the samples influenced the bioactivity in a significant way (1-2). The surface roughness and wettability properties of the HAP incorporated composites were enhanced when compared to the pristine samples. Some of the fabricated composites exhibited better stability, mechanical property and haemocompatibility and hence could be used as a composite for tissue engineering and drug delivery. The nitrogen implantation significantly enhanced permittivity, ac conductivity, photoluminescence and pore size. In addition, discussion on the irradiation studies using swift heavy ions on HAp will be presented (3-5). The surface was modified in most of the cases leading to considerable changes in surface properties. The ion implantation/irradiation could be used to modify the surface and tailor the properties to fabricate multifunctional materials.

References:

1. K. Thanigai Arul, J. Ramana Ramya, K.R. Karthikeyan, S. Narayana Kalkura, A novel and rapid route to synthesize polyvinyl alcohol/calcium phosphate nanocomposite thin films by microwave assisted deposition, Materials Letters 13, 2014, 191 – 194
2. .N. K. Elayaraja, V. S. D.Colon, P. A. Sindu, V. S. Chandra, K.R.Karthikeyan, M. SBabu, S. M. Sundaram, M. Palanichamy, S. Narayana Kalkura Effect of solvent; enhancing the wettability and engineering the porous structure of a calcium phosphate/agarose composite for drug delivery, RSC Adv., 2015, 5, 18301-18311
3. K.Thanigai Arul, J.Ramana Ramya, S.C. Vanithakumari, P. Magudapathy, U. Kamachi Mudali, K.G.M. Nair, S. Narayana Kalkura, Novel ultraviolet emitting low energy nitrogen ion implanted magnesium ion incorporated nanocrystalline calcium phosphate, Materials Letters153, 2015, Pages 182–185
4. G.M. Shanthini, N. Sakthivel, R. Menon, P.Y. Nabhiraj, J.A. Gómez-Tejedor, J.M. Meseguer-Dueñas, J.L. G. Ribelles, J.B.M. Krishna, S. Narayana Kalkura, Surface stiffening and enhanced photoluminescence of ion implanted cellulose – polyvinyl alcohol – silica composite, Carbohydrate Polymers, 153, 2016, Pages 619-630
5. J Ramana Ramya, K ThanigaiArul, P Sathiamurthi, K Asokan, N Rajmuhon Singh, S Narayana Kalkura, Enhanced magnetic behaviour and cell proliferation of gamma irradiated dual metal ions co-doped hydroxyapatite–poly (methyl methacrylate) composite films, Reactive and Functional Polymers 123, (2018), Pages 34–43

****

IT-24

Enhancement of the growth rate of the Crystal in TG-SR Method

V.Govindan and K.Sankaranarayanan*

Department of Physics, Alagappa University, Karaikudi
***Email:** hhrsankar@yahoo.com*

The principle of this method involves a temperature gradient between the nutrient zone (let, the temperature be T1) and the growth zone (let the temperature be T2). Usually the temperature T1>T2 to ensure the solute transport to the seed either by natural or forced convection and owing to the temperature difference the solution becomes supersaturated and the growth occurs on the seed surface. In TG-SR method, the unidirectional growth along a specified crystallographic direction is feasible due to the single crystal seed which is kept at the bottom of the ampoule. In the present experimental set-up, the temperature driven flow directs the growth units towards the seed with the aid of gravity induced flow regimes. A typical arrangement for temperature gradient SR method with bottom seeding is shown in Figure 1. Using this set-up, the triphenylmethane unidirectional single crystal was grown successfully for the potential application in the detection of high energy particle [1]. Generally the temperature gradient solution method has the capability of producing large size single crystals irrespective of technical limitations in transferring the mother liquor through different zones without favouring multinucleations.

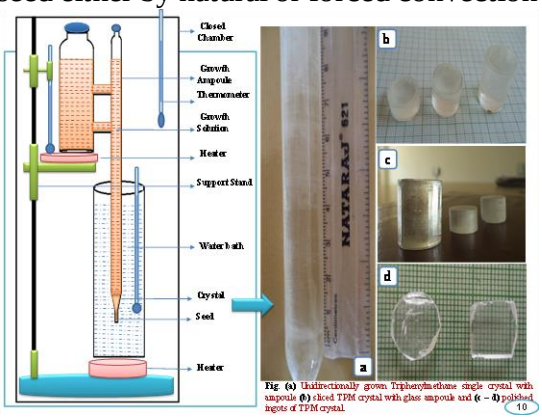


Fig. (a) Unidirectionally grown Triphenylmethane single crystal with ampoule (b) sliced TPM crystal with glass ampoule and (c – d) polished ingots of TPM crystal

Fig. 2 depicts the experimental growth apparatus of the temperature gradient SR crystal growth system. It features two hot zones and two cold zones, which can be kept at the desired temperatures with the aid of a temperature controller within ± 0.5 ºC. The zones are connected through tubes which facilitate the natural convection driven by the temperature gradient across the two zones. For a given solution with defined physicochemical characteristics, the convective flow velocity largely depends on the temperature gradient which ultimately dictates the growth rate of the crystal through the supply of growth units. The occurrence of the growth units in the cold/growth zone is directed towards the growth interface by the gravity. The constant supply of the growth units to the interface is ascertained through the observation on the elevation of the interface. The temperature gradient was fixed based on the experimental parameters like a solvent and its volume, concentration of the solute and the seed. The successful application of this set-up felicitated the growth of a unidirectional 1,3,5 triphenylbenzene at a much faster growth rate than the previous experimental set-up as shown in figure 1.

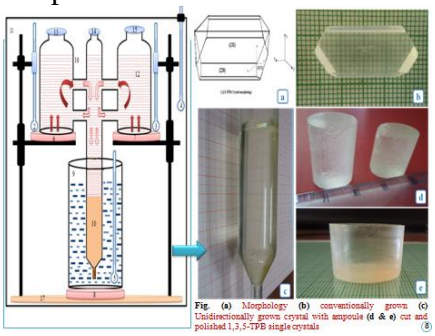


Fig. (a) Morphology (b) conventionally grown (c) Unidirectionally grown crystal with ampoule (d & e) cut and polished 1,3,5-TPB single crystals

References:

1.Materials Chemistry and Physics, Volume 223, 1 February 2019, Pages 183-189.

IT-25

Investigations on the gray tracking effects of potassium titanyl phosphate single crystals for electro-optic applications

Rajesh Narayana Perumal*, P. Ramasamy

Center for Radiation Environmental Science and Technology (SSN-CREST),
SSN College of Engineering, Kalavakkam - 603 110, India.
***Email:** rajeshnp@ssn.edu.in*

The contemporary trend in industrial and medical fields is to adopt solid state lasers with high average power, this requires technologies of higher harmonics generation with efficiency and stability. The efficiency of nonlinear crystal long-wavelength laser emissions to the visible and ultraviolet spectral ranges has led to a constant increasing use of these crystals. Among them KTP is one of the nonlinear crystal frequently opted for its excellent properties like a large nonlinear optical coefficient, wide acceptance angles, thermally stable phase-matching additionally to its attractive nonlinear optical characteristics. It is also utilized in electro-optic applications such as waveguide modulators and Pockels cells because of its large electro-optic coefficients and low dielectric constants. However, this crystal suffers from an important disadvantage, that is the formation of the colour centre called gray tracking.

Gray tracking is a fatigue damage arises due to defect in crystal characterised by a coloured appearance in them which is commonly known as darkening that reduces the non-linear property of crystal through optical power losses(by absorption) that is said to be as chromic damage and so as lowering its performance in applications. Mostly flaws in crystal will decrease the efficiency of their property, experiments show that gray tracking modifies the parametric gain and also many experiments proved that this damage lowers the SHG efficiency and causes astigmatism of the output laser beam and limits the overall lifetime of optical elements. So as if gray tracks once initiated, absorb a significant portion of the propagating beams causing optical power losses and continued operation often leads to catastrophic damage especially in KTP ($KTiOPO_4$). The scope of this research is concerned with propagating the overall knowledge of gray tracking including their mechanism and effects. This work aims to provides detail concept of gray tracking that mainly involves mechanism that lead to initiation of gray track, by laser and electric field.

The research presentation deals with the growth and characterization of neodymium doped $KTiOPO_4$ single crystal and its characterizations. Nd doped KTP crystal was grown using TSSG technique with self flux. The XRD studies have been used to describe the structural level modification and strain presence in the grown crystal. The Nd doping presence in the crystal was studied by EDX and ICP-MS. The FTIR spectra have been used to study the inclusion in the crystal. The effect of neodymium in the structure was evaluated using intensity and broadening behaviour of the Raman shift for grown crystal. The UV–Vis–NIR and EPR technique has been used to evaluate the defect presence in the grown crystal. The thermal properties have been studied by specific heat capacity measurement and increasing the specific heat capacity due to the neodymium doping is observed. The effect of doping in the dielectric permittivity, dielectric loss factor, ac electrical conductivity, complex resistivity and modulus properties has been studied. The reduction of low frequency ac electrical conductivity was measured. The electric field induced grey tracking in $KTiOPO_4$:Re dopants was investigated. Discussed the dependency factors like wavelength, threshold, moisture, repetition rate of laser, dopant addition, polarisation that

influence the gray track to signify the effects of graytracking in KTP and discoursed the measures to control and eliminate the gray tracking. The results will discussed in detail.

****

IT-26

Laser Shock Peening Employed Materials Science Tetrahedron Approach on Ferrous and Non-Ferrous Metal Alloys

Kalainathan Sivaperuman[1*] S. Prabhakaran[1]

Vellore Institute of Technology[1], Vellore
E-mail: *s.kalainathan@gmail.com*

Laser Shock Peening is a promising surface enhancement technique applied to variety of metal materials to improve their surface, microstructure and mechanical properties. The induced compressive residual stress through laser shock peening is beneficiary to retard the crack initiation and propagations to extend the fatigue life of the engineering components. In order to commercialize laser shock peening as a successful surface modification technique, there are few drawbacks identified and they are Cost of laser shock peening process, and Inconsistency in inducing compressive residual stress due to improper process parameters

In view of resolving the above mentioned issues, the present work tried to bring necessary developments to implement low energy laser shock peening technique on few ferrous and non-ferrous metal alloys using Q-switched Nd: YAG laser with the fundamental wavelength of 1064 nm. Also, we have implemented laser shock peening without any protective layer coating called laser shock peening without coating technique for cost-effective processing. The work initially tried to optimize the laser pulse density or pulse overlapping to induce maximum compressive residual stress in case of laser shock peening without coating for the metal alloys such as Medium Carbon Spring Steel SAE 9254 and Austenitic Stainless Steel AISI 304. Later, we tried to apply laser shock peening for the severe surface plastic deformations called laser shock surface nano-crystallization by optimizing the number of impacts for the metal alloys Medium Carbon Spring Steel SAE 9254, Duplex Stainless Steel SAF 2205 and Nickel base Super alloy Inconel 718. The work also tried to find the solution in performing Warm Laser Shock Peening. Laser shock peening without coating technique was not suggestible for the all metal alloys especially for Aluminum-Graphene composites, one need to give protective coating due higher surface roughness induced during direct laser ablation.

****

IT-27

Characterization of some organic NLO crystals grown by solution method

P. Selvarajan

Department of Physics, Aditanar College of Arts & Science,
Tiruchendur-628 216, Tamilnadu, India
Email: *pselvarajanphy@yahoo.co.in*

Organic nonlinear optical (NLO) crystals are interested due to their large high order polarizabilities and rapid response in electro-optic effect compared to inorganic NLO materials and they play important roles in second harmonic generation (SHG), third harmonic generation (THG), frequency mixing, electro-optic modulation (EOM) and optical parametric oscillation etc. Moreover, these materials may be desirable to replace electronic switching circuits in computing and telecommunication systems with future optical devices such as optical processing, optical computing and optical storage devices. In this work, some organic NLO crystals viz. gamma glycine crystal, urea adipic acid crystal and lauric acid crystal are considered. Gamma glycine crystal is a second harmonic generator as well as a third harmonic generator. Urea adipic acid crystal is a centrosymmtric crystal and hence it is a useful third harmonic generating material. Lauric acid crystal is an important second harmonic generator. Growth of gamma glycine crystal was carried out using alpha-glycine and ammonium chloride as the reactants. Urea and adipic acid were mixed in 1:1 molar ratio to form urea adipic acid crystal and lauric acid chemical and ethanol solution were used to crystallize the lauric acid crystal. All the crystals were grown by solution method with slow evaporation technique. The harvested crystals were studied by various characterization techniques such as XRD, FTIR, UV-vis-NIR transmittance, microhardness, dielectric, thermal, SHG and Z-scan studies.

References:

1. Benjamin G. Penn, Beatriz H. Cardelino, Craig E. Moore, Angela W. Shields, D.O. Frazie Progress in Crystal Growth and Characterization of Materials, 22 (1991) 19-51.
2. P.Selvarajan, J.Glorium Arulraj, S.Perumal, J. Crystal Growth, 311 (2009) 3835.
3. B Helina, P Selvarajan and A S J Lucia Rose, Physica Scripta 85 (2012) 055803.
4. J.Uma Maheswari,, CKrishnan, S Kalyanaraman and P Selvarajan, Mater. Res. Express, 3 (2016) 105101.
5. Shanthi, C. Krishnan, P. Selvarajan, Spectrochimica Acta Part A, 122 (2014) 521–528.

****

IT -28

Growth of 1, 3, 5 - Triphenylbenzene Scintillator Single Crystal by Modified Vertical Bridgman Method and its characterization for Scintillation Application

P. Rajesh*, M. Manikandan, P. Ramasamy

Centre for Crystal Growth, Department of Physics, SSN College of Engineering, Kalavakkam, Tamilnadu - 603 110.
Email: *rajeshp@ssn.edu.in*

Radioactive materials are often detected and identified by measuring gamma-rays and neutrons emitted from the materials. The ability to detect gamma rays and neutrons is a crucial tool for many areas of research. The applications are found in medical diagnostics, in industry, and science. The organic molecule crystals are used for particle identification process due to its pulse shape discrimination property. In recent years different authors analyzed several organic crystals for studying neutron-gamma (n-γ) discrimination property. Few organic crystals possess combined properties like Second Harmonic Generation (SHG) under laser illumination and scintillation efficiency in the high energy radiation background.

1, 3, 5-Triphenylbenzene (TPB) single crystal is one of the organic crystal to detect the neutron in the gamma-ray background. TPB single crystal (length 100 mm and diameter 10 mm) has been successfully grown for the first time by the modified vertical Bridgman technique (VBT). This method is developed for the growth of enhanced quality. Physical, optical and scintillation properties such as crystalline nature, thermal stability, transmittance, radioluminescence and lifetime were investigated. The polished TPB sample has good transmission in the wavelength range between 300-1500 nm. The thermal properties of the grown crystal were analyzed by thermogravimetric and differential thermal analyses. The refractive index at five different wavelengths in the range between 407 to 1551 nm and optical birefringence properties of TPB crystal were studied using the prism coupling method. Birefringence study reveals that the grown crystal has good optical homogeneity. Scintillation properties such as radioluminescence light yield using Sr-90 as a source and decay time were also investigated. 1, 3, 5-triphenylbenzene can be potentially used as NLO and scintillator for high-energy neutron detection application in the presence of gamma radiation background.

References:

1. G. Hull, et al, IEEE Transactions on Nuclear Science, 2009, 56, 899-903.
2. E.V. van Loef, et al, IEEE Nuclear Science Symposuim & Medical Imaging Conference, 2010, 1007-1009. IEEE.
3. N. Zaitseva, et al, J. Cryst. Growth, 2011, 314, 163-170.
4. M. Manikandan, et al, J. Mol. Struct.., 2019, 1195, 659-669.
5. N. Durairaj, et al, DAE Symp. Nucl. Phys. 2017, Vol. 62, 1046-1047).

****

IT-29

Synthesis, Growth and Physical characterization of $AgIn_{0.5}Ga_{0.5}S_2$ single crystal for Mid-IR applications

N.Karunagaran and P. Ramasamy

Department of physics, S.R.M University, Ramapuram, Chennai
Center for crystal growth, SSN College of Engineering, Kalavallam-603110
Email: *karthickkaruna@gmail.com*

Silver Indium Gallium Sulfide ($AgIn_{0.5}Ga_{0.5}S_2$) belongs to the family of $A^IB^{III}C_2^{VI}$ ternary compound semiconductors which crystallize in the chalcopyrite structure. The growth of $AgIn_{0.5}Ga_{0.5}S_2$ single crystal is a two step process. Synthesis of the polycrystalline material from the starting elements is achieved using melt temperature oscillation method. The synthesized material is used to grow a single crystal. The $AgIn_{0.5}Ga_{0.5}S_2$ single crystals have been grown by the vertical Bridgman technique. The synthesized $AgIn_{0.5}Ga_{0.5}S_2$ polycrystalline charge was confirmed by powder XRD. The peak positions are in good agreement with the powder diffraction file. Thermal property was analyzed using **TG-DTA** technique. The melting point of the crystal is 896 ºC and freezing point is 862 ºC. The unit cell parameters were confirmed by single crystal X-ray. The grown crystal was subjected to IR transmission. The stoichiometric composition of $AgIn_{0.5}Ga_{0.5}S_2$ was measured using energy dispersive spectrometry (EDS).

****

IT -30

Unidirectional Growth and Quantum Chemical Studies On NLO Active L-Alanine and L-Histidine Single Crystals

Robert R

PG & Research Department of Physics, Govt. Arts College for Men, Krishnagiri-1
Email: *roberthosur@yahoo.co.in*

The development of crystal growth technology is highly essential in view of its important role in the expansion of several important technologies. The mesmerizing features exhibited by the crystals are due to the periodic arrangement of atoms or molecules. The process of crystal growth essentially involves a change of phase in which the material loses its random character and achieves a long-range order.

In recent years, there has been considerable attention among scientists in the development of large size novel nonlinear optical (NLO) materials, which combine the high optical nonlinearity and chemical flexibility of organics with the high mechanical strength of inorganics. The key factors for material selection depend not only on the laser conditions but also on the physical properties of the crystal, such as transparency, damage threshold, conversion efficiency, phase matching, and temperature stability. In view of this, there has been shown palpable interest in the synthesis of semi-organic materials due to their large nonlinearity, high resistance to laser-induced damage, low angular sensitivity and good thermal and mechanical properties.

Amino acid crystals have been intensely investigated due to their potential NLO properties. Amino acid-based nonlinear organic and semiorganic crystals have proven to be attention-grabbing candidates for a second harmonic generation. However, to enable the material to be potentially useful for nonlinear optical applications, the material should be available in bulk form. There are different techniques to grow bulk crystals in which solution and melt growth techniques are mostly used. In the solution growth technique, there are different methods to grow bulk single crystals. However, a potential method called Sankaranarayanan - Ramasamy method gives bulk unidirectional crystals with good quality from the solution.

The present investigation is aimed at growing a few bulk forms of nonlinear optical organic amino acid single crystals.

The grown single crystals were characterized and discussed using various techniques such as X-ray diffraction (XRD), Fourier transforms infrared (FTIR), UV spectral analysis, dielectric analysis, microhardness studies, thermal analysis, photoluminescence studies and the Quantum Chemical approaches such as ab initio, DFT and semi-empirical methods.

Keywords: Nonlinear optical (NLO) materials - Amino acid crystals - solution growth - bulk unidirectional crystals - Sankaranarayanan - Ramasamy method

****

IT -31

Assessment of Sustainability of Molecular and Structural Properties of Crystals by Shock Waves

S.A.Martin Britto Dhas

Department of Physics, Abdul Kalam Research Center, Sacred Heart College, Tirupattur Tamilnadu, India - 635 601
Email: *martinbritto@shctpt.edu*

In recent years, there are few thousands of organic and inorganic crystals proposed for variety of technological applications. But, unfortunately, most of the materials do not fit to the actual standard in terms of efficiency, environmental resistance, cost effective, availability, durability and so on. Hence, searching of the most suitable materials for technological applications is highly demanded. Shock waves are one the simplest tool to identify materials against high temperature and high pressure resistance for aerospace, nuclear power plant, high power laser applications and so on. From the recent publications, it is very well proved that during the propagation of shock waves in materials, it generates different types of crystalline defects and structural changes which leads to the change of their inherent properties. Even a crystal can generate shock waves when it drops down and hit the ground. This generated shock wave is enough to create the above said defects in the crystals. Hence, we should be aware this particular problems while a material is suggested for the technological applications especially in aerospace devices and high power laser applications. In the present research, we have chosen few popular non-linear optical materials such as ammonium dihydroegn phosphate (ADP), potassium dihydroegn phosphate (KDP), Glysine phosphate (GPI), Benzophonon and copper sulfate crystals for the assessment of structural stability. Raman and powder X-ray diffraction (XRD) techniques are utilized to evaluate the molecular and structural performance of the above said material against the

impact of shock waves and obtained crystallographic structural properties. Each material has shown different shock response and produced interesting changes in structural, crystalline perfection, defect density, transparency, etc. The observed results will be discussed during the conference.

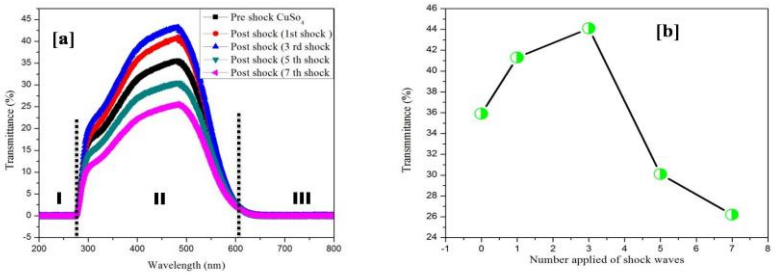


Figure: [a] Optical Transmittance of copper sulphate against number of shock waves [b] Transmittance at 480 nm with respect number of shock pulses

****

IT -32

Growth and characterization of Semi-organic and Organic Single Crystals for Nonlinear optical Applications

A. Senthil*, and P. Ramasamy[1]

Department of physics, SRM Institute of Science and Technology, Ramapuaram Campus, Chennai-600089
[1]SSNRC, SSN College of Engineering, Kalavakkam-603110, Chennai
****Email:*** *tasenthil@gmail.com*

In the last few years, there have been intensive research efforts in exploring and developing useful and efficient second-order nonlinear optical materials for various applications such as electro-optic switching or modulation for telecommunication and frequency conversion for laser sources at new wavelengths. Molecular materials such as organic systems in which chemically bonded molecular units interact in the bulk through week Vander Waals forces. Optical nonlinearities in these systems are often considered to be primary. Semiorganic materials. It is generally believed that organic-inorganic nonlinear optical crystal material compound not only possesses the high optical nonlinearity of a purely organic compound but also the favorable thermal and mechanical properties of an inorganic compound. They do not have pi electrons as organic NLO materials have. Sodium di(L-malato) borate (NaDMB) single crystals are the good candidates for SHG applications in the semi-organic malic acid family. Optically good quality, bulk single crystal of <100> directional Sodium Di (L-Malato) Borate **(**NaDMB**)** was successfully grown by Sankaranarayanan-Ramasamy (SR) method and New organic single crystals of Dicyclohexylammonium dioxalate hydrate (DHADO) were grown by slow evaporation solution method at 30 ºC temperature. Optical, thermal, structural and mechanical properties were analysed by UV-vis-NIR spectrum TG/DTA, X-ray diffraction rocking curve measurement and Vickers microhardness test. The results will be discussed in detail.

****

IT -33

Modeling and Simulation of mc-Silicon Crystal Growth Process: Investigation of Transport Effects in Melt and Crystal Phases

M. Srinivasan & P. Ramasamy

SSN Research centre, SSN College of Engineering, Chennai-603110.
Email: *srinisastri@gmail.com*

Numerical simulation is a comprehensive tool in modern process development which is extensively used for promotion of crystal growth processes. Multi-crystalline silicon is an important material with advantages of low-production cost and moderately conversion efficiency of PV solar cells[1]. The control of grains as well as the grain boundaries is particularly important to the crystal quality and thus the solar cell efficiency. Flow in the molten phase is indispensable for transport of heat and mass convection in bulk crystal growth systems. Understanding transport of heat, mass and momentum is especially essential in bulk crystal growth processes. To grow high quality bulk crystals, i.e. the crystals with acceptable defect density and good dopant uniformity, understanding of transport processes coupled with the melt and gas chemistry is crucial[2]. Direct experimental investigation and in-situ observation of species transport are quite difficult due to the high-temperature environment. Therefore, crystal growth modelling attracts much attention in developing the technology and in finding an effective way to control mass transport during crystal growth. The work is broadly categorized into following:

To study the melt flow properties of small-scale molten silicon based on the dimensionless numbers such as Marangoni, Peclet and Reynold's numbers.

To investigate the melt flow properties for large scale molten silicon based on the dimensionless numbers like Rayleigh, Reynolds and Prandtl numbers.

To study the non-metallic impurities such as carbon, oxygen, nitrogen and their inclusions based on Schmidt number during directional solidification and its effect on the solar cell efficiencies.

To analyse the generation of stress and dislocation densities in grown mc-silicon at various growth stages in industrial scale DS system.

To introduce the bottom groove DS furnace and investigate some of the thermo-mechanical properties in grown mc-silicon ingot.

Also, many modifications are made on DS system for developing high performance of mc-silicon ingots such as heater modification, varying insulation movement, crucible rotation, crucible vibration and magnetic field application.

References:

1. B. K. Sahu, Renewable and Sustainable Energy Reviews, **59**, 927-939 (2015).
2. J. Friedrich et al. *Journal of Crystal Growth,* **447,** 18–26 (2016).

****

IT -34

Single crystals: Potential candidate for reference material for technological applications

Anuj Krishna[1,*], Nahar Singh[1], R.P.Pant[1]

[1]Indian Reference Materials (BND) Division, CSIR-National Physical Laboratory, New Delhi -110012
***Email:** anuj.krishna@nplindia.org*

CSIR- National Physical Laboratory is 'National Metrology Institute' by act of Parliament and has responsibility to disseminate traceability to the needs of country. Certified Reference Materials (Bhartiya Nirdeshak Dravyas (BNDs)) plays an important role in disseminating SI traceability. Reference materials based on single crystals can be of wide importance as they can be utilised for calibration of instruments like UV-Vis spectrophotometer, photoluminescence spectrophotometer, seebeck coefficient standard etc. Owing to disadvantage in solution based reference materials due to volume inaccuracies and weighing errors, reference materials based on single crystal possess advantage as they have defined surface, easy to clean and possess higher chemical stability. Hence the talk will focus on growth and characterization of some single crystals and their application as reference material for technological applications.

Keywords: Bhartiya Nirdeshak Dravyas, Certified Reference Materials, Photoluminescence, Seebeck coefficient.

****

IT -35

Characterization of surface treated $Cd_{0.9}Zn_{0.1}Te$ Single Crystals

P.Vijayakumar1, E.P.Amaladass1,2, K.Ganesan1,2, R.M.Sarguna1, S.Chinnathambi1 S.Ganesamoorthy1,2,*, V.Sridharan1,2, Awadhesh Mani1,2 and N.Subramanian1,2

1Materials Science Group, Indira Gandhi Centre for Atomic Research, Kalpakkam 603 102, Tamil Nadu, India
2Homi Bhabha National Institute, Mumbai 400 094, India
***Email:** sgm@igcar.gov.in*

To get high spectral resolution, good detection efficiency, high sensitivity and functionality at room temperature, the semiconductor material used as gamma radiation detector should have high atomic number (~ 50: to get high stopping power of gamma radiation), wide band gap (>1.3 eV), high resistivity (>10^9 Ω cm: to get low leakage current), homogenous crystal composition (for low trapping of charge carriers), a good mobility (to have high carrier drift length and maximum charge collection) and be non-polarized (not to be affected by electric fields). $Cd_{0.9}Zn_{0.1}Te$ (CZT) single crystals satisfy almost all the above requirements of gamma radiation detection. CZT gamma ray detectors are used in many fields like medical imaging, security, astronomy, science and industrial analysis. In the present reported work CZT single crystals were grown by traveling heater method using Te as a solvent. The grown crystals were cut into wafers and polished. The polished wafers generally contain grain boundaries, sub-grains and damages induced by

mechanical polishing. This results in higher leakage current. In order to reduce the leakage current, we have optimized Br-Methanol etching concentration and etching time. The structural quality of the grown CZT single crystals is characterized by X-ray diffraction and Laue back diffraction studies. The surface roughness and transparency range of the prepared CZT wafers were analyzed by atomic force microscopy, NIR transmission and Raman spectroscopy studies. I-V characteristics of the CZT wafers are performed under different surface preparation conditions. Highest resistivity of about 1.36 x $10^{11}\Omega$.cm is obtained for the CZT wafer using gold electrodes with post-deposition thermal annealing.

****

IT -36

Studies on integration of Piezo thin films on Si substrates for realizing MEMS devices

E. Varadarajan and V.Natarajan

Research and Innovation Centre, IITM Research Park, Chennai
Email: *evaradarajan@ric.drdo.in*

During the past four decades, development of high efficiency piezoelectric materials enabled to design and fabricates numerous novel devices for various applications. In recent years, there has been increased interest in ferroelectric lead zirconate titanate (PZT) films for device applications including high-frequency ferroelectric sonar transducers, micro-electromechanical system devices, elastic surface wave devices, hydrophones, sensors and actuators. Piezo film based devices not only work at low voltage and wide frequency bandwidth, as they are compatible with semiconductor integrated circuit, but also possess superior electrical properties approaching values of bulk piezo ceramics. Naturally, processing of PZT films has become an increasingly popular field of study. Lead free piezoceramic and relaxor ferroelectrics are being investigated to enhance the efficiencies of sensors, actuators and simultaneously reducing the dimensions of the devices.

In this lecture we will give an overview of the development of different peizo thin film processing technologies and integration of peizo materials onto Si wafers to understand their influence on existing Si foundry processes and brings out the compatible process for realizing the Piezo MEMS devices for various applications. In order to realize these devices various miniaturization approaches such as Integrative, Bulk and Surface micromachining techniques are explored to realize the piezo MEMS sensors and actuators. Further results are discussed in detail the device fabrication procedures and testing methods, respectively.

****

IT -37

Hydrothermal Synthesis of Glutamic acid Cobalt based Mesoporous Microspheres with a large Size and High Porosity

M.Sakthi and M.Annalakshmi
ERK Arts and Science College, Erumiyampatty, Tamil Nadu 636905

A novel 3-dimensional Co(II)/glutamic acid based mesoporous metal–organic framework complex was synthesized by hydrothermal method. The porous organo-metallic complex in microspheres shape with high porosity, controllable morphology, and large particle size. The Brunauer–Emmett—Teller (BET) analysis reveals that maximum amount of N_2 sorbed at 77K founded to be 1550 cc/gm and surface area of 1374 $m^2 g^{-1}$ and high thermal and chemical stability compare glutamic based microspheres. The hysteresis loop for the complex was suggested contributions of type C hysteresis, indicating the presence of Wedge-shaped pores in the microspheres.

Keywords: Mesoporous, Microspheres, BET analysis, Wedge shaped pores.

****

IT -38

Ab initio prediction of the High energetic and biological molecules – A validation study

P. Srinivasan[1] and A. David stephen[2]
PG & Research Department of Physics, Chikkaiah Naicker College, Erode, India
Department of Physics, Sri Shakthi Institute of Engineering and Technology, Coimbatore, India
Email: *sriniscience@gmail.com*

The key importance of the a*b initio* crystal structure prediction method lies in the application area where a successful prediction method can give a good understanding of the crystallisation process, and also the prediction of highly energetic molecules might decrease the level of experimental risks. It also got much importance in the field of pharmaceuticals where the prediction of organic drug molecules with a specific action may create a revolution. Organic drug molecules are flexible compared to CHNO-based energetic crystals. Such flexible molecules have the tendency to show high degrees of polymorphism. Presence of a polymorph of an organic molecule in a crystal structure can differently affect the action of the organic molecule or alter the molecular geometry, which may lead to the development of a new drug or to opt out the negative effect of the concerned drug system. The crystal structure prediction method allows the theorists to discover new polymorphs of such molecules. In a different way, some polymorphs can have good application values. The current aim of the *ab initio* crystal structure prediction is to find the possible conformers of the flexible novel polymorphic/High energetic molecule using gas phase optimisation with an MP2/6-31G(*d*,*p*) basis set, and the lattice energy minimization in the presence of a repulsion-dispersion electrostatic potential.

***Keywords*:** Ab initio crystal structure prediction; polymorphs; PES scan; lattice energy minimisation; HEDM.

****

Best Thesis Presentation

BT-01

Growth and Characterization of Some Amino Acid Doped ADP Crystal

Dr. Joshi Jaydeep Hitendrakumar

Saurashtra University, Rajkot – 360 005 (Gujarat)
***Email:** jaydeep_joshi1989@yahoo.com*

The Ammonium Dihydrogen Phosphate (ADP) is an excellent nonlinear optical material used as second, third and fourth harmonic generator for Nd:YAG and Nd:YLF lasers. The amino acids have molecular chirality, Zwitter ionic nature, non-centro symmetry, which is beneficial for the nonlinear optical and other properties enhancement in ADP crystal. The author has grown single crystals of pure and amino acids like L-threonine, L-serine and L-phenylalanine doped ADP crystals using the slow solvent evaporation technique. The powder XRD study suggested that all the grown crystals are belonging to the tetragonal structural symmetry. The FT-IR spectra show the shifting of characteristic absorption bands of ADP crystal on doping. The FT-Raman study confirmed that the dopant unaltered the H_2PO_4 structural symmetry. The photoluminescence study suggested that the amino acids doping in ADP crystal causes L-defect and D-defect in hydrogen bonding. Also the PL study indicated existence of the Self Trapped Excitons with enhanced Stoke's shift and presence of vibration relaxation state. The TGA/DTA study shows that the amino acids reduce the thermal stability of ADP crystal slightly. The presence of various elements of host and guest material is confirmed using the EDAX and CHN. The UV-Visible transmittance study shows that the amino acids doping enhances the optical transparency, the optical energy band gap, the skin depth and reduces the refractive index and the extinction coefficient. The refractive index dispersion using the Wemple-DiDomenico Single Oscillator Model is studied. The complex admittance study of pure and amino acids doped ADP crystals are found to be in accordance with the dielectric and conductivity study. The pure and amino acids doped ADP crystals exhibited the Negative Photoconductivity. The dielectric constant and the dielectric loss of pure and amino acids doped ADP crystals shows the universal behaviour over angular frequency range and temperature range considered. The A.C. electrical conductivity study revealed that the amino acid doping in ADP crystals leads to enhance the hydrogen bonding defect in ADP unit cell. The Correlation Barrier Hopping (CBH) and Non-Overlapping Small Polaron Tunnelling (NSPT) kind of conductivity mechanisms are extensively studied for pure and amino acids doped ADP crystals. The presence of grain and grain boundary in pure and amino acids doped ADP crystals are indentified and modelled in terms of R-CPE circuits using the Complex Impedance and the Complex Modulus spectroscopy. The Nonlinear Optical Second Harmonic Generation Efficiency of ADP crystal is enhanced on doping the amino acids in it. The Z-scan study suggested that the pure and amino acids doped ADP crystals consist phenomenon such as self focusing and self defocusing also saturable and reverse saturable absorption. Alike SHG efficiency, the magnitude of third order nonlinear optical susceptibility is increased on doping the amino acids in ADP crystal. The Laser Threshold Damage study shows that the amino acids doping provides excellent resistance to the ADP crystal against the energetic laser beam. Ultimately, the aim of entire study to improve the nonlinear and other properties of ADP crystal on the account of amino acid doping is satisfied.

****

BT-02

Synthesis, Characterization and Structure-NLO property relationship of certain organic single crystals

Jesby George

Department of Physics, Bishop Moore College Mavelikara, Alappuzha, Kerala, India- 690 110

The thesis deals with third-order nonlinear optical properties of six synthesized organic crystals, structural confirmation analyzed by Single crystal X-ray diffraction (SXRD) and Powder X-ray diffraction (XRD) techniques. Spectroscopic characterization using infrared (IR), Raman and UV-visible spectra and NLO characterization using Z-scan technique have been carried out. The experimental data are interpreted by computational studies using density functional theory (DFT) and Atoms in Molecules (AIM). The intra and intermolecular hydrogen bonds within the crystal system and photoluminescence spectra revels the applications in the field of nonlinear optics and OLED. The major features of the six crystals are follows:

Protonated N-H...O and intermolecular interactions are responsible for the NLO activity in Diglycine Barium Chloride Monohydrate (DGBCM). Photoluminescence spectrum shows that the luminescence is at the blue region. The third order nonlinear optical properties investigated by Z-scan technique.

Proton transfer complex interconnected through water molecule via strong N^{+}-H….O^{-} and O^{+}-H...O^{-} hydrogen bonds of Picolinium Tartrate Monohydrate (PTM). FT-IR and FT-Raman spectra revels the red shifting of N-H and O-H stretching vibrations due to the proton transfer. Third order nonlinear optical properties like self-defocusing, saturable absorption and optical limiting at 532 nm are identified by Z-scan technique. High third order nonlinearity in the form of self-defocusing and two-photon absorption with saturable absorption revealed from z-scan technique. The red shifted NH stretching wavenumbers and the broadening of corresponding bands in the FTIR and FT-Raman confirmed the presence of N-H···O hydrogen bonding in G4AB.Single crystals of pure and crystal violet dye doped L-Argininium bis dihydrogen phosphate (LADP) were grown using slow evaporation technique. Blue and red shifting hydrogen bonds were predicted by DFT on the basis of vibrational spectral (FT-IR & FT-Raman), AIM and NBO analyses. Doped LADP crystal shows enhancements in the wavelength and longer life times as identified from photoluminescence spectra and decay analysis respectively. Enhancement in non linear optical parameters in dye doped LADP crystal was revealed from the Z-scan technique.Morpholin-4-ium hydrogen tartrate (MHT) linked via N-H…O and O-H…O hydrogen bonds. The photoluminescence spectrum shows luminescence at the blue region with an appreciable lifetime leading to applications in blue OLEDs. Third order nonlinear optical properties identified by Z-scan analysis and laser damage threshold (LDT) have been measured. The crystalline nature and lattice parameters of synthesized compounds of three cyclohexanone derivatives were confirmed by powder X-ray diffraction technique. The doublet of the C=O mode band in FTIR originates from Fermi resonance. Fluorescence lifetime measurement of the title compound exhibits a lifetime of order 2-3 ns and blue emission observed from CIE chromatic diagram.

****

BT-03

Growth and Characterization of 4–Dimethylamino–N–Methyl–4–Stilbazolium Tosylate (DAST) Crystal for Photonic Applications

M. Manivannan, S.A. Martin Britto Dhas, M. Jose *

** Department of Physics, Sacred Heart College (Autonomous), Tirupattur 635601, Tamilnadu, India*

**Email: mjosh1231@gmail.com, jose@shctpt.edu,Tel: +91-9944825036*

The synthesis and growth of novel materials with enhanced NLO properties is significant consideration for their potential apperiations, which can be accomplished by adopting the existing crystal growth methods and making some modification on them for better results. This research contribution witnesses the exponential growth of large size Pure, EDTA and DTPA doped organic DAST crystal by slow solvent evaporation and cost effective seed rotation techniques. The crystal structure and crystalline nature of the grown crystals was confirmed by SXRD, PXRD and HRXRD analysis. The functional groups and mode of vibrations have been confirmed by NMR, FTIR and FT-Raman spectral analysis. The optical band gaps, Linear refractive indices of pure, EDTA and DTPA doped DAST crystals were calculated using UV-Visible study. The photoluminescence spectral study shows enhanced blue light emission and significantly reducing defect-related red emission. Photoacoustic spectroscopy analysis reveals that the DTPA added DAST crystal has better thermal diffusivity, thermal effusivity and thermal conductivity than pure and EDTA added DAST crystal. The saturation polarization of the grown crystal is analysized using the hysteresis loop. The Mayer's index (n) has been found to be higher than 1.6, confirming that the DAST belongs to a soft material category. Crystalline perfection of crystal is identified from both the etch pattern and hardness test. The dielectric analysis demonstrates that the grown crystals have low dielectric constant and dielectric loss at higher frequencies, which substantiate the optical quality with minimum defects. The activation energy of the grown pure and additives added DAST crystals were found to be increasing with increasing frequency, which confirms the conductivity is thermally activated process. DTPA added DAST crystal exhibits higher laser damage threshold than those of the other crystals. Photoconductivity study reveals that the pure and EDTA doped DAST crystals possesses negative photo conducting behaviour while DTPA doped DAST crystal shows positive photo conducting behaviour.

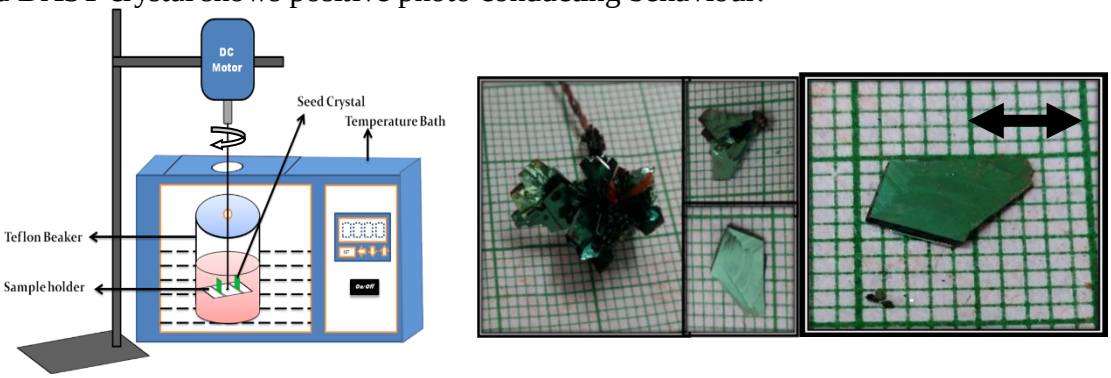


Figure: Schematic diagram of experimental setup and photograph of as grown DAST single crystal

References:
[1] S. R. Marder, J W. Perry and W P. Schaeferet, Science, **1989**, 245, 626–628.
[2] T Thomas, J V. Ramaclus, F P. Mena, P. Sagayaraja and E A. Michael, Cryst. Eng. Comm, **2015,** 17. 1989–1996.
[3] F. Pan, G. Knopfle, Ch. Bosshard, S. Follonier and R. Spreiter, Appl. Phys. Lett. **1996,** 69 (13), 13–15.
[4] A. S. Haja Hameed, S. Rohani, W.C. Yu, C.Y. Tai and C.W. Lan, Mater. Chem. Phy. **2007**, 102, 60–66.

****

BT-04

Structural, spectral and optical analysis of some 4-methylbenzylamine based crystals

Aarthi. R and Ramachandra Raja. C

Government Arts College (Autonomous), Kumbakonam-612 002, Tamilnadu.
**Email: crrajaphy@gmail.com*

This thesis deals with the growth and characterization of the following seven 4-methylbenzylamine (4MLBA) based crystals using low temperature solution growth technique.

4-methylbenzylammonium nitrate (4MLBANO_3)
Bis(4-methylbenzylammonium) tetra chloridocadmate (II) (4MLBACD)
Bis(4-methylbenzylammonium) tetra chloridozincate (4MLBAZN)
4-methylbenzylammonium chloride hemihydrate (4MLBACH)
4-methylbenzylammonium bromide hemihydrate (4MLBABH)
Bis(4-methylbenzylammonium) tetrabromido zincate (4MLTBZ)
Catena-poly[bis(4-methylbenzylammonium)[[dibromidocadmate(II)]-di-l-bromido]] (4MLBCDB)

These crystals were grown by reacting certain inorganic acids and inorganic salts with 4-methylbenzylamine. In this reaction inorganic acids donates H^+ cation to NH_2 group of 4MLBA and protonates it as NH_3^+ and forms hydrogen bonded supramolecular structures. Out of these seven, 4MLBACH, 4MLBABH, 4MLTBZ and 4MLBCDB are new crystals and their structures are reported in IUCr data. The grown crystals were subjected to various characterization techniques to identify the suitability towards applications. Single crystal X-ray diffraction analysis reveals that the 4MLBANO_3. 4MLBACD, 4MLBACH, 4MLBABH and 4MLBCDB were crystallizes in centrosymmetric space groups and 4MLBAZN and 4MLTBZ crystalizes in non-centrosymmetric space groups. Also, 4MLBCDB crystallizes in polymeric structure. In all the seven crystal structures 4-methylbenzylammonium cation linked among themselves by C-H---π intramolecular interactions. This organic cation linked to inorganic anion through [N-H---X and C-H---X (X = Br, Cl, NO_3)] hydrogen bonded intermolecular interactions. Sharp peak observed in the powder X-ray diffraction pattern of grown crystals establishes their good crystalline nature.

Linear optical transmission window was observed from 260 to 1100 nm for 4MLBAZN, 4MLBACH, 4MLBABH, 4MLBTBZ and 4MLBDCB crystals. For 4MLBANO_3 and 4MLBACD it is observed from 231 to 1100 nm and 219 to 1100 nm respectively. The intra and intermolecular

interactions were authenticated by the shifts observed in the stretching and bending vibrations of functional groups. NH, OH and CH stretching vibrations were shifted to lower frequency and their bending vibrations to higher frequency when compared with pure 4MLBA vibrations. The protonation of amine group to NH_3^+ was confirmed through the observed NH_3^+ vibration. Also, the respective metal halide vibration predicted through Raman spectral analysis ensures the association of inorganic anion in the molecular structure of grown crystals.

The molecular structural framework of the grown crystals was established through ^{13}C and ^1H NMR spectral analysis. In ^1H NMR, the signal for protonated NH_3^+ group of grown crystals were shifted towards downfield when compared with the value of pure 4MLBA. Intermolecular C-H---X and N-H---X interactions were ascertained by observed signals. In ^{13}C NMR the intramolecular interactions was ensured by shift observed for aromatic carbons. Signal observed for carbon present in CH_2 group of 4MLBA cation is shifted towards upfield. These observations clearly establishes the protonation and the presence of inter and intramolecular interactions in the molecular structure of grown crystals. These hydrogen bonded intermolecular interactions changes the electronic distribution and promotes the charge transfer which results in enhanced NLO efficiency. According to this the noncentrosymmetric crystals 4MLBAZN and 4MLTBZ reports SHG efficiency as 1.14 and 1.41 times of KDP. Also, all the grown crystals gives enhanced third order nonlinear susceptibility values and it is determined through Z-scan technique. Third order nonlinear refractive index and absorption coefficient are also found and reported for all the seven crystals. The results reveals that they can be used for laser mode locking, optical bistability applied in optical memory, optical transistor, Q-switches in pulsed laser system and also useful for cleaning up pulse shapes. Based on the observed results, these crystals can be used in optoelectronic and photonic applications.

The thesis consists of nine chapters. Chapter 1 illustrates the brief introduction of crystal growth, theoretical concept of nonlinear optics and scope of the thesis. Chapter II, III, IV, V, VI, VII and VIII discusses the synthesis method and structural interpretation of the grown crystals. Chapter IX presents the summary of the present work and suggestions for the future work.

****

BT-05

Synthesis, Structural Elucidation and Pharmaceutical Activities of Heterocyclic Based Salts and Co-Crystals

Dr. R. Mekala

The recent progress in pharmaceutical materials science has advanced our understanding of the relationships between the molecular, crystal structure and the functional properties of the active pharmaceutical ingredients (API). This improved knowledge has brought about the possibility of producing pharmaceutical materials by design. The main aim of the multicomponent crystallisation has become an important research area in the recent years for the great potential of fine-tuning the physicochemical and pharmacological properties of the active pharmaceutical ingredient (API) as well as the ability of the separation. The multi component crystals such as polymorphs, co-crystals, salt, hydrates and solvates offer opportunities for varied physico-chemical properties.

The thesis consists of six chapters which contributes to the field of pharmaceutical science by advancing our understanding of crystallisation processes and formulation development, thus enabling pharmaceutical co-crystal and salt into drug products. The crystals of this thesis were grown by the following combinations at very first time, benzimidazole and benzotriazole with *m*-nitrophthalic acid (BZD^{+}·*m*NPA and BTA^{+}·*m*NPA^{-}·H_2O, CCDC ID 1429137 and 1518121), *o*-picolinic acid with *p*-nitro aniline zwitterionic co-crystal (PANAC ,CCDC ID 1452472) , 2-amino 4,6 dimethyl pyrimidine with gallic acid and pimelic acid (ADP^{+}·GA^{-} and ADP·PA ,CCDC ID 1541058 and 1541059), 8-hydroxy-2-methylquinoline with 5-chloro salicylic acid (HMQ^{2+}·CS^{2-} ,CCDC ID1585421) and these new crystals were deposited in Cambridge crystallographic data centre (https://summary.ccdc.cam.ac.uk/structure-summary-form).

The addition of 'N' in the benzotriazole moiety showed potent anti-cancer activity against Hela cell line, compared to benzimidazole. Compared to all crystals, the PANAC zwitterionic co-crystal showed both anti-microbial and anti-fungal activity. Even though ADP^{+}·GA^{-} and ADP·PA crystals did not show anti-microbial activity, they exhibit anti-cancer activity. The strong interaction between the aromatic acid (GA) with ADP showed an effective anti-cancer activity compared to ADP·PA. Anti-cancer activity of ADP^{+}·GA^{-} crystal exhibited the lowest IC_{50} value (8.781µM) compared to all the other crystals, which illustrated that the crystal can be tuned for the anti-cancer drug delivery process.

An interesting anti-microbial activity was identified for the HMQ^{2+}·CS^{2-} sample. The four crystals namely BZD^{+}·*m*NPA, BTA^{+}·*m*NPA^{-}·H_2O, ADP^{+}·GA^{-} and ADP·PA showed violet emission. The red emission was observed for the PANAC crystal and HMQ^{2+}·CS^{2-} exposed green emission, which clearly indicates that the different chemical environment showed different emission property. The future work will be focused on the formation of drug discovery process. The drug product of co-crystal and salt is a long time process to deliver in the market.

****

BT-06

Crystal Growth of Some Correlated Metal Oxides Using the Optical Floating-Zone Technique

Rabindranath Bag* (Thesis Supervisor: Surjeet Singh) Institute of Science Education and Research Pune, India

***Email:** *rabindra.bag89@gmail.com*

The discovery of strongly correlated materials showing interesting and potentially useful properties is important for scientific progress. To understand the properties of such complex materials, their availability as high-quality single crystals is essential. In this regard, the floating-zone (FZ) method associated with an optical image furnace (Figure 1) is a highly successful tool for growing high-quality crystals of correlated oxides.

My doctoral research focusses on crystal growth and properties of low-dimensional quantum magnets showing interesting properties arising due to the interplay of strong electronic correlations and low- dimensionality or frustrated interactions. The systems that I have grown as single crystals, and investigated during my PhD includes: (i) The noncongruently melting, composite chain-ladder compound $Sr_{14}Cu_{24}O_{41}$ with doped impurities, (ii) rare-earth

orthoferrites $RFeO_3$, (iii) manganites $RMnO_3$, and titanates Co_2TiO_4, $CoTiO_3$ and $NiTiO_3$. Using the FZ technique very high-quality, cm-size crystals were obtained. In Figure 1, a $HoFeO_3$ (HFO) crystal boule grown during my thesis is shown as a representative example. Optical microscopy under polarized light and scanning electron microscopy on highly polished sections cut at various distances along the length of the boule were carried out to infer the crystal quality. The Laue technique was used to orient the grown crystal for various physical properties measurements. As a representative case, highly anisotropic magnetization (M) of a single crystalline specimen of HFO is shown along the principal crystallographic axes.

In this talk, I will present various crucial steps involved in the successful implementation of the FZ technique. In particular, I will show how the FZ technique can be modified as a travelling solvent floating-zone (TSFZ) to grow high-quality crystals of non-congruently melting compounds, which is so far the most appropriate growth technique to obtain these compounds as large and high quality of single crystals.

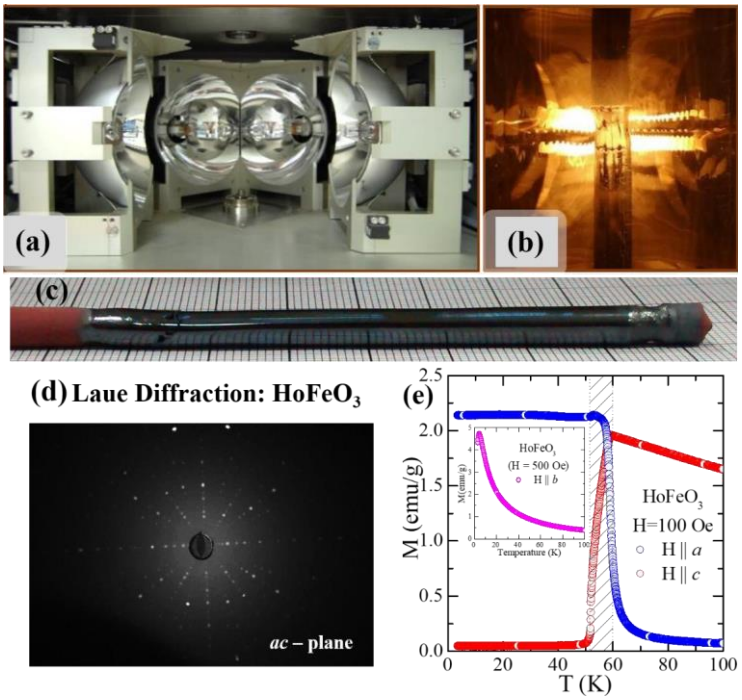


Figure1: (a) Four mirror optical furnace; (c) Photograph during the growth process showing feed, molten zone and grown crystal; (c) as-grown HoFeO3 crystal, (d) a Laue image showing that the crystal is of high-quality and it is oriented parallel to the *ac*-plan, (e) Anisotropic magnetization of HFO along *a*, *b* and *c* axes.

****

BT-07

Growth, Spectral, Thermal and Other Properties of Some Single Crystals for Optical Applications

D. Shanthi

Aditanar College, Tiruchendur,
***Email:** shanthid20@yahoo.com*

The study of light is called as the optics and the materials in connection with optics are classified into linear optical and nonlinear optical (NLO) materials. For nonlinear optical phenomena like second harmonic generation (SHG), third harmonic generation (THG), higher harmonic generations, sum and difference frequency generation, stimulated light scattering, optical parametric amplification, optical rectification etc, high intense laser light is necessary. In this investigation, some novel NLO crystals like L-alanine alaninium picrate (LAAP), beta-alanine, beta-alaninium picrate (BAP), beta-alaninium perchlorate (BAPC) and beta-alaninium maleate (BAM) were grown by aqueous solution method. The grown crystals were subjected to various studies like structural studies, UV-visible spectral studies, microhardness studies, dielectric studies, impedance studies, thermal studies, photoluminescence studies, photoconductivity studies, SHG studies, Z-scan studies. Since the grown and studied crystals in this work have better NLO properties, they could be useful in many applications such as optical communication, laser technology, optical computing, optical power limiting, image manipulation, optical data processing and storage, photonics. The Ph.D. thesis is divided into nine chapters. The first chapter deals with general introduction, crystal growth techniques, literature survey and objectives of the work. The second chapter covers the basics of nonlinear optical phenomena and the NLO materials. The principle and working of the experimental techniques and instruments that are adopted for characterization of the grown crystals are given in the chapter-3. The fourth chapter deals with the nucleation kinetics, growth and characterization of L-alaninium alaninium crystals. The fifth chapter covers the growth, results and discussion of beta alanine crystals. The sixth chapter gives the explanation of crystal growth and studies of beta-alaninium picrate crystals. The seventh chapter gives the explanation of crystal growth and studies of beta-alaninium perchlorate crystals and the eighth chapter covers the characterization of beta-alaninium maleate crystals. The summary and conclusions of the research work are given in the chapter-9. Finally, references, biodata, list of publications and list of seminars/conferences attended are provided at the end of the thesis. The important features of the work are briefly given here. Out of five crystals, some of the crystals were grown for the first time. Many characterization techniques have been adopted to study the grown crystals. The grown crystals could be used for second order and third order NLO applications.

****

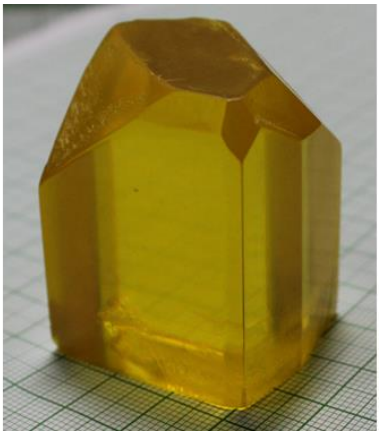
BT-08

Crystal Growth and Characterization of 4-Nitrophenol Derivative Single Crystals for Nonlinear Optical Applications

Scholar: P. Karuppasamy,*[1] Supervisor: Muthu Senthil Pandian[1], P. Ramasamy[1]

[1]SSN Research Centre, SSN College of Engineering, Chennai-603110, Tamil Nadu,
**Email:* karuppasamyp75@gmail.com *;* karuppasamyp@ssn.edu.in*; Tel: +91-9791552297*

Single crystals are the basic pillars of modern science and technology. Crystal growth is an interdisciplinary subject covering many areas such as physics, chemistry, materials science, chemical engineering, metallurgy, crystallography, mineralogy, etc. Large size single crystals with good physico-chemical properties are the prerequisite for the above mentioned applications. Since recent years the organic material of 4-nitrophenol (4NP) has attracted due to its interesting physical and chemical properties. In this view, the present thesis deals with synthesis, growth and physico-chemical investigations on 4-nitrophenol derivative single crystals such as triphenylphosphine oxide 4-nitrophenol (TP4N), 2-amino-4,6-dimethylpyrimidine 4-nitrophenol (AMP4N), 4-nitrophenol 4-aminobenzoic acid monohydrate (4NPABA) and 2-aminopyridinium 4-nitrophenolate 4-nitrophenol (2AP4N) for NLO applications. Initially, the slow evaporation solution technique was used to grow the nonlinear optical single crystals. The structure of grown crystals were confirmed by Single crystal X-ray Diffraction (SXRD) and the crystalline purity and planes were analyzed by Powder X-ray Diffraction (PXRD). Functional groups were confirmed by Fourier Transform Infrared (FTIR) spectral analysis. The optical quality of the grown crystals were confirmed by the UV-Vis NIR spectral analysis. The thermal behaviour was investigated by Thermogravimetric and Differential Thermal Analysis (TG-DTA). Vickers microhardness analysis was carried out to identify the mechanical stability of the grown crystal. Chemical etching study was carried out to find the dislocation density. The dielectric permittivity (ε) and dielectric loss (tan δ) as a function of frequency were measured. Laser Damage Threshold (LDT) value was measured by using Nd:YAG laser (1064 nm). The Z-scan technique was carried out to analyzed the nonlinear optical parameters such as refractive index (n_2), absorption coefficient (β) and the third order nonlinear optical susceptibility ($\chi^{(3)}$). Among those crystals and their properties, the 2AP4N single crystal has good in optical and physical properties. Hence, the 2AP4N single crystal was subjcted to the bulk growth. The optically high 2AP4N single crystals have been grown by (i) Sankaranarayanan–Ramasamy (SR) method and (ii) Rotational Sankaranarayanan–Ramasamy (RSR) method and (iii) Point seed rotation method. The effect of rotation on unidirectional crystal growth method (RSR) have been reported for the first time. The apparatus was specially designed and developed for the growth of high quality crystals by slow cooling under several rotational conditions. The high-quality crystals have been achieved under forced convection and the quality of the crystal is high compared to the crystals grown under free convection conditions. Refractive index measurement was carried out with different wavelength using prism coupling method. The phase matching angle of 2AP4N was find out by fitting Sellmeier equation. Based on the phase matching angle, the grown 2AP4N crystal was cut and the type-I and type-II SHG elements were fabricated.



Acknowledgement:

The authors gratefully acknowledge DAE-BRNS, Government of India for the financial support (Ref. no. 34/14/06/2016-BRNS/34032).

****

BT-09

SYNTHESIS, GROWTH AND PHYSICO-CHEMICAL INVESTIGATIONS ON PYRIDINE BASED SINGLE CRYSTALS FOR NONLINEAR OPTICAL (NLO) APPLICATIONS

V. Sivasubramani, Muthu Senthil Pandian*, P. Ramasamy

[1]SSN Research Centre, SSN College of Engineering, Chennai-603110, Tamilnadu
Email: senthilpandianm@ssn.edu.in, sivasubramaniv1989@gmail.com,
***Tel**: +91 9791802135*

Modern science and technology realize the inevitable role of crystals for the development of new-generation devices. In recent days, considerable attempts are being made to design and growth of efficient nonlinear optical (NLO) single crystals for the wide range of photonic and optoelectronic applications. Among the organic/inorganic compounds, pyridine based single crystals have attracted attention for crystal growth researchers due to their ability to form ionic co-crystals through the hydrogen bonding with many numbers of counterparts. Among the pyridine based materials, the 2-amino-5-nitropyridine is one of the attractive materials for NLO applications due to their Donor-π-Acceptor (D-π-A) charge transfer structure. It consists of electron donor (amino) and electron acceptor (nitro) groups to induce a high NLO response. Moreover, the pyridine ring acts as a cationic bonding site, then the pyridinium nitrogen acts as a proton acceptor and the amino group acts as a proton acceptor. Owing to the interesting molecular structure, the 2A5NP based single crystals are well recognized as NLO building blocks for organic and semi-organic molecular complexes. The present thesis deals with synthesis, growth and physico-chemical investigations of pyridine based single crystals such as 2-amino-5-nitropyridinium nitrate (2A5NPN), 2-amino-5-nitropyridinium bromide (2A5NPBr), 2-amino-5-nitropyridinium dihydrogen phosphate (2A5NPDP), 2-amino-5-nitropyridinium p-phenolsulfonate (2A5NPP) and pyridinium 2-carboxylate: 4-nitrophenol (P2C4N) for NLO applications. The merits of low-temperature solution growth techniques such as slow evaporation solution technique (SEST), slow cooling and unidirectional Sankaranarayanan-Ramasamy (SR) method have been discussed. The promising NLO pyridine based single crystals have been grown by SEST and unidirectional

methods. The crystalline structure and morphology of the grown crystals were ascertained by single crystal X-ray diffraction (SXRD) analysis. The crystalline quality of the grown crystals has been evaluated by high-resolution X-ray diffraction (HRXRD) analysis. The Fourier Transform Infrared (FTIR) spectroscopy analysis reveals the existence of various vibrational modes of functional groups in the grown crystals. The optical quality was evaluated by UV-Vis NIR spectroscopic analysis and it is observed that the grown crystals possess good optical transparency in the range of 400-1100 nm. The thermal stability of the grown crystals was ascertained using Thermogravimetric (TG) and Differential Thermal Analysis (DTA). The chemical etching study was employed to reveal the quality of the grown crystals. The electrical properties have been studied by dielectric and photoconductivity analyses. The mechanical strength of grown crystals was analyzed by Vickers microhardness tester. The Laser Damage Threshold (LDT) analysis shows that the grown crystals have large LDT value and this experiment was carried out using Nd:YAG laser operating at 1064 nm. Second Harmonic Generation (SHG) and Third Harmonic Generation (THG) have been measured by Kurtz-Perry and Z-scan techniques, respectively. The overall results show that the pyridine based single crystals possess attractive characteristics such as high crystalline perfection, good optical transmittance in the visible and NIR region, good thermal stability and larger nonlinear optical response, which leads to the positive sign for the crystals to be used for optoelectronic and photonic applications.

****

Oral Presentation

OP-01

Nonlinear optical and antibacterial activities of $Zn/Cu/Al_2O_4$ nanoparticles prepared by microwave-assisted combustion method

A. Lakshmanan[a], P. Surendran[a], S. SakthyPriya[a], K. Balakrishnan[a], Tejaswi Ashok Hegde[b], G. Vinitha[b], G. Ramalingam[c], P. Rameshkumar[a],*

[a]PG and Research Department of Physics, Periyar E.V.R. College (Autonomous), Tiruchirappalli-620 023.
[b]Division of Physics, School of Advanced Sciences, VIT Chennai, Chennai-600 127. [c]Department of Nanoscience and Technology, Alagappa University, Karaikudi-630 003.
***Email:** rameshkumarevr@gmail.com*

Nonlinear optical nanoparticles of $Zn/Cu/Al_2O_4$ were synthesized by microwave assisted combustion method with different fuel to oxidizer ratio. And, these nanoparticles were characterized by various analytical techniques to examine their suitability in fascinating applications. XRD results enunciate that the nanoparticle crystallizes in *cubic spinel* structure. The morphology and quantitative chemical compositions of Zn, Cu, Al and O elements were obtained from SEM with EDAX analysis. The prepared compound was confirmed by FTIR spectrum. The optical energy bandgaps are studied from UV-Vis absorption spectra. The luminescence emission peaks are observed at 371 nm (Violet), 425 nm (violet), 471 nm (blue) and 637 nm (red). In the application point of view from the Z-scan technique, the third order nonlinear optical parameters such as nonlinear refractive index (n_2), nonlinear absorption coefficient (β), and third-order nonlinear susceptibility (χ^3) of title compound are calculated. For biological application, the antibacterial activities were tested against *Bacillus cereus, Staphylococcus aureus, Shigella flexneri, and Vibrio cholera* bacterial species by measuring the inhibition zone.

Keywords: $Zn/Cu/Al_2O_4$ nanoparticles; Combustion method; Optical properties; Luminescence; Z-scan; Antibacterial activity

****

OP-02

Fluorescent carbon quantum dots from orange waste peels for nonlinear optical applications

P. Surendran[1], A. Lakshmanan[1], S. Sakthy priya[1], K. Balakrishnan[1], G. Vinitha[2], G. Ramalingam[3], P. Rameshkumar[1]*

[1]PG and Research Department of Physics, Periyar E.V.R College (Autonomous), Tiruchirappalli-620 023.
[2]Division of Physics, School of Advanced Science, VIT Chennai, Chennai-600 127.
[3]Department of Nanoscience and Technology, Alagappa University, Karaikudi-630 003.
***Email*:** rameshkumarevr@gmail.com

Using natural waste peels, the simple and eco-friendly hydrothermal method was used to prepare carbon quantum dots (CQDs). The synthesized CQDs are well dispersed and it was found that the average diameter is 2.9 ± 0.5 nm. Fluorescence spectrum exhibited blue emission peak at

432 nm. The fluorescence quantum yield of the CQDs was found to be around 11.37 % at an excitation wavelength of 330 nm. The third-order NLO properties were examined by Z-scan technique which was operated at a wavelength of 532 nm. The encouraging results of the Z-scan analysis suggest that the CQDs are a promising material for photonic devices applications. Fig 1 shows the schematic diagram of the synthesized CQDs.

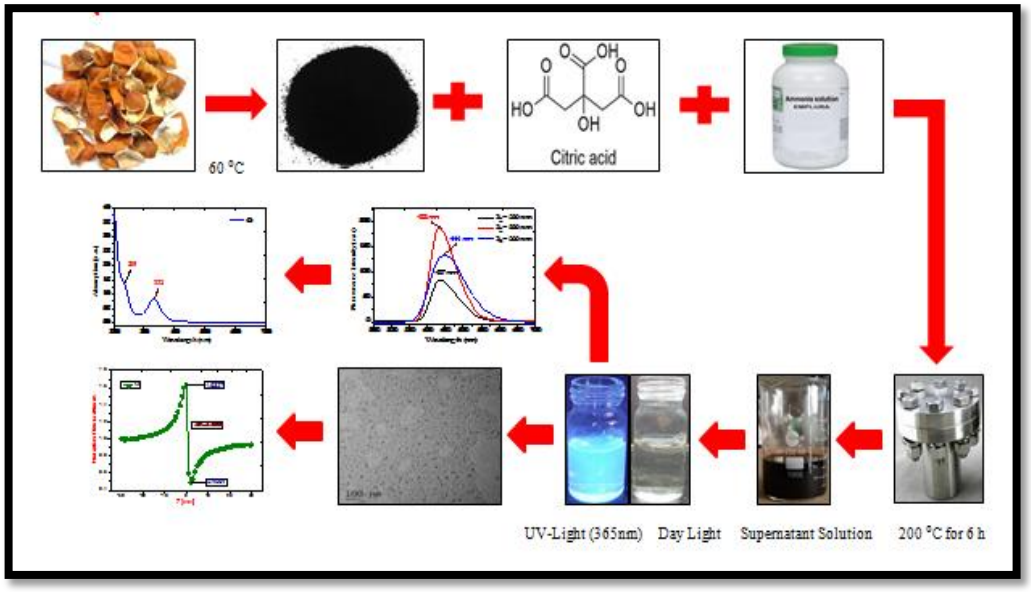


Figure 1: Schematic diagram of the synthesized CQDs

Keywords: Hydrothermal method, CQDs, HR-TEM, fluorescence, Z-scan analysis

****

OP-03

Studies on growth and characterization of nonlinear optical L-tartaric acid–nicotinamide single crystal

P. Rameshkumar*, P. Surendran, S. Sakthy Priya, A. Lakshmanan, S.Pushpalatha

PG and Research Department of Physics, Periyar E.V.R College (Autonomous), Tiruchirappalli-23, Tamilnadu, India.

***Email:** *rameshkumarevr@gmail.com*

Nonlinear optical (NLO) single crystal of L-tartaric acid–nicotinamide (LTN) has been grown by slow evaporation solution technique as shown in Fig 1. The grown crystals were subjected to various characterization techniques in order to examine their suitability for various applications. Powder X-ray diffraction (PXRD) analysis revealed that the compound is formed without any impurities. Functional groups and formation of the title compound were confirmed using FTIR analysis. Optical behavior of the material was examined using UV–Vis NIR spectrum and optical band gap energy were calculated. Microhardness, dielectric and piezoelectric studies have been carried out at ambient conditions. Electronic properties such as valence electron plasma energy, Penn gap, Fermi energy and electronic polarizability were calculated by Clausius–Mossotti relation. Photoluminescence analysis was carried out to study the luminescence nature of

the crystal and its defect states. In addition photoconductivity, and powder Kurtz and Perry second harmonic generation (SHG) test were carried out.

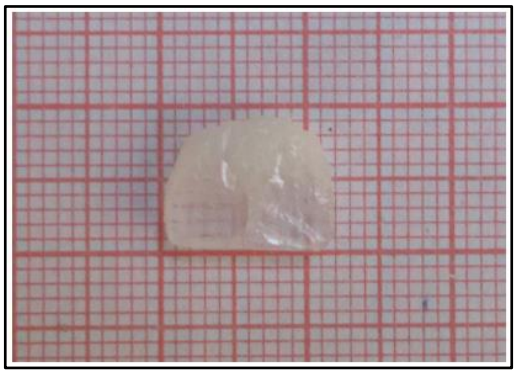


Figure 1: As grown LTN single crystal

****

OP-04

Modification of Optical Properties of Ammonium Dihydrogen Phosphate Crystal by Employing Shock Waves

A.Sivakumar and S.A. Martin Britto Dhas Sathiyadhas*

Department of Physics, Abdul Kalam Research Center, Sacred Heart College, Tirupattur, Tamilnadu, India- 635 601
***Email**: martinbritto@shctpt.edu*

We describe the investigation into tailoring the optical properties of ammonium dihydrogen phosphate (ADP) crystal by the influence of mild shock waves (Mach number 1.7) produced by a shock tube. An ADP crystal was grown by employing the Sankaranarayana–Ramasamy method with (101) orientation. The test crystal was subjected to different numbers of shock pulses such as 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, and 13, respectively. Pre- and post-shock wave-loaded test crystals were experimented with a ultraviolet-visible spectrometer for recording the optical transmission. From the observed results, it is known that, on increasing shock pulses, optical transmission is enhanced from 55% to 66% in such a way that optimization is attained. Thereafter, it reduces to 47% by further increasing the number of applied shock waves. Following the optical transmission, optical constants such as extinction coefficient, optical density, skin depth, real and imaginary parts of the dielectric constant, optical conductivity, and electrical conductivity are also greatly altered if the ADP crystal is exposed to shock pulses. From this experiment, an alternative way to boost the optical properties of an ADP crystal without modifying the original crystal system and without adding any dopants is proposed.

***Keywords*:** shock waves; ammonium dihydrogen phosphate crystal; optical properties; recrystallization; crystal defects.

****

OP-05

Development and Certification of Bharatiya Nirdeshak Dravaya (α-Alumina): Standard used for the calibration of Powder X-ray diffractometer

Ravinder Kumar[1, 2], N. Vijayan[2*], Naghma Khan[1,2], R. P. Pant[2]

[1]Academy of Scientific and Innovative Research, CSIR – National Physical Laboratory, New Delhi 110012, India
[2]CSIR –National Physical Laboratory, Dr K. S. Krishnan Road, New Delhi 110 012, India.
***Email:** bhoria.ias@gmail.com*

CSIR –National physical laboratory certifies a suit of Bharatiya Nirdeshak Dravya (BND®) as Certified Reference Material (CRM) to address specific aspects of the performance of Powder X-Ray Diffraction (PXRD) instruments. This article describes α-Alumina (BND®2001) powder, the standard used for the quantitative analysis of powder X-ray diffraction. A unit of BND®2001 consists of approximately 5g of α-Alumina powder bottled in the laboratory environment is certified with respect to relative intensities and lattice parameter. The powder X-ray diffraction patterns, along with Rietveld refinement analysis was used to make the certification measurements for lattice parameter. In addition to this international round robin test was also carried out used to evaluate the uncertainty to characterize the materials according to the prescribed standard operating procedure (SOP). Homogeneity testing and stability study of this BND were examined within the lab PXRD results as well as inter laboratory round robin test by other two NMIs. Additionally, the expanded uncertainties originating from the process of BND development were comprehensively evaluated. The experimental results indicate that the certified value of this BND is homogeneous and stable at laboratory environment condition for at least three years. The new CRM (BND®2001) can be applicable to calibration of instrument and assurance of accuracy and comparability of results in routine measurement.

***Keywords*:** Powder X-ray diffraction, Certified reference materials, Uncertainty

****

OP-06

Growth of Potassium Acid Phthalate (KAP) single crystal by conventional slow evaporation solution technique (SEST) and Sankaranarayanan-Ramasamy (SR) unidirectional method: A comparative Investigation

Manju Kumari[1, 2 *], N.Vijayan[2], Debabrata Nayak[1, 2] and R.P.Pant

[1,2]Academy of Scientific and Innovative Research, CSIR – National Physical Laboratory, New Delhi 110012, India
[2]CSIR – National Physical Laboratory, Dr K.S. Krishnan Road, New Delhi 110012, India
***Email:** manjukumari1794@gmail.com*

In the recent development of innovative technologies, the nonlinear optical (NLO) single crystals have fascinated the researchers and industries due to their wide applications such as second harmonic generation (SHG), color display, electro-optic switches, optical limiting etc. In the present work a semi-organic single crystal of potassium acid phthalate (KAP) was grown from

unidirectional Sankaranarayanan-Ramasamy method as well as slow evaporation solution growth technique. The concentrated solution was taken in a 'V' shaped container and directionally oriented seed was taken at the bottom of the container. Then the saturated solution was housed in a constant temperature bath (CTB). The non-destructive characterization techniques were performed to know about the structural, crystalline and optical properties of the title compound. The powder X-ray diffraction was performed to know the orientation of the seed as well as lattice dimension of the grown single crystal. The high resolution X-ray diffraction (HRXRD) study has been performed to know the crystalline perfection of the grown ingot. To know the optical properties of grown single crystal UV-Vis, photoluminescence (PL) and time resolved PL studies have been carried out. The observed results will be presented in detail.

***Keywords*:** Nonlinear optics (NLO), KAP, Unidirectional growth, Crystalline Perfection

****

OP-07

Growth of Ethyl P-hydroxybenzoate single crystal by Solution and Vertical Bridgeman technique

Debabrata Nayak[1,2], *, N. Vijayan1,[2], Manju Kumari[1,2], Nikhilesh Kumar Dilwaliya[3], R.P.Pant[1,2]

[1]Academy of Scientific and Innovative Research, CSIR – National Physical Laboratory, New Delhi – 110012, India
[2] CSIR – National Physical Laboratory, Dr. K. S. Krishnan Road, New Delhi – 110012, India
[3] National Institute of Technology Srinagar, Hazratbal, Kashmir, 190006.
Email: *debabratanayak254@gmail.com*

The numerous applications of nonlinear optical single crystals have made interest of research community to grow bulk size single crystals. People started growing these crystals obtaining various techniques from different existing chemicals by melting or making saturation solution of it. Usually the conventional slow evaporation technique is considered as the simplest way of growing single crystals. Especially for organic single crystal one can say it might be the best technique for growing bulk size single crystal as it takes less effort than the melt growth technique. But most of the organic materials are insoluble in water or solvent. Those chemicals mostly dissolved in organic solvent like methanol, ethanol, acetone, etc. These materials based single crystal can be grown using these organic compounds as solvent but the main difficulty in this process is inclusion of solvent. In this work we try to grow single crystal of ethyl p-hydroxybenzoate by slow evaporation solution growth technique using methanol, and mixed solution but we could not avoid the inclusion of solvent in the grown crystal. Therefore, we opted vertical Bridgman technique to grow this crystal. We also made some specific changes in the vertical Bridgman growth process to get better quality crystal. This work will be presented in details during conference.

****

OP-08

Growth and Second order NLO Characterization of tetrakis-thiourea nickel sulphate crystals (TTNS) by slow evaporation method

U. Rajesh Kannan[1*], G. Narayanasamy[1], P. Selvarajan[2], M. Malathi[3]

[1]Assistant Professor, Department of Physics, Kamaraj College, Tuticorin, 628003, Tamilnadu, India*
[1]Associate Professor, Department of Physics, Kamaraj College, Tuticorin, 628003, Tamilnadu, India
[2]Associate Professor, Department of Physics, Aditanar College of Arts and Science, Tiruchendur-628216, Tamilnadu, India
[3]Assistant Professor, Department of Physics, Seethalakshmi Achi College For Women, Pallathur-630 107, Tamilnadu, India. ***Email:** rajeshphymsu@gmail.com*

A semi-organic crystal namely tetrakis-thiourea nickel sulphate (TTNS) crystal was prepared. Slow evaporation technique was adopted to grow the single crystals of tetrakis-thiourea nickel sulphate after the growth period of 25 days. Bulk crystals were harvested from the supersaturated solution at room temperature. The harvested crystals have been subjected to various characterization techniques like TG/DTA, SHG, Z-scan and dielectric studies. Thiourea is one of the few simple organic compounds having high crystallographic symmetry. Thiourea is an interesting inorganic matrix modifier due to its large dipole moment and its ability to form an extensive network of hydrogen bonds. The TTNS salt was synthesized by dissolving nickel sulphate and thiourea in the ratio 4:1 in deionized water. From the results, it is observed that the grown crystal crystallizes in orthorhombic crystal system with space group of $P2_12_12_1$. The Kurtz and Perry powder SHG method is used to measure the SHG efficiency of the grown crystal. The obtained relative SHG efficiency of TTNS crystal is 1.15. The output from SHG test confirms the nonlinear nature of the crystal. The calculated value of the nonlinear refractive index (n_2) is + 6.463 x 10^{-11} m^2/W. As sample has positive refractive index, it results in focusing nature of the material.

Keywords: Single crystal; Solution method; TG/DTA; NLO; Z-scan, SHG

****

OP-09

Supersaturation dependent nucleation control of paracetamol polymorphs through swift cooling process

S. Kavipriya and K. Srinivasan*

Crystal Growth Laboratory, Department of Physics, Bharathiar University, Coimbatore - 641046.
***Email:** nivas_5@yahoo.com*

The polymorphic behaviour of the pharmaceutical solid paracetamol has been investigated under different concentrations of the solute from ethanol and cyclohexanone solutions. The

variation in the induction period of nucleation at different ranges of supersaturation was studied. In addition, different templates such as polymers, metals and non-metals were introduced into the saturated solution and nucleation of either mono or ortho or both polymorphic forms of paracetamol were induced at well distinguished supersaturation regions. Whereas pure aqueous solution without any template yielded only monoclinic form. The external morphology of the grown polymorphs was identified and their internal crystallographic structure was confirmed by powder X-ray diffraction and single crystal X-ray diffraction analyses. Differential scanning calorimetry analysis revealed that the grown metastable ortho polymorph undergoes solution mediated polymorphic phase transformation at 114 °C, whereas the mono form does not show any phase transformation throughout the experimental temperature range of 40 °C - 190 °C. Results will be presented.

****

OP-10

Nucleation, growth morphology and characterization of Methyl-p-Hydroxybenzoate (p-MHB) single crystals in selected solvents

V.Manikandan, M. Kowsalya and K.Srinivasan*

Crystal Growth Lab, Department of Physics, Bharathiar University, Coimbatore -641046.
***Email:** nivas_5@yahoo.com*

Methyl-p-Hydroxybenozate ($C_8H_8O_3$), also known as p-MHB, identified as a potential material for nonlinear optical applications specifically for second harmonic generation or frequency doubling of a fundamental infrared frequency into visible one, has been grown as a single crytal from solution with two different solvents such as ethanol and ethyl acetate by slow evaporation at ambient conditions. Nucleation events of the crystals was monitored through in-situ studies under mircroscope and reocorded through digital imaging. Growth morphology of the nucleated single crystals was examined and different crystal faces were indexed accordingly. Differnece in morphology of the grown crystals from solutions with ethanol and ethyl acetate as solvents were studied and the dependence of growth along different growth directions with resepct to the solvents used was analysed. Grown single crystals were subjected to various instrumental technques such as PXRD, FTIR and UV-Vis Near IR studies and from which the lattice parameters of the unit cell, presence of different functional groups and the percentage of optical transmittance in the uv-visible-near infrared region were determined. Finally, the second harmonic generation efficiency of one such grown p-MHB crystal was studied in comparision with that of the inorganic standard KDP by Kurtz powder method. Resuslts will be presented.

****

OP-11

Control of oiling-out phenomena and nucleation of stable polymorph of vanillin through vapor diffusion crystallization process at selected solvent environments

S. Supriya, S. Sushmitha and K. Srinivasan*

Crystal Growth Laboratory, Department of Physics, Bharathiar University, Coimbatore -641046.
Email: *nivas_5@yahoo.com*

An effective way of controlling the occurrence of oiling-out and nucleation of vanillin from aqueous solution was achieved through vapor diffusion crystallization process in selected solvent environments. Dimethyl sulfoxide and sulfuric acid solvent environments generate a sufficient level of supersaturation due to their significant hygroscopic and water absorbing capabilities and induce crystal nucleation within shorter periods well before the occurrence of oiling-out, whereas in the case without any solvent environment, nucleation occurs only at longer periods. Also, in the case of ethyl acetate as the solvent environment, due to its non-hygroscopic nature and high vapor pressure when compared to water molecules, no crystal nucleation was attained even after a month period owing to the dominance of oiling-out in the solution. A powder x-ray diffraction study reveals that the nucleated plate-like crystals belong to monoclinic Form-I polymorph of vanillin, and differential scanning calorimetry and Fourier transform infrared spectroscopic analyses reveal that the diffusion processes have no effect on the thermal stability and chemical purity of the grown vanillin single crystals. This method proves to be an effective means of controlling the occurrence of unwanted oiling-out phenomena prior to the crystal nucleation and to promote the crystallization of a stable polymorph of vanillin from aqueous solution. Results will be presented.

****

OP-12

Crystallization of DL-Methionine polymorphs in the presence of structurally compatible additives

M. Suresh and K. Srinivasan*

Crystal Growth Laboratory, Department of Physics, Bharathiar University, Coimbatore -641046.
Email: *nivas_5@yahoo.com*

The alpha and beta polymorphs of DL-Methionine, one of the significant amino acids used in pharmaceutical industry, were crystallized from aqueous solution in the presence of the structurally similar additive DL-Leucine. The variation in the solubility of DL-Methionine in the presence of different concentrations of DL-Leucine was determined gravimetrically. Pure aqueous solution yields only the stable beta form of DL-Methionine which crystallizes in monoclinic system with space group C2/c whereas the presence of DL-Leucine as an additive induces the nucleation of metastable alpha form which belongs to monoclinic system with space group $P2_1/c$. At lower range of concentrations of DL-Leucine, solution yields both alpha and beta forms. When

the concentration of DL-Leucine was increased in the solution, the nucleation of beta form getting reduced and that of alpha form found increased. After a critical level of the additive concentration, the solution yields only the alpha form of DL-Methionine. The variation in the induction period of nucleation of alpha and beta forms with the additive concentration was estimated. The morphology of the nucleated polymorphs were analysed and investigated under in-situ microscopic study. The form of crystallization of the nucleated polymorphs was confirmed by powder x-ray diffraction (PXRD) and single crystal x-ray structural analysis. Results will be presented.

****

OP-13

Growth of non-linear optical γ glycine single crystals from aqueous solution in the presence of potassium carbonate and their characterization

T. Anitha and K.Srinivasan*

Crystal Growth Laboratory, Department of Physics, Bharathiar University, Coimbatore -641046.
Email: *nivas_5@yahoo.com*

Organic non-linear optical γ glycine single crystals were grown from aqueous solution in the presence of potassium carbonate by slow evaporation method. The variation in the solubility of glycine with various concentrations of potassium carbonate was determined gravimetrically. Nucleation and growth morphology of the γ glycine single crystals were viewed under microscope through in-situ observation by fast evaporation method. The grown γ glycine single crystals were characterized by powder x-ray diffraction (PXRD), differential scanning calorimetry (DSC) and second harmonic generation (SHG) analyses. PXRD analysis reveals that the grown γ glycine single crystals belong to hexagonal crystal system with space group $P3_1$. Thermal characteristics of the grown crystals were analyzed through DSC. Second harmonic generation efficiency of the grown γ glycine crystals was studied by Kurtz method. Results will be presented.

****

OP-14

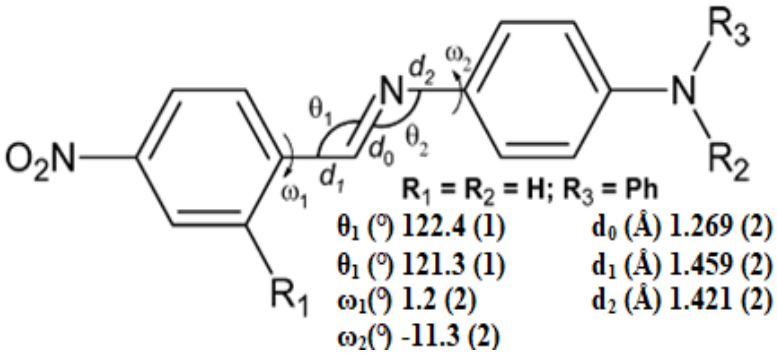
Crystal structure and thermal kinetic approach on benzylideneaniline derivative:p-nitrobenzylidene-p-phenylamineaniline

N. Sivakumar[1]* G. Anbalagan[2] and R. Jayavel[1]

[1]Crystal Growth Centre, Anna University, Chennai 600 025.
[2]Department of Nuclear Physics, University of Madras, Guindy Campus, Chennai - 600 025.
Email: *nsivakumar1986@gmail.com*

Organic crystal of p-nitrobenzylidene-p-phenylamineaniline (PNBPDA) was synthesized by mechano-chemical method at ambient temperature. Single crystal X-ray diffraction analysis confirms that PNBPDA crystallizes in monoclinic system with space group Cc. The obtained lattice parameters are a = 10.64 Å, b =17.10 Å, c = 8.98 Å, a = 90°, $ß$ = 98.02°, γ = 90° and V = 1619 (Å^3). Fourier Transform Infrared spectroscopy study reveals the presence of various

functional groups in the material. Thermo gravimetric analysis at two different heating rates (5, 10 and 15°C min^{-1}) to study the thermal decomposition behavior of the crystal. Non-isothermal studies on PNBPDA reveal that the decomposition occurs in three stages. Kinetic parameters (effective activation energy (Ea), pre-exponential factor (ln A)) of each stage were calculated by model free method: Kissinger, Kim-Park and Flynn-Wall method and the results are discussed. A significant variation in effective activation energy (Ea) with conversion progress (α) indicates that the process is kinetically complex. The result indicates that the surface crystallization dominates overall crystallization process.



****

OP-15

Solvatochromic effects on the properties of Sodium Acid phthalate crystals

C. Ramalakshmi @ sathya[1], K. Sangeetha[1,*]

[1]School of Electrical and Electronics Engineering, SASTRA Deemed to be University, Thanjavur 613 401, Tamil Nadu, India
Email: *sangeetha.bdu.physics@gmail.com*

Solvatochromism is fascinating subject of research in solution chemistry because the environment has an essential role on the solute behaviour and therefore on the thermodynamics and kinetics of reaction in solution. Also, solvents are reported [1-3] to have control over the absorption and emission wavelengths of the solute molecules by shifting their energy levels. In this direction, Sodium acid phthalate (NaAP), a polar molecule, was chosen to investigate the optical behaviours of the molecule in different solvent environment. The type and extent of wavelength and energy level shifts in NaAP molecule were identified for two different solvents and were interpreted based on the interactions between the solvent and the solute. The experimental results obtained will be supported by the computational results and the same will be discussed briefly in the seminar.

References:

1. M. Saravanana,b,∗, A. Senthila, S. Abraham Rajasekarb,c, N. Vijayan," *Effects of semi-organic additives on the solubility, growth, optical,thermal, mechanical, dielectric and NLO behaviors of ADP crystalsfor optoelectronic applications"*, Optik 127 (2016) 1463–1470

2. Mihaela Homocianu*, Anton Airinei, *"Solvent effects on non-linear optical properties and intramolecular charge transfer (ICT) characteristics of disperse red 19 dye"* Optik - International Journal for Light and Electron Optics 202 (2020) 163606
3. Umesh Warde, Nagaiyan Sekar*,"*NLOphoric mono-azo dyes with negative solvatochromism and in-built ESIPT unit from ethyl 1,3-dihydroxy-2-naphthoate: Estimation of excited state dipole moment and pH study"* Dyes and Pigments 137 (2017) 384-394.

****

OP-16

Bulk Crystal Growth, Optical, Raman, Thermal and Third Order NLO Properties of 2-[4-(Diethylamino)benzylidene] malononitrile (DEBM) Single Crystals

S. Anand[a], S. Kalainathan[a*], Elisabetta Landini[b], R. R. Sumathi[b]

[a] Centre for Crystal Growth, VIT University, Vellore –632 014, India.*
[b] Materials Science and Crystallography institute, Ludwig-Maximilians-University, D-80333 Munich, Germany
Email: *kalainathan@yahoo.com*

An organic nonlinear optical (NLO) single crystals of 2-[4-(Diethylamino)benzylidene] malononitrile (DEBM) crystal was successfully grown in ethyl acetate solution by the slow evaporation solution growth method at room temperature. The grown crystal belongs to monoclinic system with $P2_1/n$ space group. The lattice parameters and crystalline purity of the grown crystal were confirmed by single crystal XRD and powder XRD, respectively. The calculated unit cell parameters of the DEBM crystal are a = 9.358(5) Å, b = 9.371(6) Å, c = 14.671(8) Å and $\alpha = \gamma = 90°$, $\beta = 98.98(7)$. UV-Vis-NIR spectral analysis signifies that the DEBM crystal is transparent in entire visible and near infra-red region, which has a lower cut-off wavelength around 476.8 nm. The various functional groups present in the crystal were analyzed by FT-IR and FT-Raman studies. The molecular structure of DEBM crystal was confirmed through proton NMR. Thermal stability and melting point (137.8ºC) were studied with TGA-DSC analysis. The third-order optical nonlinearities of the DEBM crystal were confirmed by Z-scan technique. The Raman spectrum has been acquired using the IR laser (λ = 785 nm). The spectrum shows several interesting features namely, a doublet at ~1600 cm^{-1} attributed to the CC ring stretching modes with a conjugated substituent. The CH bending modes appear in the region between 1400 cm^{-1} and 1100 cm^{-1}. The CH out-of-plane bending mode appears at 862.6 cm^{-1} and it is typical of para-substituted benzene rings, while the in-plane ring deformation is found at 613.4 cm^{-1}. Some more additional features due to the presence of two ethyl groups have also observed. The complete peak assignments will be summarized and presented.

****

OP-17

Linear and nonlinear optical properties of mercury cadmium bromide thiocyanate (MCBT) crystal for laser applications

S.M. Ravi Kumar [a,*], S. Sivaraj[a] and G.J. Shanmuga Sundar[b]

[a]PG Department of Physics, Sri Subramaniyaswamy Government Arts College, Tiruttani 631 209, Tamil Nadu, India
[b]Department of Physics, Rajeswari Vedachalam Government Arts College, Chengalpattu - 603 002, Tamil Nadu, India ***Email:** smravi78@rediffmail.com

Single crystal of mercury cadmium bromide thiocyanate (MCBT) was grown by slow cooling technique using mixing solvent of ethanol and deionised water (1:1). The cell parameters of the MCBT crystal measured from single crystal XRD analysis which shows MCBT belongs to orthorhombic crystal system. The SHG efficiency of MCBT is 5.64 times greater than KDP crystal. The transmission spectrum gives UV cut off wavelength 328nm. Third order nonlinear optical properties were determined and its various parameters like nonlinear refractive index (n_2), nonlinear absorption coefficient (β), real part of the third-order susceptibility [R_e ($\chi^{(3)}$)], imaginary part of the third-order susceptibility [I_m ($\chi^{(3)}$)] Third-order nonlinear optical susceptibility ($\chi^{(3)}$) were also determined.

***Keywords*:** Slow cooling; X-ray diffraction; Linear and nonlinear optical properties; UV-Vis-NIR; Microhardness studies

****

OP-18

Synthesis, Structure and Electrical Characterization of $TlBiSe_2$ Crystal for Thermoelectric Application

K. Aravinth, P. Ramasamy

SSN Research Centre, SSN College of Engineering, Chennai -603 110
***Email:** aravinthk@ssn.edu.in*

Thermoelectric materials are capable of direct by converting thermal energy into electrical energy. These are potential candidates for waste heat recovery and or other specialized applications without any hazardous emissions or moving parts. The performance of a thermoelectric material is given by its figure of merit ZT, with $ZT = \sigma S^2 T/\kappa$, where σ is the electrical conductivity, S is the Seebeck coefficient, Tis the absolute temperature, and κ is the thermal conductivity consisting of electronic and lattice thermal parts. A suitable material for thermoelectric applications should have a high conductivity, large Seebeck coefficient, and low thermal conductivity. In recent past thermoelectric properties of materials are connected with different quantum states of matter like topological insulators, semimetals, Dirac materials etc, and studies proved that significant number of TE materials are topological insulators. In the last decade, it has been more fully appreciated that thallium chalcogenides tend to possess very low thermal conductivities. Practical applications of the high temperature thermoelectric materials developed so far are partially obstructed by the costly and complicated fabrication process. High quality $TlBiSe_2$ polycrystalline is successfully

synthesized by horizontal furnace for investigating fundamental properties. The structure properties were measured by combination of powder X-ray diffraction and Raman spectroscopy. The average elemental compositions of the samples were found by using scanning electron microscopy (SEM, S-5500 Hitachi) and energy dispersive X-ray spectroscopy (EDS). The electrical properties were obtained by Hall effect measurements, performed in a 0.45 T magnetic field in the van der Pauw geometry. The thermoelectric properties (S and κ) were measured by a Physical Property Measurement System.

****

OP-19

Investigations on 4-methyl benzophenone (4MB) single crystal grown by Czochralski method and its characterization

V. Mohankumar*, K. Ramachandran, M. Senthil Pandian and P. Ramasamy

SSN Research Centre, SSN College of Engineering, Chennai-603110, Tamil Nadu
***Email:** mohaphysics@gmail.com*

Bulk size 4-methyl benzophenone (4MB) single crystals have been grown by Czochralski method in a period of 8 h. The unit cell parameters of the grown crystals were confirmed by single crystal X-ray diffraction analysis. The lower UV cutoff wavelength of 4MB crystal was studied by UV–Vis NIR spectrum analysis and the cut-off wavelength was found to be 379 nm. The FTIR spectrum confirms the presence of different functional groups present in the crystal. The luminescence properties of 4MB single crystal were described by Photoluminescence spectra. Thermal stability, material decomposition and melting point of the grown crystals were determined by Thermogravimetric/differential thermal analysis measurements. The mechanical stability of the 4MB single crystal was examined using Vickers microhardness test and it was found that the crystal belongs to soft material category. Laser damage threshold measurement was carried out by using Nd:YAG laser. The nonlinear refractive index, nonlinear absorption coefficient and third order nonlinear susceptibility were measured from Z-Scan measurements. The density functional theory calculations for isolated 4MB molecule were performed with B3LYP/6-311++G(d,p) level. The electronic properties and polarizabilities of title molecule were calculated.

****

OP-20

Synthesis and structural evaluation of silicon nanowires by PECVD using Indium catalyst

Nafis Ahmed*, P. Ramasamy, P. Balaji Bhargav

SSN Research Centre, SSN College of Engineering, Kalavakkam, Tamilnadu, INDIA
***Email:** nafisa@ssn.edu.in*

In this work, we report a detailed investigation on the growth of In catalyzed SiNWs using SiH_4-H_2 gas mixture by PECVD. The In catalyst of thickness 2 nm is deposited ex-situ by evaporating 5N pure In pellets in a thermal evaporation system. The effect of growth-temperature and time-duration on the structure of grown SiNWs is studied. Morphology obtained from FESEM shows tapered growth of NWs with a distinctively sharp tip. The diameter of NWs is measured at two places (near the base and tip of NW) to evaluate the tapering effect, which decreased with an increase in temperature. An increase in temperature also increases the density of NWs and promotes axial growth. HRTEM, GIXRD spectra and Raman spectroscopy show high crystallinity of the grown NWs. GIXRD spectra show the grown NWs have crystallized along (111), (220) and (311) plane orientation, where (111) being preferred orientation as demonstrated by HRTEM. The surface chemistry analysis performed using XPS shows the presence of Si besides the native oxide as the major element with no trace of In.

***Keywords*:** Silicon nanowires, Indium, PECVD, Growth morphology

****

OP-21

Comparative study of Experimental results of various Crystals grown by Slow Evaporation method and Sankaranarayanan–Ramasamy (SR) method.

Pankaj D.Ghodke*, Dr.S.S.Hussaini, Dr.M.D.Shirsat.

Rashtriya Uchchatar Shiksha Abhiyan (RUSA), Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, Maharashtra, India.
Email: ghodkepd@gmail.com

From the recent development in the field of optics, the Non-linear optical (NLO) crystals have been given much prominence on account of their distinct applications in the field of telecom industry, frequency conversion devices and data storage on optical devices. Many nonlinear optical materials have been characterize and analyze on the basis of their structural, optical, chemical and physical properties. Here in present study we have compared 4 different crystals viz. dimethyl ammonium picrate (DMAP), potassium dihydrogen phosphate (KDP), ammonium dihydrogen phosphate (ADP), L-alanine formate (L-AF), L-arginine phosphate (L-AP) and sulphamic acid (SA) grown by two well known methods Slow evaporation method and Sankaranarayanan–Ramasamy (SR) method. Grown single crystals have been analyzed with Fourier infrared spectrometer, Ultra violet (UV) and visible spectrometer, Vickers micro hardness test, dielectric

studies, thermo gravemetric analyses (TGA) and differential thermal analysis (DTA). Functional groups present and vibration modes of the grown crystals was confirmed by FTIR studies.

***Keywords*:** NLO single crystals, slow evaporation, Sankaranarayanan–Ramasamy (SR) method, Fourier infrared spectrometer, Ultra violet (UV) and visible spectrometer, Vickers microhardness test: Dielectric studies

References:

1) Crystal Growth and Characterization of KDP and ADP Single Crystal. Dr.M.Selvapandiyan al., Asian Journal of Engineering and Applied Technology (AJEAT) Vol.2.No.1 2014 pp 71- 77

2) Babu, G. Anandha, S. Sreedhar, S. Venugopal Rao, and P. Ramasamy. "Synthesis, growth, structural, thermal, linear and nonlinear optical properties of a new organic crystal:

****

OP-22

Synthesis and characterization of a Nonlinear Optical Property of Urea Nickel Ammonium Sulfate (UNAS)

G. Sathishkumar, R. Oviya and M.Lenin

PG & Research Department of Physics, Thiru.A.Govindasamy Government Arts College, Tindivanam- 604307

***Email**: gsathishbsc@gmail.com*

The semi organic nonlinear optical single crystal of Urea Nickel Ammoniumsulfate (UNAS) was grown from aqueous solution by slow evaporation method at room temperature. The cell parameters were determined by using single crystal X –ray diffraction method. The different functional groups with different modes of vibrations were confirmed using FT-IR spectral studies. Theoptical absorption studies shows that materials have wide optical transparency in the entire visible region. UNAS crystals is transparency in UV visible optical ranges representing a phase matched on nonlinear semi organic crystalline materials, which shows the high purity of the grown crystals. The second harmonic generation efficiency was confirmed by the Kurtz powder method using Nd: YAG laser with fundamental wavelength of 1064 nm.

***Keywords*:** Urea nickel ammonium sulfate (UNAS), Second Harmonic Generation (SHG), Single crystal X- ray diffraction, NLO.

****

OP-23

Crystal structure and Computational evaluation of a novel intermediate salt of N-cyclohexyl-N-(cyclohexylcarbamoyl)-4-(trifluoromethyl)benzamide as potential Potassium channel blocker in Epileptic paroxysmal seizures

Natchimuthu V[1,*], Srinivas Bandaru[2], Anuraj Nayarisseri[2], Ravi S[3]

[1]Department of Science & Humanities (Physics), M.Kumarasamy College of Engineering (Affiliated to Anna University), Karur- 639 113, Tamilnadu, India.
[2]Bioinformatics Research Laboratory, Eminent Biosciences, Vijaynagar, Indore - 452010, Madhya Pradesh, India.
[3]PG & Research Department of Physics, National College (Affiliated to Bharathidasan University), Tiruchirapalli - 620 001, Tamil Nadu, India.
***Email:** natchimuthu88@gmail.com* ***Phone:** +91-9597955314*

The narrow therapeutic range and limited pharmacokinetics of available Antiepileptic drugs (AEDs) have raised serious concerns in the proper management of epilepsy. To overcome this, the present study attempts to identify a candidate molecule targeting voltage gated potassium channels anticipated to have superior pharmacological than existing potassium channel blockers. The compound was synthesized by reacting (S)-(+)-2,3-Dihydro-1H-pyrrolo[2,1-c][1,4] benzodiazepine 5,11(10H,11aH)-dione with 4-(Trifluoromethyl) benzoic acid ($C_8H_5F_3O_2$) in DMF and N,N'-Dicyclohexylcarbodiimide (DCC) which lead to the formation of an intermediate salt of N-cyclohexyl-N-(cyclohexylcarbamoyl)-4-(trifluoromethyl)benzamide with a perfect crystalline structure. The structure of the compound was characterized by FTIR, ^{1}H-NMR and ^{13}C-NMR analysis. The crystal structure is confirmed by single crystal X-ray diffraction analysis. The Structure-Activity Relationship (SAR) studies revealed that substituent of fluoro or trifluoromethyl moiety into the compound had a great effect on the biological activity in comparison to clinically used drugs. Employing computational approaches the compound was further tested for its affinity against potassium protein structure by molecular docking in addition, bioactivity and ADMET properties were predicted through computer aided programs.

***Keywords*:** Fluorinated N,N'-Dicyclohexylcarbodiimide; X-ray crystal structures; Molecular Docking; ADMET property prediction; paroxysmal seizures; K^+ blocker.

****

OP-24

OFZ Growth of $Y_2Ti_2O_7$ Single Crystal and its Characterization

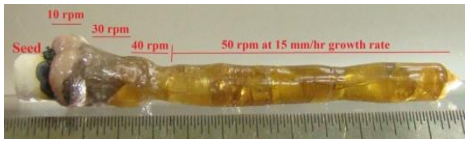
M. Suganya[1], P. Vijayakumar[2], Amirdha Sher Gill[1*], R. Ramaseshan[2] and S. Ganesamoorthy[2]

[1]School of Science and Humanities, Sathyabama Institute of Science and Technology, Chennai-600119.

[2]Materials Science Group, IGCAR, Kalpakkam-603102.

Email: *amirdhashergill@gmail.com*

Yttrium Titanate ($Y_2Ti_2O_7$) belongs to the $A_2B_2O_7$ pyrochlore family and it exhibits symmetrical cubic structure. Growing crack free and striation less single crystal is a challenging task. By optimizing the growth parameters such as rotation rate (10-60 rpm) and growth rate (10 - 15 mm/h), efforts are made to grow good quality single crystals of length 60 mm and Ø 5 mm by OFZ technique. The quality of the grown single crystal is confirmed using X-Ray diffraction and Laue diffraction pattern. The optical band gap energy 3.56 eV is calculated by Tauc plot using UV-Vis-NIR absorption spectra. The calculated hardness value reveals that the material possesses high creeping strength.



References:

[1] Hossain. M.M, Walauchi.S, Naga. M, Tanaka. I, Effects of lamp power and mirror position on the interface shape of the silicon molten zone during infrared convergent heating, Cryst Eng Comm., 2014, **16**, 4619-4623.

[2] Watauchi. S, Sarkar. M.A.R, Nagao. M, Tanaka I, Watanabe T, Shindo I, Crystal growth of rutile by tilting mirror type floating zone method, J. Cryst. Growth, 2012, **360**, 105-110.

[3] Changyou Liu, Antoni Dabkowski, Wangi Jie, Bruce D.Gaulin, Hanna. A. Dabkowska, Optical observation of striation of $Y_2Ti_2O_7$ single crystals, Crystals, 2019, **9**, 233-243.

****

OP-25

Effects of 1,2-dichloroethane on the optical, thermal, mechanical and NLO behaviors of ADP crystals

M. Saravanan

Department of Physics, SRM Institute of Science and Technology, Ramapuram Campus, Chennai, Tamilnadu,

The effects of 1,2-Dichloroethane (DCE) over a concentration range from 1 to 5 mol% on the optical absorption, hardness, thermal, microhardness behaviors and SHG efficiency of ammonium dihydrogen phosphate (ADP) single crystals grown by slow evaporation solution growth technique have been investigated. The powder X-ray diffraction and FT-IR analyses indicate that the crystals undergo considerable stress as a result of doping and these also confirm the slight distortion of the structure of the crystal in the presence of a high concentration of dopant

(5 mol%). UV–vis studies reveal that the absorption of the DCE doped crystals is less than that of pure ADP. Thermal studies (TG/DTG) disclose that the decomposition temperature of doped ADP is more than that of pure ADP. Vicker's microhardness study reveals that the addition of DCE increases the hardness of the ADP. SHG efficiency of DCE doped ADP is higher than that of pure ADP. Presence of dopant was confirmed by energy-dispersive spectrometry.

Keywords: Crystal growth, TGA, Optical materials and properties,Mechanical properties,SHG

****

OP-26

Experimental study of parametric dependency of ZnO nanorods based vibration sensor

Iyappan Gunasekaran[1], Govindaraj Rajamanickam[2], Ramasamy Perumalsamy[2], Kiruthika Ramany[3], Radha Shankararajan[3]

[1,2] SSN Research Centre, Department of Physics, SSN College of Engineering, Kalavakkam, India.
[3] ECE Department, SSN College of Engineering, Kalavakkam, India.

Zinc oxide (ZnO) nanorods were grown on rigid substrate (Fluorine doped tin oxide, FTO) with different molar concentrations (0.025 M, 0.075 M and 0.125 M) using a low temperature hydrothermal process. The XRD analysis revealed the formation of hexagonal wurtzite structured ZnO nanorods with (002) plane c-axis orientation of all the samples. Morphological analysis through FESEM analysis confirmed the formation of ZnO nanorods with hexagonal top surfaces. The electrical properties of the fabricated devices were identified using photoconductivity and Impedance studies. Less turn on voltage of 0.2 V, internal resistance of 1.12 kΩ for 0.075 M sample depicted better piezoelectric property. At 9 Hz resonant frequency a maximum voltage of 2.3 V and for 1 g acceleration input, the output voltage obtained was 2.34 V for 0.075 M sample which is better compared to the other two precursor molar concentration varied samples (0.025 M and 0.125 M). The sensitivity of this sample was found to be 30.56 V/g.

Kewwords : ZnO, Hydrothermal process, Nanorods, Vibration sensor

****

OP-27

Temperature dependent photoluminescence of 4-Methoxybenzyl ammonium chloride (4-MBACl)

E. Anu Ranjani[1], K. Sangeetha[1,*]

[1]School of Electricals & Electronics Engineering, SASTRA Deemed to be University, Thanjavur – 613 401, Tamil Nadu, India
***Email**: sangeetha.bdu.physics@gmail.com*

4-Methoxybenzylammonium chloride (4-MBACl), a semi-organic material has been synthesized and grown as single crystals by slow solvent evaporation technique. The material crystallized in centrosymmetric space group and was found to be stable up to 490 K. Temperature dependent photoluminescence of 4-Methoxybenzylammonium chloride (4-MBACl) have been investigated in order to reveal the photo physical properties of the material [1,2]. The material was observed to emit a delayed near UV light when excited at 275 nm and the emission was found to exists down to a temperature of 10 K. Intersystem crossing (ISC) between excited singlet and triplet states may be responsible for delayed PL emission. Charge-transfer (CT) excitons created in this conjugated system (4-MBACl) after the excitation processes have interacted with optical and acoustic phonons at different temperatures. These phonons have significant role in affecting the emission wavelength, emission intensity and FWHM of the emission peaks at every temperatures. The importance of phonon-exciton coupling at low temperatures in influencing the optical behaviour of the material will be briefly discussed in this seminar [3].

References:

[1] R Aarthi, C Ramachandra Raja, "Spectral and optical characterization of the new semi-organic crystal: 4-methylbenzylammonium chloride hemihydrates, to establish protanation and the effect of resultant hydrogen bonding", Bull. Mater. Sci. (2019) 42:209

[2] Daniel Ramirez, Jose´ Ignacio Uribe, Luca Francaviglia, Pablo Romero-Gomez, Anna Fontcuberta i Morral, Franklin Jaramillo, "Photophysics behind highly luminescent two-dimensional hybrid perovskite $(CH_3(CH_2)_2NH_3)_2(CH_3NH_3)_2Pb_3Br_{10}$ thin films", J. Mater. Chem. C, 2018, 6, 6216

[3] S.P. Ramteke, S. Kalainathan, Mohd Anis, G.G. Muley, M.I. Baig, H. Algarni, "Novel report on luminescence, linear and laser induced optical traits of potassium aluminium sulphate crystal for photonic device applications" Optik, 201 (2020) 163509.

****

OP-28

Enhanced nonlinear polarizabilityof Cu doped L-tartaric acid single crystals

S. Rajkumar[1] and K. Sangeetha[1,*]

[1]*School of Electrical and Electronics Engineering, SASTRA Deemed to be University,Thanjavur 613 401, Tamil Nadu, India*
***Email:** sangeetha.bdu.physics@gmail.com*

For over 3 decades, investigations on organic crystals have been the forefront for many material scientists due to their promising optical nonlinearity. Several growth aspects and physicochemical parameters have been modified during the growth of organic materials in order to analyze the changes in their nonlinear optical properties. Doping metals in organic materials [1, 2] has become a convenient way to increase the mechanical stability as well as nonlinear polarizabilities of the materials. In this viewpoint, L-tartaric acid (LTA), a well-established nonlinear optical (NLO) and ferroelectric material [3,4],has been doped with copper to investigate the property changes. Pure and doped LTA crystals were grown by solvent evaporation technique under ambient conditions and were confirmed by FT-IR and TG-DTA analyzes. Other preliminary measurements such as optical transmittance, birefringence, refractive index and microhardness were also performed and significant differences between the pure and doped crystals were observed. The SHG efficiency was tested by Kurtz-Perry powder technique and it is found that efficiency is increasing for pure than doped LTA. The reason behind the enhancement of optical nonlinearity and properties of LTA upon doping Cu will be discussed briefly in the seminar.

References:

1) P.S. Rohith, N. Jagannatha and K.V. Pradeep kumar, “Growth and characterization of pure and magnesium doped copper cadmium oxalate single crystals”, Journal of Master Today-Proc, vol. 8, p. 1, p. 85-93, 2019.
2) A.Vijayakumar, A.Ponnuvel and A.Kala, “Growth and characterization of pure and lanthanum doped L-Histidine Acetate crystals”, Journal of Master Today-Proc, vol. 8, p. 1, p. 484-491, 2019
3) S. Arulmani, A. Venkatesan, M.E. Rajasaravanan, S. Senthil, “Growth and spectroscopic studies on the L-Tartaric acid doped Ammonium Dihydrogen Phosphate Non-Linear Optical single crystals”, Journal of Master Today-Proc, vol. 8, p. 1, p. 136-141, 2019.
4) B. Deepa and V. Rajendran, “Pure and copper doped tungsten trioxide prepared via co-precipitation method and studies on their structural, morphological, electrochemical and optical properties”, Journal of P soc photo-opt ins, vol. 16, p. 185-192, 2018.

****

OP-29

Effect of Molybdenum Shield on Non-metallic Impurities in mc-silicon Grown by Directional Solidification Process

M. Avinash Kumar, M. Srinivasan*, P. Ramasamy

SSN Research Centre, SSN College of Engineering, Chennai-603110, India.
***Email:** srinisastri@gmail.com*

A transient global heat transfer simulations are done to analyse the impact of molybdenum shield on carbon impurity concentration and silicon carbide particle formation in mc-silicon grown by Directional Solidification (DS) process. The molybdenum shield is installed to control the incorporation of carbon from the graphite furnace elements and it also acts as a gas flow guidance that enhances argon gas flow near the melt free surface. Simulations are done for the whole DS growth process with furnace which has no molybdenum shield and for the furnaces having molybdenum shield fixed at three different positions. The applied molybdenum shield modification in DS furnace shows significant impact on uniformity and reduction of carbon, oxygen impurity concentration in as-grown mc-silicon ingot.

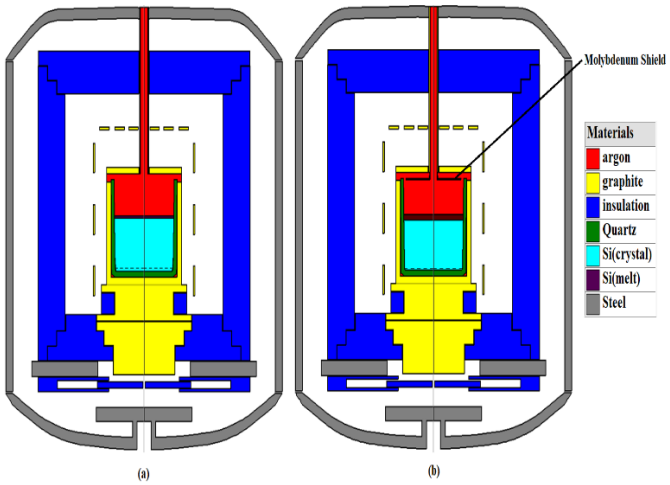


Figure: Conventional DS furnace (a) and modified DS furnace with molybdenum shield (b)

****

OP-30

Electrical impedance analysis and optical analysis of Chalcone (BMP) crystal grown by VASR method.

N. Madhavan, S.A. Martin Britto Dhas*

Department of Physics, Abraham Panampara Research Center (APRC), Sacred Heart College, Tirupattur, Tamil Nadu, 635 601 India ***Email:** brittodhas@gmail.com*

Chalcone derivative crystal 1,3-bis (4-methoxyphenyl) prop-2-en-1-one (BMP) was grown by Vacuum Assisted SR technique using acetone as a solvent. The grown crystal was subjected to

various characterization studies like power XRD analysis to determine the crystalline nature and FTIR analysis to investigate the functional group present in the material. The optical properties such as optical band gap, absorption coefficient, excitation coefficient, dielectric constant for real and imaginary part, electrical conductivity, optical conductivity and refractive index of the crystals were analyzed using UV-Vis spectrophotometer. Dielectrical analysis like dielectric constant, dielectric loss, resistivity, ac and dc conductivity, etc were carried out at different temperatures viz 30, 50 and 75 ^{o}C in the frequency ranging from 1 Hz - 10 MHz. The results will be discussed in the conference.

Keywords: Chalcone crystals, absorption coefficient, Electrical impedance analysis, optical conductivity, refractive index, etc.

****

OP-31

Rare-earth ions integrated silica nanocrystals derived from rice husk via microwave-assisted combustion method for bioimaging applications

T. Saravanan, G. Suresh Kumar

[a]Department of Physics, K.S. Rangasamy College of Arts and Science (Autonomous), Tiruchengode 637 215, Tamil Nadu, India
***Email:** gsureshkumar1986@gmail.com; **Tel:** +91 9944429261*

Silica nanoparticles have received great interest in biomedicine due to their high biocompatibility. In this study we report the preparation of rare-earth ions integrated silica nanoparticles using rice husk biomass through a rapid and simple microwave-assisted combustion techniques for making cost-effective bioimaging contrast agents. XRD, EDX and TEM studies indicate that rare earth (europium/gadolinium) ions were strongly integrated with silica matrix *via* electrostatic interaction with environmental oxygen atoms. Europium integrated silica nanoparticles exhibits a strong red fluorescence imaging capability which was attributed from $^{5}D_{0}\rightarrow{}^{7}F_{1}$ and $^{5}D_{0}\rightarrow{}^{7}F_{2}$ transitions of europium ions in the silica host matrix whereas gadolinium integrated silica nanoparticles demonstrate paramagnetism with T_1 weighted MR imaging capability ascribed to magnetic moment originated from a spin-orbit coupling of partially filled 4f electrons of gadolinium in silica host matrix. The obtained results indicate that prepared rare-earth ions integrated silica nanoparticles can have significant potential in developing new bioimaging contrast agents at low cost.

Keywords: Rare earth; Rice husk; Silica; Bioimaging; nanoparticles.

****

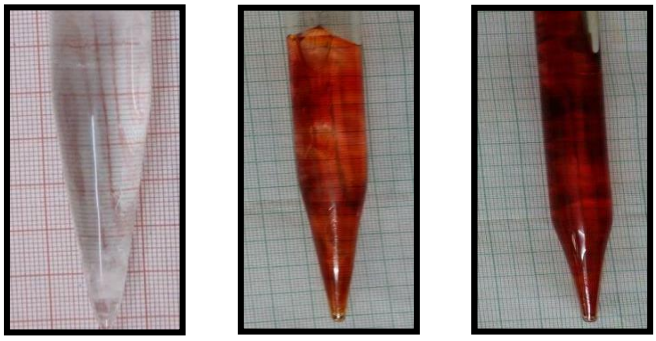
OP-32

Investigation on the impact of xylenol orange dye on the growth and properties of unidirectional grown KDP crystals for photonic applications

Saranraj[1], S. Sahaya Jude Dhas[2], M. Jose[1], S. A. Martin Britto Dhas*[1]

[1] Department of Physics, Abraham Panampara Research Centre, Sacred Heart College, Tirupattur - 635 601, India.
[2] Department of Physics, Saveetha Engineering College, Chennai – 602 105, India.
corresponding author: Telephone +91-8903101253, ***Email: brittodhas@gmail.com*

Unidirectional (101) bulk size xylenol orange dye-doped potassium dihydrogen phosphate single crystals were grown by Vacuum Assisted Sankaranarayanan-Ramasamy (VASR) method so as to improve the properties of the crystal. The objective of this study is to know the impact of organic dyes on properties of the crystal and also to understand how it could be used for relevant applications. Optical transmission decreases and thermal properties remain the same for the dye-doped crystals whereas the addition of dye improves mechanical, dielectric and photoconduction properties. On comparison, a stronger absorption is identified at 480 nm for the dye-doped crystal. Laser damage threshold confirms that 0.01 M dye-doped crystal has the value 12.40 GW/cm^2 as compared to 8.59 GW/cm^2 for pure crystal, whilst, second harmonic efficiency was determined by Kurtz method, it has been decreasing with increases dye concentration such that crystals of pure, 0.001 M and 0.01 M dye-doped have the respective values of 26.4 mV, 18.1 mV and 17.6 mV.



Photographs of as grown crystals a) Pure KDP b) 0.001M of xylenol orange dye-doped KDP c) 0.01M of xylenol orange dye-doped KDP

Keywords: Inorganic compound, Crystal growth, X-ray diffraction, Dielectric properties

****

OP-33

INVESTIGATIONS ON L-VALINE) DOPPED IMIDAZOLINIUM L-TARTRATE SINGLE CRYSTAL

P. Dhivya[1], R. Arun Kumar[2]

[1]Department of Physics, PSG College of Technology, Coimbatore, India
[2]School of Sciences (Physics), National Institute of Technology, Tadepalligudem, Andhra Pradesh, India
***Email:** rarunpsgtech@yahoo.com*

The slow cooling method was adopted for the growth of pure and L-valine doped IMLT crystals in 1, 3, 5 molar percentage. The incorporation of the dopant L-valine was confirmed using the cell parameters measured using powder X-ray analysis. The development of lattice strain in doped crystals are due to the high concentration of the dopant has been studied using Debye-Scherrer method. The FTIR spectrum reveals the assignments of characteristic bonding present in the grown crystals. The frequency dependent dielectric constant and dielectric loss of pure and L-valine doped IMLT crystals have been investigated by the dielectric measurements. Doping has improved the optical parameters and was studied using UV-Vis-NIR spectral studies. The cutoff wavelengths of pure and 1 mol% L-valine doped IMLT crystals were observed at 234 nm and 229 nm respectively. The etching study examines the growth mechanism and surface morphology of the pure and L-valine doped IMLT crystals. The CHN analysis conveys the percentage of carbon, hydrogen and nitrogen elements present in pure and L-valine doped IMLT crystals. The consequences of doping L-valine in IMLT single crystal and their dominance in various properties of the crystal grown in aqueous solution by slow evaporation technique have been explored.

****

OP-34

CVD grown graphene on commercial and electroplated Cu substrates-analysis & suitability

Balaji C, Ganesh Kumar, P. Balaji Bhargav, Arokiyadoss R, Nafis Ahmed

SSN Research Centre, SSN College of Engineering, Kalavakkam 603110

***Email:** balajic@ssn.edu.in*

Copper has emerged as a suitable substrate material for the synthesis of graphene using CVD. It is imperative to make the CVD process sustainable. Understanding the growth of graphene on electroplated Cu substrates is an important step towards realising this objective. Cu, after transfer of graphene, can be recycled into a new substrate using electrolysis. In this work graphene was grown on commercial and electroplated copper substrates. The substrates were analysed using AFM and EBSD. Raman spectroscopy was used to analyse the synthesised graphene. The suitability of electroplated Cu substrates for graphene synthesis was evaluated. The average roughness (Ra) of commercial copper foil was observed to be 30.5 nm while that of electroplated copper foil was observed to be of 4 nm. EBSD analysis revealed the average grain size of

commercial copper foil and electroplated copper foil to be 7 µm and 5 µm respectively. Raman analysis of the synthesized graphene revealed average $I_{2D}/I_{G\ ratio}$ of 1.56 for commercial copper foil and 1.89 for that of electroplated copper foil. The suitability of the synthesized graphene was evaluated.

****

OP-35

Physicochemical and quantum chemical calculations of new bis (2-amino-6-methylpyridinium pyrimidinetrioate) tetrahydrate organic single crystal for nonlinear applications

R. Kaliammal, G. Parvathy, K. Velsankar, G. Maheswaran, S.Sudhahar

Department of physics, Alagappa University, Karaikudi-03.

***Email:** sudhaharsalagappauniversity.ac.in@gmail.com*

In the present work, new bis (2-amino-6-methylpyridinium pyrimidinetrioate) tetrahydrate organic single crystal was eminently grown by slow evaporation method in the technique of solution growth with the dimensional value 15 × 4 × 10 mm^3. To confirmation the grown crystal structure via single crystal X-ray diffraction. It is revealed that synthesized 2A6MP compound crystallizes in triclinic crystal system with centrosymmetric space group $P\bar{1}$.To find out the diffracting planes of the synthesized 2A6MP crystal by powder X-ray diffraction and it confirms the crystalline nature. ^{1}H NMR spectra were carried out to observe the various hydrogen expose in 2A6MP structure and the series of functional groups were elucidated by FTIR spectral analyses. Optical properties were analyzed by UV, PL analyses. In TG-DSC measurement to investigated the thermal stability of the grown 2A6MP crystal. The Vicker's microhardness test was arranged at room temperature and the gathered results were perceived under classical Meyer's law. The chemical etching was analyzed and the results were expressed that growth feature of the crystal. Second order nonlinear optical property of synthesized 2A6MP crystal was conscious by (SHG) second harmonic generation. Density functional theory (DFT) computations were used by B3LYP/6-311++G (d, P) basis set to optimize molecular geometry and the HOMO-LUMO energies confirm the presence of charge transfer within the molecule, Mulliken population analyses to find out the charge distribution in the atomic level, molecular electrostatic potential to established the electrophilic and nucleophilic reaction. NBO showed that the possible interaction between bonding and antibonding orbital molecular system with respect to the donor and an acceptor and first -order hyperpolarizability also confirmed the nonlinear property.

****

OP-36

Crystal growth and characterization of 3,4-diamino benzopheone: A novel benzophenone derivative for NLO applications

S. Usharani1, J.Judes1, V. Natarajan2*, M. Arivanandhan3, P. Anandan4

[1]University VOC College of Engineering, Anna University: Tuticorin Campus, Tuticorin 628 008, India
[2]Department of Physics, Dr. Sivanthi Aditanar College of Engineering, Tiruchendur 628215, India
[3]Centre for Nanoscience and Technology, Anna University, Chennai 600025, India
[4]Department of Physics, Thiru Kolanjiappar Government Arts College 606001, India
***Email:** Dr.V.Natarajan (vnatarajan@gmail.com)*

Benzophenone and its derivatives are the promising organic materials for NLO applications. Therefore, a series of benzophenone derivatives were grown as bulk single crystal and their NLO properties were studied. Being one of the benzophenone derivatives, 3, 4-diaminobenzophenone (3,4DABP) was selected and grown as a bulk single crystal by slow evaporation growth technique from mixed solvents of ethanol and o-xylene in the ratio of 1:3 at ambient temperature. Grown crystals were subjected to various characterization studies like XRD, FTIR analysis, TG/DTA, UV-Vis NIR spectroscopy, Vicker's microhardness testing and NLO studies to reveal their structural, thermal, mechanical and optical properties. Powder XRD studies indicated the pure crystallinity nature of the grown crystals. The presence of various functional groups was analyzed from FTIR spectrum. Optical studies revealed that the material can be used in photonics as optical filters. Microhardness study revealed that 3,4 DABP belongs to soft material and also exhibit Reverse Indentation Size Effect (RISE). SHG study confirmed that the frequency conversion efficiency of the crystal 3,4 DABP is 2.3 times that of KDP crystal.

Keywords: Organic NLO material, mixed solvents, Powder XRD, SHG efficiency, Photonics

****

OP-37

Bio-Supramolecular gel metal organic framework and its transformation to metal complexes by controlled pH

Sasikala Vadivel and Kalyana Sundar Jeyaperumal *

Materials Science Laboratory,
Department of Physics, Periyar University, Salem-636 011, Tamil Nadu, India.
***Email:** jksundar50@gmail.com*

Study of supramolecular gels component comprising molecular moieties sensitive to external entities is interesting as it controls the gelation process and alters the properties of the gel suitable for different applications. Here we reported the gel formation using simple organic arginine with 1, 3, 5 benzene tricarboxylic acid (BTCs) as a coordination network and cobalt for metal coordination, and the role of pH on the gelator containing pH-sensitive environment. The

supramolecular gel with the morphology of 1D microfibers was obtained at pH=5. It was transformed to metal complexes of 2 D micro sheets (pH 7), to 3D rugged surfaces (pH 8), to 3D hexagonal microcrystals, baton and finally spongy (pH 9). The gel was associated with tetragonal crystal system and the formed metal complexes were confirmed by X-ray powder diffraction. From the FTIR spectra, the coordination between cobalt ion and carboxyl group was clearly identified and this interaction strength varies for different metal complexes. This metal coordination combined with other noncovalent interactions controls the phase transformation from gel to complexes at different pH values. The gel displayed a pronounced fluorescence enhancement compared to metal-organic complexes. From the BET studies, the surface area of the complexes has increased compared to gels. For the metal complexes, the surface area has increased and reached a maximum of 1895 m^2/g at pH 8. This study insight the gelator molecules containing functional moieties for example carboxylic acid sensitive to pH environment can tune the gel properties suitable for gas storage and luminescence applications.

Keywords: Supramolecular gel; microfibers; arginine-based gel; gel transformation; photoluminescence.

****

OP-38

Growth and Low frequency Raman study of meta nitro aniline crystals

S. Boomadevi[*1], S.K.Pandiyan[2], M. Kaliwoda[3], R.R.Sumathi[3] and D.Sastikumar[1]

[1]Department of Physics, National Institute of Technology, Tiruchirapalli
[2]Center for Nonlinear Science and Engineering, Sastra University, Thanajvur
[3]Materials Science and Crystallography institute, Ludwig-Maximilians-University, Munich, Germany
***Email:** e-mail id: boomadevi@nitt.edu*

Metanitroaniline (mNA)$C_6H_6N_2O_2$ has been extensively studied for its second order nonlinear applications such as SHG and THz wave generation.The present works discusses the crystal growth and low frequency Raman analysis of the grown meta nitro aniline single crystals.Commercially available meta nitroaniline (mNA) from Sigma Aldrich (purity 99.99%) was used for growing the crystals. Single crystals of mNA of dimensions about 1.7 cm x 0.8 cm x 0.6 cm were obtained by slow evaporation technique for a period of about ten days. Acetone was used as the solvent.

The grown crystals had prismatic morphology and c axis as its growth axis.The as- grown single crystals were subjected to powder x-ray diffraction analysis,which revealed the crystal structure of mNa is to be orthorhombic with lattice parameters a= 6.4578Å, b=19.1911Å,

c=5.074Å. The point group is mm2. The results agreed well with JCPDS card no 381961. The melting point was found to be 112°C from TG analysis as compared to the theoretical value of 114°C. The Raman spectrum was acquired using both the IR and red lasers at room temperature.Low frequency Raman study has been carried out in the region 50-3000 $cm^{-1}$to understand the vibrational, vibration-rotational assignments of mNA crystal which gives rise to THz waves. The results will be discussed in detail.

****

OP-39

Growth and characterization of pure and L-lysine doped sulphamic acid single crystals

J. Arumugam [1, 2, 3], M. Selvapandiyan[2]*

[1]Department of Physics, Sri Vidya Mandir Arts & Science College, Uthangarai- 636902, Tamil Nadu, India
[2]Department of Physics, Periyar University PG Extension center, Dharmapuri- 636 705, Tamil Nadu, India
[3]Department of Physics, Periyar University, Salem- 636 705, Tamil Nadu, India

Optically transparent single crystals of pure and L-lysine doped sulphamic acid (SA) were grown by solvent evaporation solution growth technique at room temperature. Orthorhombic structure and lattice parameters of grown crystals were confirmed by X-ray diffraction analysis. UV-Vis spectral analysis shows the crystals have lower cut-off wavelength was observed less than 215 nm with high transmittance in the entire visible region. Thermal properties of the title material have been investigated by thermo-gravimetric (TG) and differential thermal analysis (DTA) studies. The hardness number of amaranth dye-doped SA crystal has been investigated by means of Vickers microhardness study by applying different loads ranging from 25 to 200 gm. From photoconductivity measurement shows that the grown crystals have negative photoconductivity nature. The *Z*-scan studies have been carried out at 632.8 nm to ascertain the influential third-order non-linear optical (TONLO) nature of amaranth dye-doped SA crystal. The *Z*-scan transmittance data have been used to determine the magnitude of TONLO susceptibility ($\chi 3$), absorption coefficient (β) and refractive index ($n2$) of amaranth dye-doped SA crystal.

Keywords: Single crystal XRD; UV visible; Microhardness; Photoconductivity; Z-Scan

****

OP-40

Structural, Optical and Electrical Properties of Benzo [e] Indolium based D-π-A chromophore Single Crystal

P. Eniya, R. Anbarasan and J. Kalyana Sundar*

Department of Physics, Periyar University, Salem 636 011, Tamil Nadu, India
***Email:** jksundar50@gmail.com*

In the field of nonlinear optics, strong second harmonic generation is widely observed in the molecules which are having electron donor and acceptor groups bridged by a benzene ring and having a heterocyclic benzo [e] indol. On these D-π-A chromophores, a novel high nonlinear optical salt of (E)-2-(4-(hydrophenyl) vinyl)-1, 1, 3-trimethyl-1H-benzo [e] indol-3-ium iodide (H-BI) is crystallized successfully by slow evaporation technique. The grown crystal was characterized by Single crystal X-ray diffraction (SXRD) analysis, which shows that crystal was perfectly crystalline in nature and belongs to Monoclinic structure with space group is P21/c. The UV-Vis NIR spectra show the crystal has wide transparency in the entire visible region with the lower cut-off wavelength is 284 nm and the bandgap value is 4.3 eV. The maximum weight loss has been confirmed by the endothermic peak of DTA. It is understood that the material P-BI is thermally stable upto 180 ºC from the analysis of TGA and DTA. The dielectric studies reveal that the crystal has low dielectric constant and low dielectric loss at high frequency range, which is a unique required property for NLO materials. The results of the structural, optical and electrical properties of this material confirm that this novel H-BI crystal will be more useful for photonic and NLO applications.

***Keywords**:* Single crystal, H-BI, dielectric, NLO, D-π-A

****

Poster Presentation

PP-01

Advancement and promising depictions of NLO organic crystal 4-nitrophenol 8-hydroxyquinoline (4n8Q) for opto electronic applications

J. Vidhya, R. Padmavathi

Department of Science and Humanities, M.Kumarasamy college of Engineeing (Autonomous), Karur-639 113
**Email: opilal@gmail.com*

Single crystals of 4-nitrophenol 8-hydroxyquinoline has grown by slow evaporation solution growth technique at room temperature. The crystal structure and crystalinity of the compound was confirmed by using X-Ray diffraction analysis. Vibrational modes of the functional groups were identified by using FTIRtechnique. Percentage of C, H and N present in the compound was confirmed by elemental analysis. Optical transmittance spectrum and Band gap was recorded by using UV-Vis-NIR spectrum. Thermal stability of the crystal was evaluated by Thermo Gravimetric and Differential Scanning Calorimetricstudies. Dielectric, DC and photoconductivity measurements were also carried for the grown crystal. The second harmonic generation efficiency of the grown crystal was found to be 7.81 times greater than that of standard KDP. Photoluminescence study was also taken for the grown crystal.

***Keywords*:** Optical materials; Crystal growth; Thermal study; SHG; Electrical conductivity

****

PP-02

Structure Property Correlation of a Series of Halogenated Schiff Base Crystals and Understanding Molecular Basis Through Nanoindentation

C. Ragaverthini[1] and Soumyajit Ghosh*[1]

[1]Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, 603 203, Chennai, India.
***Email*:** *soumyajs@srmist.edu.in*

Organic molecular crystals were perceived as brittle and inelastic entity; however, very recently there is a sudden spurt of reports of soft molecular crystals. We describe a family of halogenated Schiff base molecular crystals.[1,2] The design protocol was aimed to achieve incorporating structural features for desired mechanical property. However, we were able to achieve two elastically bendable crystals and remaining three were brittle. One of them is dimorphic means one form is brittle while another form is elastically bendable. Delicate rebalancing between weak and dispersive noncovalent interactions along with packing features ultimately give rise to two different polymorphs having different mechanical properties.[3] Further, nanoindentation technique was employed to understand the role of weak interactions so that design of crystals with desired properties can be done more precisely in future.[4] Elastic bending flexibility and fluorescence optical properties of molecular crystals can be combined to find applications in flexible optoelectronics.[5]

***Keywords*:** Polymorph, Nanoindentation, Optoelectronics

***References*:**

1) Ghosh, S.; Reddy, C. M. *Angew. Chem. Int. Ed.* 2012, *51*, 10319–10323.
2) Ghosh, S.; Mishra, M. K.; Kadambi, S. B.; Ramamurty, U.; Desiraju, G. R. *Angew. Chem. Int. Ed.* 2015, *54*, 2674 –2678.
3) Raju, K. B.; Ranjan, S.; Vishnu, V. S.; Bhattacharya, M.; Bhattacharya, B.; Mukhopadhyay, A. K.; Reddy, C. M.. *Cryst. Growth Des*. 2018, *18(7)*, 3927–3937.
4) Kiran, M. S. R. N.; Varughese, S.; Reddy, C. M.; Ramamurty, U.; Desiraju, G. R. *Cryst. Growth Des*. 2010, *10(10)*, 4650-4655.
5) Liu, B.; Di, Q.; Liu, W.; Wang, C.; Wang, Y.; Zhang, H. *J. Phys. Chem. Lett*. 2019, *10*, 1437–1442.

****

PP-03

Design of Mechanically Flexible Fluorescent Molecular Crystals

***Nipun. P*[1] *and Soumyajit Ghosh**[1]

[1]*Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, 603 203, Chennai, India.*
***Email:** soumyajs@srmist.edu.in*

Very recently, Flexible organic crystals have attracted wide attention among researchers worldwide. Incorporation of flexibility in organic single crystals find a wide range of applications such as optical waveguides, flexible optoelectronics, flexible light emitting diodes, optical switches, smart actuators etc.[1,2] So far poor processing abilities and fragilities of organic crystals limits their applicability in flexible optoelectronics. However, recently it has been observed that crystalline fluorescent materials serve as good candidates for flexible wave guides over non crystalline counterparts such as polymers etc.[1] Ordered alignment of molecules in densely packed system facilitates transduction of light even in bent state. In our exploration to design fluorescent flexible molecule crystals, we have chosen halogen substituted benzothiazole molecules.[3-5] These molecules meet the primary requirements of i) planar conformation ii) rigid structure and iii) π conjugated system.[6] The restorative nature of these interactions in combination with packing features gives rise to elastic bendable properties to few of them in this series. Rest does not comply packing requirements of elasticity therefore rendered as brittle in nature.

***References*:**

(1) Liu, H.; Lu, Z.; Zhang, Z.; Wang, Y.; Zhang, H. *Angew. Chem. Int. Ed*. **2018**, *57(28)*, 8448–8452.
(2) Ou, E. C. W.; Hu, L.; Raymond, G. C. R.; Soo, O. K.; Pan, J.; Zheng, Z.; Park, Y.; Hecht, D.; Irvin, G.; Drzaic, P.; Gruner, G. *ACS Nano* **2009**, *3*, 2258–2264.
(3) Hayashi, S.; Koizumi, T. *Angew. Chem. Int. Ed.* **2016**, *128(8)*, 2751-2754.
(4) Ghosh, S.; Mishra, M. K.; Kadambi, S. B.; Ramamurty, U.; Desiraju, G. R. *Angew. Chem. Int. Ed.* **2015**, *54*, 2674 –2678.
(5) Hayashi, S.; Koizumi, T.; Kamiya, N. *Cryst. Growth Des*. **2017**, *17(12)*, 6158– 6162.
(6) Saha, S.; Mishra, M. K.; Reddy, C. M.; Desiraju, G. R. *Acc. Chem. Res*. **2018**, *51(11)*, 2957–2967.

PP-04

Microwave combustion synthesis of tin oxide decorated silica nanostructure using rice husk template for supercapacitor applications

R. Vijayan [a,c,*], G. Suresh Kumar [b], N. Surumbarkuzhali [c], S. Prabhu [d], R. Ramesh [d]

[a]Department of Physics, Padmavani Arts and Science College for Women, Salem 636 011, Tamil Nadu, India.
[b]Department of Physics, K.S. Rangasamy College of Arts and Science (Autonomous), Tiruchengode 637 215, Tamil Nadu, India
[c]Department of Physics, Government Arts College (Autonomous), Salem 636 00, Tamil Nadu, India.
[d]Department of Physics, Periyar University, Salem 636 011, Tamil Nadu, India.
***Email:** nldvijay97@gmail.com*

Supercapacitors are emerged as leading energy storage device and developing new electrode materials for supercapacitors has received much scientific interest from the researchers. In this study we have synthesized tin oxide decorated amorphous silica (SnO_2@RH-SiO_2) nanostructures using rice husk template as a silica source *via* simple microwave combustion method for supercapacitor applications. XRD, FTIR and EDX studies obviously characterize that silica is present in amorphous form along with crystalline SnO_2 having a rutile tetragonal structure in the prepared SnO_2@RH-SiO_2 sample. Further, TEM observation indicates that prepared sample is consisting of amorphous silica nanospheres decorated with agglomerated tin oxide nanoparticles having size of 5-10 nm. Cyclic voltammetry and galvanostatic charge/discharge studies characterize the supercapacitaive behaviour of working electrode fabricated from prepared SnO_2@RH-SiO_2 nanostructure. The specific capacitances of SnO_2@RH-SiO_2 nanostructure are about 448, 330, 275, 240, 225 and 200 F/g with the current density value of 1, 2, 4, 6, 8 and 10 A/g, respectively. The presence SnO_2 species in SnO_2@RH-SiO_2 nanostructure can provide reactive surfaces for the adsorption/desorption charges and it facilitates the charge storage at the surface of sample. The above results suggested that the prepared SnO_2@RH-SiO_2 nanostructure has potential application for making electrochemical supercapacitors.

***Keywords*:** Tin oxide; Nanoparticles; Amorphous silica; Supercapacitors.

****

PP-05

A new non-linear optical material and mechanical studies for pure and sarcosine doped L-tartaric acid of single crystal by Slow Evaporation Method

A.T. Ravichandran[1], S. Aron Rabi[1,2]*
1. Department of Physics, National College (Autonomous), Trichy-620001, India.
2. Department of Physics, Loyola College of Arts & Science, Mettala, Namakkal-636202 India.
***Email:** atrnct@gmail.com, aron.rb@gmail.com*

A new non-linear optical material of sarcosine doped L-tartaric acid crystal grown by slow evaporation method by room temperature. The vibrational frequencies of functional groups doped L-tartaric acid in the grown crystal identified by FTIR spectral analysis. The optical transmission study reveals the improved is good transparency of doped crystal in the entire visible region for NLO applications. The crystalline size and cell parameter were characterized by powder X-Ray diffraction and Single X-Ray diffraction analysis. The presence of dopent in the sample grown by L-tartaric acid crystal with addition of sarcosine was determined by the spectral analysis. The presence of elements the dopent of grown crystal confirmed by energy dispersive X-ray analysis (EDAX). The Vickers Microhardness studies reveal that the mechanical strength of the grown crystal. The SHG efficiency of pure sarcosine doped L-tartaric acid crystal confirmed by Nd:YAG pulsed laser employing the Kurtz- Perry powder technique.

Keywords: Sarcosine, L-tartaric acid, FTIR, UV, Vickers hardness test, Single crystal XRD, EDAX, SHG

****

PP-06

Investigations on structural, electrical, third order nonlinear optical and antibacterial activity of Benzimidazolium maleate single crystal

S. Sakthy Priya[a], K. Balakrishnan[a], P. Surendran[a], A. Lakshmanan[a], S. Pushpalatha[a], G. Vinitha[b], P. Rameshkumar[a,*]

[a]PG and Research Department of Physics, Periyar E.V.R. College (Autonomous), Tiruchirappalli – 620 023.
[b]Division of Physics, School of Advanced Sciences, VIT Chennai, Chennai – 600 127.
**e-mail: rameshkumarevr@gamil.com*

An efficient organic single crystal of Benzimidazolium maleate (BIMA) has been grown by slow solvent evaporation method. The lattice parameters and crystallinity of the crystal was determined by powder x-ray diffraction analysis. Various chemical bond and vibrations present in BIMA crystal was confirmed by FTIR spectroscopy analysis. The dielectric constant and dielectric loss of the grown crystal as a function of frequency was measured. In addition solid state parameters like plasma energy, penn gap and fermi gap are evaluated. Z-scan technique was used to determine the refractive index (n_2) and nonlinear absorption coefficient β and third order nonlinear susceptibility (χ^3). For the first time antibacterial activity was done against gram positive and gram negative bacterial strains. *Shigella flexneri* shows high antibacterial activity and confirms

the suitability in Pharmacological applications. Fig 1 shows the Z-Scan pattern and zone of inhibition of some bacteria of BIMA crystal.

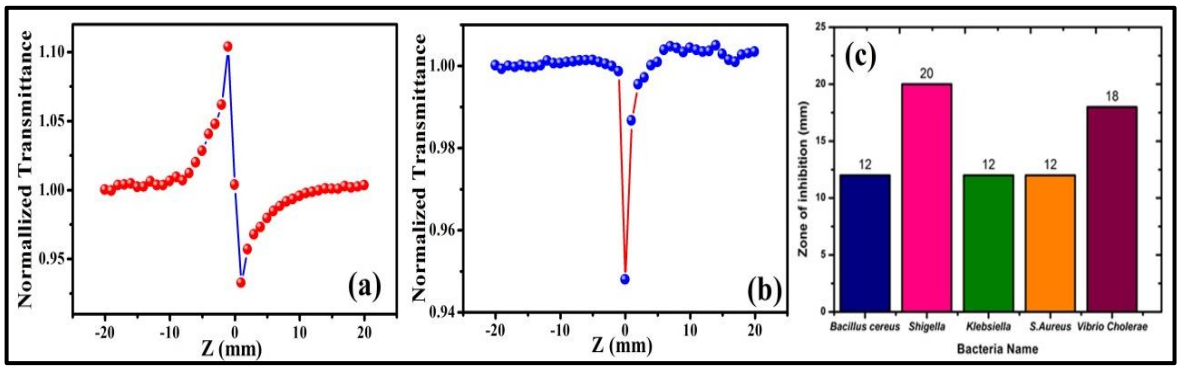


Figure 1. Z-Scan pattern and zone of inhibition of some bacteria of BIMA crystal.

Keywords: Organic crystal; Polarizability; Z-scan; Antibacterial activity

****

PP-07

Effect of precursor concentration of calcination Temperature dependent investigation on the properties of the La2O3 nanoparticles: Photocatalytic application

S.Karthikeyan , M.Selvapandiyan *

Department of Physics, Periyar University PG Extension Centre, Dharmapuri 636701.
Email: *skarthiphysics@gmail.com*

Different morphologies of the La_2O_3 nanostructures (nanorods and nanoparticles) were successfully synthesized with a facile sol gel method with reaction time (6hr) at 100°C. The morphology was transformed from nanorods to nanoparticles when the calcination time is increased. The effect of calcination time on the morphology, particle size, band gap and photocatalytic performance of the La_2O_3 products have been investigated. The La_2O_3 nanostructures have been formed with lanthanum nitrate and cerium nitrate as starting reactants, urea as the reaction medium and double distilled water as the structure-directing reagent. The obtained products are characterized by Powder X-Ray Diffraction, SEM, EDAX, UV-Vis Spectroscopy, PL and FT-RAMAN. XRD patterns show that the La_2O_3 nanoparticles obtained are of hexagonal structure. The Scanning electron microscopic images confirm the formation of nanoparticles. The results of the energy dispersive analysis of X-ray (EDAX), UV-Visible spectroscopy (UV-Vis), FT-IR studies are compared and discussed. The photocatalytic activity studies reveal that the synthesized La_2O_3 nanorods exhibit excellent photocatalytic performance in degrading methylene blue dye solution under UV irradiation.

Keywords: La_2O_3 nanoplates; Morphology; SEM; FT Raman Spectroscopy

****

PP-08

Growth and Comparative Studies Of Third Order Nlo Organic Crystals: Beta Alanine (Ba) And Beta-Alaninium Maleate (Bam)

D.Shanthi[a], P. Selvarajan[b] and S. Perumal[c]

[a]Department of Physics, Aditanar College of Arts and Science, Tiruchendur-628 216, Tamilnadu, India.
[b]Associate Professor, Department of Physics, Aditanar College of Arts and Science, Tiruchendur-628 216, Tamilnadu, India.
[c]Associate Professor & Principal (Rtd.), Physics Research Centre, S.T. Hindu College, Nagercoil-629 002, Tamilnadu, India.
***Email:** shanthid20@yahoo.com*

Beta alanine (BA) and beta-alaninium maleate (BAM) have been successfully grown by slow solvent evaporation solution growth technique at room temperature. The grown BA and BAM crystals were subjected to the various studies and their results have been compared. The crystalline structure of BA and BAM were confirmed by single crystal X-ray diffraction measurement. The various functional groups and vibrational modes for the grown crystals have been found by FTIR and FT-Raman studies. The TG/DTA study was carried out to determine the thermal stability of the grown crystals. Dielectric properties of the samples were studied at various frequencies. The optical transmission window of the grown crystals has been identified by UV-visible spectral studies. The mechanical strength of the grown crystals were analyzed by Vickers microhardness tester and the hardness number, Meyer's index, yield strength, stiffness constant and Hays-Kendall relations were evaluated. The second harmonic generation efficiency of the grown crystals were analysed by Kurtz-Perry test. The grown crystals have been studied by Z-scan technique using a He-Ne laser operating at 632.8 nm. The closed and open aperture Z-scan configurations have been used to determine the nature of refraction, nonlinear absorption coefficient, nonlinear refractive index and third-order nonlinear optical susceptibility. The photoluminescence studies were carried out for the grown crystals at room temperature. Also, impedance properties of the BA and BAM samples were analyzed.

***Keywords*:** Solution method; XRD; FTIR; FT-Raman; spectroscopy; NLO; Z-Scan; TG/DTA; dielectric; impedance; PL.

****

PP-09

Investigation on Growth, Structural and Optical studies of Potassium Sulphamate single crystal –A Material for Non-Linear Optical application

Ravinder Kumar[1, 2], N. Vijayan[2*], Naghma Khan[1, 2]

[1]Academy of Scientific & Innovative Research, CSIR – National Physical Laboratory, New Delhi
[2]CSIR –National Physical Laboratory, Dr K. S. Krishnan Road, New Delhi 110 012, India
Email: *bhoria.ias@gmail.com*

Nonlinear optical single crystal of Potassium Sulphamate (PSM) has been successfully grown from the aqueous solution by the slow evaporation method at room temperature. Powder X-ray diffraction analysis was employed to estimate the cell parameters and to confirm the structure for the grown crystal. The functional group exist in PSM was accomplished using Fourier transform infrared spectroscopy. The optical transparency and the band gap energy were elucidated by utilizing UV-visible spectrum. The Photoluminescence spectral studies revealed the photon excitation in the crystal system. Non-linear optical absorption coefficient estimated from open aperture Z-scan analysis revealed that crystal can be act as a promising aspirant for optical limiting applications.

Keyword: Nonlinear optical material, Z-scan, X-Ray Diffraction, UV-Vis, Photoluminescence

****

PP-10

Growth, and analysis of Optical and Mechanical properties of L-Asparagine Monohydrate Single Crystal for Nonlinear Optical Applications

Naghma Khan[1,2], N. Vijayan[2], Ravinder Kumar[1,2]

[1]Academy of Scientific & Innovative Research, CSIR – National Physical Laboratory, New Delhi
[2]CSIR – National Physical Laboratory, Dr K. S. Krishnan Road, New Delhi 110 012, India.
Email: *aayat22@gmail.com*

In the past few years, nonlinear optical single crystals are getting attention towards different areas of research. A semi organic nonlinear optical single crystal of L-Asparagine monohydrate (LAM) is one of the potential materials, and it has been successfully grown from the aqueous solution by the slow evaporation method at room temperature of size 10 x 5 x 4 mm^3. The grown single crystal was analyzed by different instrumentation techniques. Powder X-ray diffraction (PXRD) analysis was employed to estimate the cell parameters and to confirm the structure of the grown crystal. The presence of functional groups was examined by Fourier-transform infrared spectroscopy (FTIR). The recorded UV-Vis (UV) spectrum shows the optical transmission property of the crystal the existence of wide transparency window and it will be useful for optoelectronic device applications. The Photoluminescence (PL) spectral studies revealed the photon excitation in the crystal system. The mechanical behaviour and work hardening coefficient were evaluated by employing Vickers micro hardness tester. The observed results will be presented in detail.

PP-11

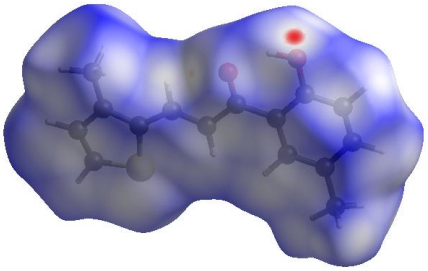
Hirshfeld surface analysis of a chalcone derivative

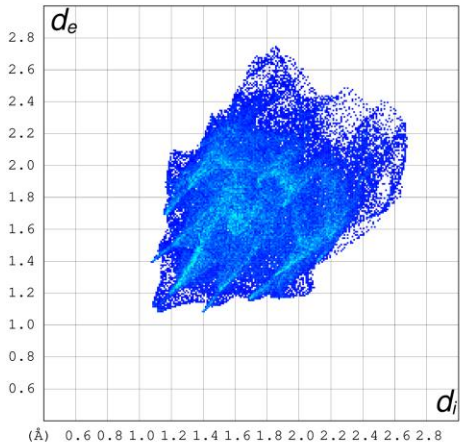
Lohith T. N[1]., Akhileshwari P[1]., Sirdhar M. A[*].

1. Department of Studies in Physics, University of Mysore, Manasagangotri, Mysuru 570 006, Karnataka, INDIA

**Email: mas@physics.uni-mysore.ac.in*

The compound 1-(2-hydroxy-5-methylphenyl)-3-(3-methyl thiophene-2-yl)prop-2-en-1-one is one of the derivative of the chalcone family. Chalcones are the aromatic ketones and enones. The chalcone skeleton has two aromatic rings bridged by three α, β-unsaturated carbonyl group. The presence of carbonyl functional group (C=O) makes chalcone more biologically active. Chalcones have been reported to show a wide spectrum of pharmacological activities like anti-inflammatory, anti-fungal, cytotoxic, anti-tumor, and etc. Hirshfeld surface analysis for the titled compound was done to visualize and analyzing the inter-molecular interactions. 2D fingerprint plots have been used to examine percentage contribution from each individual inter-molecular interactions to the surface. The d_{norm} and fingerprint plot of the titled compound is shown in the figure.





****

PP-12

Growth and characterization of nicotinium tartrate single crystal: An efficient organic nonlinear optical material

S.Pushpalatha, S.Sakthy Priya, K. Balakrishnan, A. Lakshmanan, P. Surendran, P. Rameshkumar*,

PG and Research Department of Physics, Periyar E.V.R College (Autonomous), Tiruchirappalli – 620 023.

***Email:** rameshkumarevr@gmail.com*

Organic single crystal of nicotinium tartrate (NT), an efficient nonlinear optical (NLO) material for frequency conversion, has been grown at a constant temperature at 40˚C within a period of 20 days by slow evaporation solution technique (SEST) as shown in Fig 1. Structural information and lattice dimensions were determined using powder X-ray diffractometer (PXRD) analysis. The functional groups and vibrational frequencies were identified using FTIR spectrum analysis with the range of 4000–450 cm^{-1}. Mechanical properties of the grown crystal were studied using Vickers microhardness tester. The optical properties of grown crystal were investigated using UV–Vis NIR spectrum analysis and it is confirmed that the crystal has very low absorption in the entire visible region. The dislocations and defects were studied by photoluminescence spectrum. The crystal has single stage melting, which was observed at 180˚C and there was no decomposition before its melting point. Piezoelectric, photoconductivity and chemical etching analysis have also been performed on the grown NT single crystals. Nonlinear optical property of the material was measured using the powder Kurtz–Perry technique.

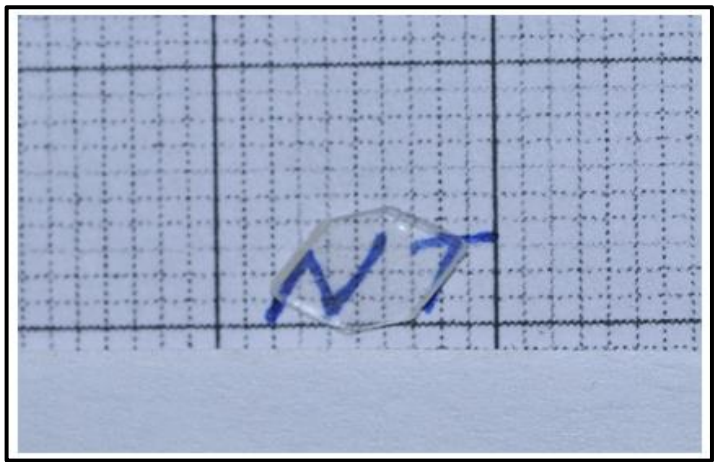


Figure 1: As grown NT single crystal

****

PP-13

Synthesis, Growth, Structural and Hirshfeld Surface Analysis of the NLO 3-Nitroanilinium chloride Single Crystals

C. S. Juliet Brintha *[a], **S. E. Joema** [b]

[a] *Research Scholar, Reg.No:18213112132001, Manonmaniam Sundaranar University, Abishekapatti, Tirunelveli 627 012, Tamilnadu, India.*
[a, b] *Department of Physics and Research Centre, Nesamony Memorial Christian College, Marthandam,TamilNadu, India.*
**Email:* *julietbrintha1985@gmail.com*

An organic nonlinear optical (NLO) single crystal of 3-nitroanilinium Chloride was grown by slow solvent evaporation technique at 30-40°C temperature, ethanol was used as a solvent. A good yellowish colour crystal of 3-nitroanilinium Chloride was obtained in duration of 21 days. The grown crystal was characterized by Single crystal X-ray diffraction (SXRD) analysis, which shows that crystal was perfectly crystalline in nature and belongs to Triclinic structure with space group is P1. The lattice parameters are a=6.89Å, b=7.66 Å and c=14.34Å. Fourier Transform Infrared Spectral analysis was recorded using spectrophotometer by KBr pellet technique in the region 4000-400 cm^{-1}. This study was recorded to confirm the functional groups of respected compounds. The intermolecular contacts in the compound was examined by Hirshfeld surfaces (HS) and fingerprint plots (FP) using the X-ray diffraction data. The second harmonic generation efficiency of the grown crystal was confirmed by Kurtz and Perry powder technique.

***Keywords*:** Nonlinear optical crystal, slow evaporation technique, SXRD, Hirshfeld surfaces (HS) and fingerprint plots (FP).

References:

1.Y.Mori, Y.K. Yap, T. Kamimura, M. Yoshimura, andT. Sasaki, Opt. Mater. 19, 1 (2002).
2.M.Ushasree, R. Muralidharan, R. Jayavel, and P.Ramasamy,J. Cryst. Growth 218, 365 (2000).
3.Z. Li, K. Wu, G. Su, and Y. He, Opt. Mater. 20, 295(2002).
4.KURTZ. S. K. Perry, T. TT. J. Appl. Physics 1968, 39, 3798-3813.

****

PP-14

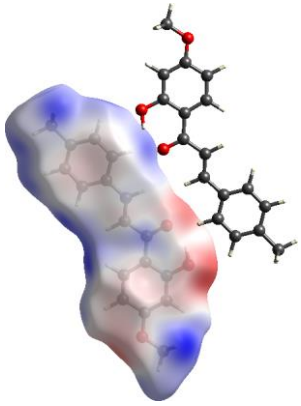
Computational studies of intermolecular interactions in a chalcone derivative

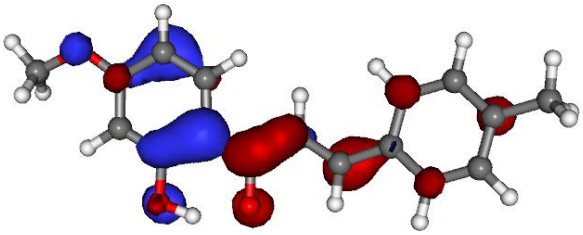
Akhileshwari P[1]., and Sridhar M. A.[1]*

[1]*Department of Studies in Physics, Manasagangotri, University of Mysore, Mysuru, INDIA 570 006.*
***Email:** mas@physics.uni-mysore.ac.in*

The molecule is a 1-(2-hydroxy-4-methoxyphenyl)-3-(4-methylphenyl) prop-2-en-1-one chalcone derivative. Chalcone is an aromatic ketone and an enone. Chalcones and its derivatives exhibit a broad spectrum of biological activity such as antioxidant, antitumor, anti-inflammatory, anticarcinogenic activity *etc*. The molecule crystallizes in the primitive monoclinic system. The space group is $P2_1/c$. The lattice parameters are a = 11.340(2)Å, b = 6.835(7)Å, c = 20.449(4)Å and β = 117.71(4)º. The final residual value is 0.0569. The molecule exhibits intramolecular

hydrogen bond of the type O-H...O. Hirshfeld surface analysis was employed to anatomize the intermolecular interactions in the crystal [1]. The frontier molecular orbitals, HOMO and LUMO were done using density functional theoretical methods study to know the chemical stability of the molecule [2]. The Hirshfeld surface mapped over $d_{norm,}$ and HOMO and LUMO of the molecule is shown in figure respectively.





***Keywords*:** Chalcone; Hirshfeld surface analysis; HOMO-LUMO.

***References*:**

1. J. J. McKinnon, M. A. spackman, and A. S. Mitchell, *Acta Cryst*., B60, 627-668, 2004.
2. Tahar Abbaz, Amel Bendjeddou, and Didier Villemin, *Pharmaceutical and biological evaluations*, 5 (2), 27-39, 2018.

****

PP-15

Investigations On Semi Organic Nonlinear Optical Single Crystal: L-Tyrosine Hydrobromide (Lthb)

D.Abila Darling[1], S.E.Joema[2]

[1] *Research Scholar, Reg.No: 18123112132039, Manonmaniam Sundaranar University, Abishekapatti, Tirunelveli-627 012, Tamilnadu, India.*

[1, 2] *Department of Physics and Research Centre, Nesamony Memorial Christian College, Marthandam, Tamilnadu, India.*
[*] ***Email:*** *abilajose.15@gmail.com*

The potential application of amino acid crystals, used in NLO applications leads to intensive investigation about the material. In the present work, L-Tyrosine Hydrobromide single crystal was grown by slow evaporation technique. The crystalline nature of the grown crystal is confirmed by powder X-ray diffraction analysis. Single crystal X-ray diffraction analysis reveals that the grown crystal belongs to monoclinic system. The Fourier Transform analysis confirms the incorporation of L-Tyrosine into Hydrobromic acid. The optical transparency of the grown crystal was studied by UV-Visible spectra. The microhardness study shows that the Vickers hardness number of the crystal increases with the increase in applied load. Its nonlinear optical response was tested by using Kurtz and Perry method.

***Keywords*:** Solution Growth, Single crystal XRD, FTIR Analysis, UV Analysis, Microhardness and NLO Activity.

References

[1] V.G. Dmitriev, G.G. Gurzadyan, D.N. Nicogosyan, Handbook of Nonlinear Optical Crystals, Springer-Verlag, New York, 1999.
[2] C. Razzetti, M. Ardoino, L. Zanotti, M. Zha, C. Paorici, Cryst. Res. Technol. 37 (2002) 456–465.
[3] M.S. Wong, C. Bosshard, F. Pan, P. Gunter, Adv. Mater. 8 (1996) 677–680.
[4] J. J. Jr. Rodrigues, L. Misoguti, F. D. Nunes, C. R. Mendonea, S. C. Zilio, Opt. Mater. 22, 235 (2003).
[5] N. Vijayan, N. Rajasekaran, G. Bhagavannaravana, R. Ramesh Babu, R. Gopal Krishnan, M. Palanichamy, and P.Ramaswamy, Cryst. Growth Des. 6, 2441 (2006).
[6] M. Narayan Bhat and S. M. Dharmaprakash, J. Cryst. Growth 236, 376 (2002).

****

PP-16

Synthesis and Characterization of ZnSe nanoparticles by Co-precipitation method

V. Beena[1], Dr. S. L Rayar[2],Dr. S. Ajitha[3]
[1]Research Scholar, Department of Physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai, Tamil Nadu, India
.[2]Principal, J P College of Arts & Science, Thenkasi, [3]Assisstant Professor, Department of Physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai.
Email: *beenarajadhas@gmail.com*

In recent years, semiconductor nanoparticles have attracted great deal of attention because of their novel optical properties and potential applications. The nanocrystalline semiconductors behave differently from their bulk semiconductors. Zinc Selenide is a II-VI compound semiconductor with the wide band gap of 2.7eV. In the present work, we report the synthesis of zinc selenide nanoparticles using the precursor materials such as zinc acetate and selenium powder by the co-precipitation method. The prepared samples are annealed at a low temperature and a high temperature. The morphology and structure of the as synthesized samples have been characterized by using the field emission scanning electron microscopy (FE-SEM), X-Ray diffraction studies (XRD), UV-Visible Diffuse Reflectance Spectroscopy (UV-Vis DRS), Fourier Transform Infrared Spectroscopy (FTIR) and Photoluminescence (PL) spectroscopy. XRD study evident that the synthesized ZnSe nanoparticles were cubic in structure. Fourier Transform Infrared Spectroscopy confirmed presence of various groups in the synthesized ZnSe nanoparticles. The band gap energy is found to be 3.4eV and 3.45eV. The Photoluminescence study also revealed the optical behaviour of the ZnSe Nanoparticles. The FE-SEM images showed that the produced ZnSe nanoparticles substantiates the cubical shape with crystalline nature.

Keywords: ZnSe nanoparticles, XRD, FTIR, UV, PL, FE-SEM

References

1. S.K Shakir Mohd, K.K Kushwaha, G. Maurya, G.Bhagavannarayana And M.A Wahab, 'Characterization Of Znse Nanoparticle Synthesized By Microwave Heating Process', Solid State Communication 149, No.45-46(2009):2047-2049
2. Anikin, K.V, N.N Melnik, A.V , Simakin , G.A Shafeev, V.V. Varanu And A.G Vitukhuovsky, ' Formation Of Znse And Cds Quantum Dots Via Laser Abilation In Liquid', Chemical Physical Latters 366,No.3-4(2002), 357-360.
3. Yanbin Wng, Chunlei Wang, Shuhong Xu, Zhuyuan Wang And Yiping Cui, Published I July 2014, Nanotechnology, Vol.25, No. 29.

****

PP-17

Structural, growth, optical and mechanical properties of Potassium 4-methyl benzene sulfonate single crystal

C.Amirthakumar, B. Valarmathi, R. Mohan Kumar*

[a]*Department of Physics, Presidency College, Chennai-600 005, India*
***Email:** mohan66@hotmail.com*

Semi-organic single crystal of Potassium 4-methyl benzene sulfonate (KOPT) was grown by slow evaporation solution growth technique. Structural parameters of the grown crystal were obtained by single crystal X-ray diffraction analysis. It reveals that the KOPT belongs to monoclinic system with non-centrosymmetric space group $P2_1$. UV-Vis spectral studies revealed the shorter cut-off wavelength, good transparency and optical band gap. The second harmonic generation efficiency was estimated for grown crystal by Kurtz and Perry powder technique. Hardness number of the crystal was estimated by Vicker's microhardness studies.

Figure: Photograph of as grown KOPT crystal

****

PP-18

Growth and Studies on Sodium Selenite Doped Tgs Single Crystals

N.Thangaraj[1], C.Gnana Sambandam[1] , N. Joseph John[2]

[1] Physics Research Centre, S.T.Hindu College, Nagercoil, Kanyakumari District,Tamilnadu-629002, India.

[2]Department of Physics, Kamarajar Govrnment Arts College, Surandai, Tirunelveli District, Taminadu-627859, India.

Email: *thangarajmscphysics@gmail.com*

An inorganic nonlinear optical single crystal, sodium selenite doped Tri Glycine Sulphate (SSTGS) was grown by slow evaporation method at constant temperature 40˚C. The grown SSTGS crystal was characterized by single crystal XRD and powder XRD technique to determine the cell parameters and the crystalline nature. The percentage of optical transmittance, optical band gap were ascertained by UV-Vis-NIR spectrophotometer. The luminescence property was examined by luminescence spectrum. These characterization studies confirmed that the nonlinear optical property of the grown crystal and suitability for nonlinear optical applications. The thermal behaviors of the grown crystal were studied by TG/DTA analyzer. The hardness of SSTGS was determined by Vicker's hardness test.

****

PP-19

Studies on bioactive single crystal 2,4,6-Triaminopyrimidinium Nitrobenzoate

M. Tamil Elakkiya, K. Anitha*

School of Physics, Madurai Kamaraj University, Madurai.
Email: *singlecrystalxrd@gmail.com*

A novel organic bioactive single crystal 2,4,6-Triaminopyrimidinium nitrobenzoate (TAPNB) which was grown by slow evaporation solution growth method. The experimental and quantum chemical investigations were carried out and their results are discussed. The solid-state structure of TAPNB is solved by single crystal X-ray diffraction. The crystallographic data reveals that the grown crystal structure is monoclinic crystal system with Cc space group. In the present crystal structure, molecules are connected through N-H…O intermolecular hydrogen bonding with $R_2^2(8)$ ring motifs and $C_2^2(13)$, $C_3^1(8)$ chain motifs along b axis. The non-covalent interactions are responsible for extending their supramolecular networks. The intermolecular hydrogen bonds were quantitatively analyzed by Hirshfeld surface and finger print analysis.

The molecular geometry of the grown crystal was optimized theoretically by using density functional theory with B3LYP/6-311++G(d,p) basis set. The optimized molecular geometry and computed vibrational spectra were compared with experimental results which showed noteworthy agreement. The atomic charge distribution on atoms of TAPNB molecule has been calculated by Mulliken charge analysis. Energy gap, ionization potential and chemical hardness of the TAPNB

molecule were carried out by HOMO–LUMO plot. In which, lower band gap of the frontier orbitals value indicates the possible bio- activity of the molecule. Mulliken atomic charge distribution and FMOs investigation clearly support the arrangement of N-H…O intermolecular hydrogen bonds. The natural bond orbital analysis was carried out to interpret the stability of the molecule and charge delocalization within the molecule. The effect of complex formation (TAPNB) molecule on the anti-bacterial activity was screened against different strains of bacteria. The theoretical evaluation of biological activity like molecular docking was studied for the present compound.

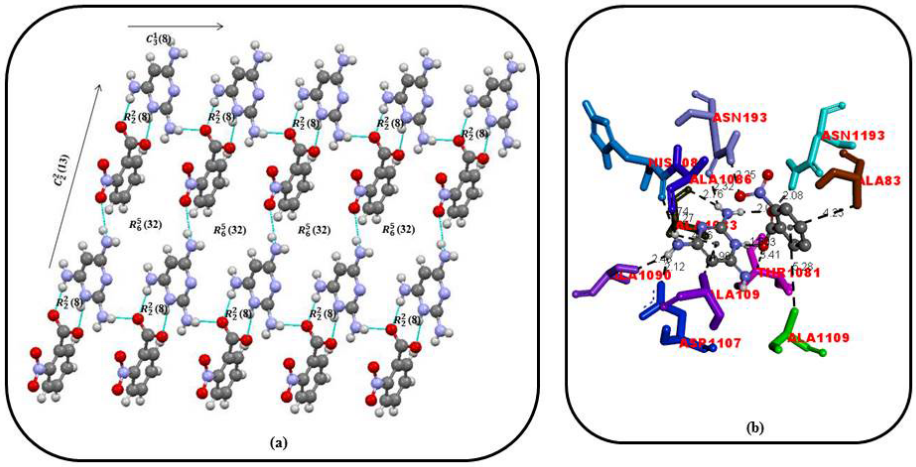


Figure: (a) Ring $R_2^2(8)$,$R_6^5(32)$motifs and chain $C_2^2(13)$, $C_3^1(8)$ motifs in TAPNB and

(b) Specific interaction of TAPNB with protein.

****

PP-20

Synthesis and properties of MgO nanoparticles doped with strontium ions

A.Suba[1*], P.Selvarajan[2], J.Jebaraj Devadasan[3]

[1]Department of Physics, Pope's College, Sawyerpuram, Tirunelveli district, Tamilnadu, India.
[2]Department of Physics, Aditanar College of arts and science, Tiruchendur-628216, Tuticorin district, Tamilnadu, India.
[3]Department of Physics, Pope's College, Sawyerpuram, Tirunelveli district, Tamilnadu, India.

***Email:** suba.aldrin@gmail.com*

Magnesium oxide is one of the most useful ceramic materials. Because of its high melting temperature (about 2800 °C), it is usually used in fire-resisting bricks or crucibles. Magnesium oxide (MgO) nanoparticles doped with strontium ions were prepared by wet thermal method. The reactants used are magnesium sulphate, urea and ethylene glycol for preparing MgO nanoparticles. To prepare strontium ions doped MgO nanoparticles, 5 wt. % strontium chloride was added into sample of MgO nanoparticles. The X-ray diffraction pattern of the material confirms that thee

prepared sample was single phase. The functional groups on the surface of material were determined by Fourier-transform infrared spectroscopy (FT-IR). The morphology and particle size were given by scanning electron microscope (SEM). The chemical composition of MgO material after adsorption was analyzed with energy-dispersive X-ray spectroscopy (SEM-EDX). Other studies like TG/DTA and particle size analysis were also carried out.

***Keywords*:** Magnesium oxide, nanomaterial; characterization; XRD, SEM, EDAX,

****

PP-21

Growth, spectral, second and third order NLO properties of L-histidine tartaric acid crystals

S.Sudharthini[1], P. Selvarajan [2], C.Gnana Sambandam[3]

[1] Department of Physics and Research Centre, S.T.Hindu College, Nagercoil-629002, Tamilnadu, India.

[2] Department of Physics, Aditanar College of Arts and Science, Tiruchendur-628216,

Tamilnadu, India.

[3]Department of Physics, S.T.Hindu College, Nagercoil-629002, Tamilnadu, India.

The importance of amino acids in NLO applications is due to the fact that, except glycine, all the amino acids have chiral symmetry and crystallize in non-centrosymmetric space groups. L-histidine tartaric acid was synthesized and was grown in the form of single crystal by solution method. L-histidine tartaric acid (LHTA) crystals were grown by solution method with slow evaporation technique using double distilled water as the solvent. The saturated solution of L-histidine and L-tartaric acid in 1:1 molar ratio was prepared. By XRD studies, the crystal structure of LHTA crystal was found to be monoclinic. The various functional groups of the sample were identified by FTIR studies and the weight percentage of different elements in LHTA crystal were determined by EDS and CHN analyses. The UV cut-off wavelength of the sample was found to be 225 nm and the relative SHG efficiency of LHTA crystal was observed to be 1.02 times that of KDP crystalline sample. The third order NLO parameters like nonlinear absorption coefficient, nonlinear refractive index and nonlinear susceptibility of the grown LHTA crystal were determined by Z-scan technique. The hardness of the sample was found at different applied loads and it is noticed that the hardness increases with increasing of applied load. Since hardness, transparency in visible region, SHG efficiency and third order NLO parameters of LHTA crystals are quite a high, this crystal could be used in NLO devices like second harmonic generator.

Keywords: Single crystal, XRD, FTIR, UV, SHG, Z-Scan, EDAX, Hardness

****

PP-22

Green Synthesis and Studies of Aluminium Nitride (Aln) Nanoparticles

M.Malathi[1], P.Selvarajan[2] and U.Rajesh Kannan[3]

[1]Assistant Professor, Department of Physics, Seethalakshmi Achi College for Women, Pallathur-630107, Tamilnadu, India.
[2]Associate Professor, Department of Physics, Aditanar College of Arts and Science, Tiruchendur- 628 216, Tamilnadu, India.
[3] Research Scholar, Department of Physics, Kamaraj College, Tuticorin-628003, Tamilnadu, India

Nowadays aluminium nitride (AlN) is becoming an attractive material, especially in the nano powder form. It is an important material for electronics and for optoelectronic devices. Other important applications of this material include surface acoustic wave devices and buffer layers for group III nitride thin film epitaxy. The main purpose of this paper was to develop a method for obtaining a pure and fine AlN nano powder with an average grain size lower than 100 nm and agglomerate size below 500 nm via a simple and cost-effective technique of synthesis. It has been reported that Aluminium nitride nanoparticles were prepared by many techniques. In this work, Aluminium nitride nanoparticles are prepared by using green synthesis. Using aluminium nitrate, urea and leaves of drum stick, aluminium nitride nanoparticles are synthesized. The sample was annealed at 700^{o}C for 7 hours. The prepared AlN nanoparticles are characterized by XRD studies, FTIR, EDAX, and TG/DTA studies.

Keywords: Nano powder, AlN, green synthesis, characterization, XRD, FTIR, EDAX

****

PP-23

XRD, Optical, NLO and thermal properties of mono-urea oxalic acid crystals doped with zinc sulfate

T. Manju[1], P. Selvarajan[2], U.Rajesh Kannan[3]

[1]Assistant Professor of Physics, Merit College of Arts and Science, Idaikal, Tirunelveli,Tamilnadu, India.
[2]Associate Professor of Physics, Department of Physics, Aditanar College of Arts and Science, Tiruchendur-628216, Tamilnadu, India.
3. Research Scholar, Department of Physics, Kamaraj College, Tuticorin, 628003

Sample of zinc sulfate doped mono-urea oxalic acid (ZMUOA) were synthesized using urea, oxalic acid and zinc sulfate as the reactants. Nucleation studies have been carried out for the synthesized sample for various supersaturation values. Single crystals of the synthesized salt of ZMUOA were grown by aqueous solution growth with slow evaporation technique. XRD studies reveal the crystal structure. Dielectric constant and dielectric loss of the grown ZMUOA crystal were measured using a parallel plate capacitor method at various frequencies and temperatures and

the results are analyzed. Mono-urea oxalic acid crystal is a centrosymmetric crystal which gives out second harmonic generation (SHG) under irradiation of the light from Nd: YAG laser. Urea is an important NLO material which can be combined to organic and inorganic materials to form many useful complexes like urea succinic acid, di-urea oxalic acid, mono-urea oxalic acid and urea malic acid. The details of crystal structure of mono-urea oxalic acid and di-urea oxalic acid crystals were given in the literature. Zinc sulfate is an inorganic material and it can be added into the organic urea oxalic acid crystal to modify its properties. it is found that the ZMUOA crystal belongs to monoclinic structure. It is observed that the space group of the grown crystal is C2/c and this is identified as the centrosymmetric space group. The XRD studies reveal that the grown crystal of ZMUOA crystallizes in monoclinic structure. The critical nucleation parameters like Gibbs free energy, interfacial tension, nucleation rate, critical radius of the sample were determined.

***Keywords*:** Organic crystal; doping; solution growth; single crystal; nucleation; XRD; dielectrics; optical conductivity

****

PP-24

Studies of L-lysine acetic acid crystals by grown by solution method

C. Anbulakshmi[1]*, P.Selvarajan[2], S.Selvaraj[3]

[1,3] Department of Physics and Research Centre,
MDT Hindu College, Tirunelveli-627010, Tamilnadu, India.
[2]Associate Professor of Physics, Aditanar College of Arts and Science,
Tiruchendur - 628216, Tamilnadu, India.
[3]Affiliated to Manonmaniam Sundaranar University, Abishekapatti-627012,
Tirunelveli, Tamilnadu, India)
**Corresponding author: sharmichandrasekaran@gmail.com*

Nonlinear optics is one of the branches of the optics and it has revealed many second order and third order optical phenomena such as second harmonic generation (SHG), third harmonic generation (THG), higher harmonic generations, optical rectification, stimulated Raman scattering etc. There are mainly three types of nonlinear optical (NLO) crystals viz., organic NLO, inorganic NLO and semiorganic NLO crystals. Organic NLO crystals have high SHG efficiency and high laser damage threshold and they can be easily fabricated. Lysine is an α-amino acid that is used in the biosynthesis of proteins. Bulk single crystals of L-lysine acetic acid (LLAA) were grown by solution method. XRD studies indicate that LLAA crystal has monoclinic structure. The density of the grown crystal was found to be 1.552 g/cc. The elements like C, N and O were identified in the sample and weight percentage was calculated. FTIR and PL studies of the sample were carried out. The mechanical properties like hardness, work hardening coefficient, corrected hardness, yield strength and stiffness constant of LLAA crystal were determined by Vickers microhardness analysis. The relative SHG efficiency of LLAA crystal was found to be 1.14 times that of KDP sample. L-lysine and acetic acid were used as the reactants to grow the single crystals of L-lysine acetic acid (LLAA) and the crystals were grown by solution method at room temperature. The crystal structure was analysed by X-ray diffraction studies. Second order NLO studies were carried out for the grown LLAA crystal. Density of the sample was found by floatation method. The functional groups of the grown LLAA crystal were identified by FTIR

analysis. The weight percentage of elements in the sample was determined by EDAX method. PL studies were carried out for the sample using the photoluminescence (PL) analyser and the obtained results were discussed.

Keywords: Amino acid complex; single crystal; solution growth; XRD; FTIR: SHG; Photoluminescence; EDAX

****

PP-25

Investigation on undoped and zinc sulfate doped magnesium iodate crystals

P.Geneva Sequirea Roche[*], A.Lesly Fathima[**], P. Selvarajan[***]

[*]*Department of Physics and Research Centre, Holy Cross College, Nagercoil-629004, Tamilnadu.*

[**]*Assistant Professor of Physics, Department of Physics and Research Centre, Holy Cross College, Nagercoil-629004, Tamilnadu*

[***]*Department of Physics, Aditanar College of Arts and Science, Tiruchendur-628216, Tamilnadu, India.*

Undoped and zinc sulfate doped magnesium iodate crystals have been grown by solution method using the double distilled water as the solvent. The reactants used here are magnesium sulfate, iodic acid and zinc sulfate and the grown crystals were harvested after a period of nearly one month. The grown crystals were subjected to XRD studies, LDT studies, UV-visible spectral studies, microhardness studies, SHG and dielectric studies. Both undoped and zinc sulfate doped magnesium iodate (ZSMI) crystals are found to be crystallizing in monoclinic crystal structure. The transmittance is observed to be decreasing when magnesium iodate crystal is doped with zinc sulfate. The hardness is found to be increasing due to doping of zinc sulfate into the lattice of magnesium iodate crystal. The NLO properties like SHG efficiency have been enhanced when magnesium iodate crystals are doped with zinc sulfate. and the obtained results are analysed and reported.

***Keywords*:** Magnesium iodate; doping; solution method; slow evaporation technique; Characterization; XRD; microhardness; SHG; dielectrics

****

PP-26

Growth of defect free non-linear optical 4-aminobenzophenone (ABP) single crystals from pure and mixed solvents

A. Mythili and K. Srinivasan*

Crystal Growth Laboratory, Department of Physics, Bharathiar University, Coimbatore -641 046.
***Email:** nivas_5@yahoo.com*

Nonlinear optical single crystals with good optical quality and preferable size are most important for potential applications. Solvent incorporation in the grown crystals is often a problem when crystallized from solutions. In this investigation, well-known nonlinear optical material 4-aminobenzophenone (ABP) was crystallized from solutions with different selected solvents having different chemical properties. Solubility of ABP in the selected solvents was determined by gravimetric method. Saturated solutions with pure as well as mixed solvents were prepared and nucleation and growth of the crystals were observed through in-situ monitoring under microscope. Morphologly of the grown crystals and growth rate along different crystallographic directions were studied with respect to solvents of differnet chemical nature. Single crystals were grown by slow evaporation method. Over all observation indicates that the single crysals of ABP grown from solution with mixed solvents of ethanol and DMSO yield good quality single crystals and they are comparatively defect free. It is well understood that the solvent incorporation was significantly reduced while using the mixed solvents of ethanol and DMSO and also the growth rate along differnet growth directions are very much controlled. Grown single crystals were characterized for their structural confirmation by powder x-ray diffraction analysis. Second harmonic genecation efficiency of one such grown single crystal was studied by Kurtz powder method. Resutls will be presented.

****

PP-27

Synthesis and Crystal Growth of Acetylsalicylic Acid from Aqueous Solution

M. Ramya, S. Supriya and K. Srinivasan*

Crystal Growth Laboratory, Department of Physics, Bharathiar University, Coimbatore - 641046.
* ***Email:** nivas_5@yahoo.com*

Acetylsalicylic acid ($C_9H_8O_4$), commonly known as aspirin, is a well-known anti-inflammatory, antipyretic and antirhumetic drug used mainly in pharmaceutical applications widely. In the present work the raw material was synthesised in the laboratory using the precursor materials such as salicylic acid, acetic anhydride and phosphoric acid in the stoichiometric ratio and the synthesised material was then purified thorough step-by-step recrystallization process in selected solvents. Solubility of the the purified material was determined by gravimetry and saturated solution was prepared at room temperatue. Crystal nucleation was observed under in-situ microscopic technique and the morphology of the nucleated and grown smaller size signle crysals of asprin was identified. The internal crystallographic structure of the grown crystal was confirmed

by powder x-ray diffraction method initially and later the structure was refined through single crystal x-ry structural refinement method. Thermal stability till the melting point was cofnired by differential scanning calorimetry analysis. Results will be presented.

****

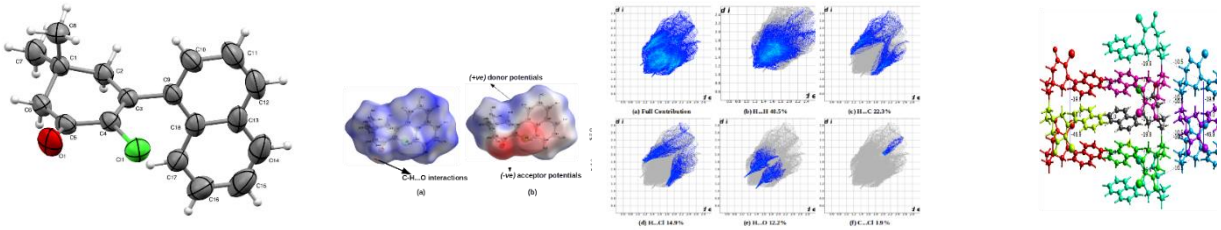
PP-28

Structural, Hirshfeld surface studies and computation of interaction energies of a compound 2-Chloro-3-(1'-napthyl)-5,5-dimethyl-2-cyclohexenone

N R Sreenatha[a, b] A S Jeevan Chakravarthy[C], B Suchithra[d] B N Lakshminarayana[a], S Hariprasad[c] and D P Ganesha[a]

[a]Department of Engineering Physics, Adichunchanagiri Institute of Technology, Chikkamagaluru - 577102, Karnataka, India.
[b]Department of Physics, Government Engineering College, Hassan - 573 201, Karnataka, India.
[c]DOS in Chemistry, Central College Campus, Bangalore University, Bengaluru - 560 001, Karnataka, India
[d]Department of Biochemistry, Jnana Bharathi Campus, Bangalore University, Bangalore - 560 056, Karnataka, India
***Email:** bnlphysics@gmail.com*

The single crystal X-ray diffraction study revealed that the title compound 2-chloro-3-(1'-napthyl)-5,5-dimethyl-2-cyclohexenone was crystallized in monoclinic crystal system with the space group $P_{21/c}$. In the molecule, cyclohexenone ring displayed puckering environment by adopting envelope conformation. The molecules are stabilized by C-H...O intermolecular interactions exhibiting independent 1D polymeric chains propagating indefenitely along *c*-axis. The intermolecular interactions are studied and analyzed by Hirshfeld surfaces mapped on d_{norm} and electrostatic potentials and percentage contribution between various intercontacts are calculated by 2D fingerprint plots towards formation of 3D Hirshfeld surfaces. Apart from these, interaction energies between the various pairs of molecules were obtained using the energy density model of B3LYP/6-31 G(d,p).



Parameters	Values
CCDC	1952185
Chemical formula and Formula weight	$C_{18}H_{17}ClO$ and 284.76

Temperature (K) & Wavelength (Å)	290 & 0.71073
Crystal system, space group	Monoclinic, $P_{21/c}$
Unit cell dimensions (Å, °)	A=20.2583(2), b=7.4914(6), c=9.9034(9), β=93.097
Cell volume ($Å^3$) and Cell formula units Z	1500.8(2) and 4
Calculated Density (Mg/m) and F (000)	1.260 and 600
Crystal size (mm)	0.40 × 0.35 × 0.31
Theta range for data collection (°)	3.0 to 28.3
Limiting indices	h=-26→27, k=-9→9, l=-13→13
No. of measured, independent and observed reflections	39386, 3717, 2586
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3717/ 0 / 184
R Value and Goodness of Fit on F^2	0.079 and 1.01

References:

1) APEX2 Bruker, SAINT-Plus and SADABS, Bruker AXS Inc., Wisconsin, Madison, USA, (2004).
2) G. M. Sheldrick, Acta Cryst. A64, 112-122 (2008)
   A. L. Spek, Acta Cryst. D65, 148-155 (2009)
   B. F. Macrae, I. J. Bruno and J. A. Chisholm et. al. J. Appl. Cryst. 41, 466 (2008).
3) S. K. Wolff, D.J. Grimwood, J.J. McKinnon, M.J. Turner, D. Jayatilaka, M.A. Spackman,
4) CrystalExplorer (Version 3.1), University of Western Australia, (2012)
5) J.J. McKinnon , M.A. Spackman , A.S. Mitchell , Acta Cryst. B60, 627-668 (2004) .
   A. Gavezzotti. J. Phys. Chem. B, 106(16), 4145-4154 (2002).
6) J. Thakkar, C. Lupinetti, S. Shyamapada, M. Christoph, and M. Samiran. Maroulis, G. Ed.; World Scientific:Hackensack, NJ, 505-529 (2006).
7) S. Grimme. J. Comput. Chem., 27:1787-1799, (2006).

****

PP-29

Synthesis of Organic Dye and Its characteristics for Dye Sensitized Solar Cell (DSSC) Applications

Kotteswaran Shanmugam* and Ramasamy Perumalsamy

SSN Research Centre, SSN College of Engineering, Chennai-603110, Tamilnadu, India
***Email:** kotties555@gmail.com*

The phenyl-conjugated Oligoene dye 2-cyano 3-(4-diphenylaminophenyl) prop 2-enoic acid (SKS) was synthesized by chemical method. The synthesized dye was purified using column chromatography. The structure of the SKS was confirmed by ^{1}H NMR and ^{13}C NMR analysis. The FTIR spectrum was carried out to identify the functional groups of the dye. From the cyclic-voltammetry analysis the information about the reversibility of electron transfer process is obtained. Cathodic and anodic redox potentials were used to determine the HOMO (Highest Occupied Molecular Orbital) -LUMO (Lowest Unoccupied Molecular Orbital) values. The cyclic voltammetry of the dye was taken using Ag/AgCl as reference electrode, Glassy carbon as working electrode and Pt as counter electrode with the scan rate of 100 mVs^{-1} at room temperature. From the UV-Visible NIR spectrum, the absorption maximum was analyzed and the molar extinction coefficients were calculated using the maximum absorption value. Fluorescence spectrum was carried out at 430 nm excitation wavelength to find out the emission behavior of the SKS dye. The TG-DTA analysis revealed the melting and decomposition point of the synthesized dye. Solar cell was made using TiO_2 (P-25) as photoanode, synthesized Oligoene SKS dye as sensitizer, I^-/I_3^- as electrolyte and Platinum as counter electrode**.** The overall power conversion efficiency of SKS dye based solar cell was 1.76 % and the photovoltaic parameters are V_{oc} – 0.67 V, J_{sc} - 4.63 mA/m^2 and FF – 56. The photo stability of SKS dye was analyzed before and after various light irradiation by UV-Vis NIR absorption spectrum.

****

PP-30

Temperature dependent dielectric study of Graphene-Chitosan-Cotton Green Fabrics

Swathi Somanathan[1], Radha Perumal Ramasamy[1*], Vinod K. Aswal[2] and Miriam H. Rafailovich[3]

[1 -] Department of Applied Science and Technology, ACT campus, Anna University, Chennai - 600 025, India.
[2 -] Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai - 400085, India
[3-] Department of Materials Science and Engineering, Stony Brook University, NewYork–11794 2275, USA.
***Email:** perumal.ramasamy@gmail.com*

Creation of light weight, conducting and environmentally friendly materials are necessary. In this research temperature dependent dielectric characteristic of graphene-chitosan-cotton fabrics

are reported. SEM analysis showed that the pores in the cotton fabric are reduced by incorporation of graphene in the fabric. Raman analysis showed that as graphene concentration increased the defects induced in the graphene due to drying. The dielectric constant increased as the graphene concentration increased resulting in high dielectric constant materials for high concentrations of graphene. Shift in relaxation peaks as the graphene concentrations changed. The conductivity of the fabrics were influenced by frequency, temperature and concentration of graphene. The activation energy was influenced by graphene concentration and water content (annealed and not annealed). The activation energy was lowest for fabrics containing 30% graphene. Water present in the samples was found to affect the dielectric characteristics and the conductivity of the fabrics. These environment friendly green fabrics can have potential applications in batteries and electronics.

***Keywords*:** Biopolymer, Dielectric Relaxation, chitosan, cotton, graphene.

****

PP-31

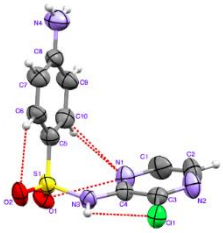
Structural, Hirshfeld surface studies and computation of interaction energies of a compound 4-Amino-N– (3-Chloropyrazin-2-yl)benzene- 1-Sulfonamide.

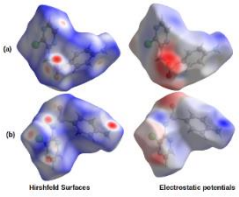
D P Ganesha,[a] N R Sreenatha, [ab] B N Lakshminarayana, [a*]

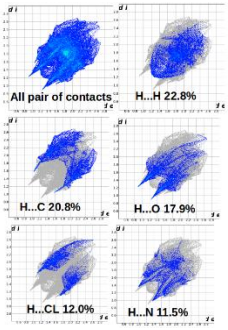
C R Gnanendra [c] and S Madan Kumar [d]

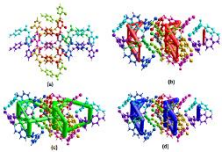
[a]Department of Engineering Physics, Adichunchanagiri Institute of Technology, Jyothinagara, Chikkamagaluru - 577102, Karnataka, ., India,
[b]Department of Physics, Government Engineering College, Dairy Circle, Hassan - 573 201, Karnataka, ., India,
[c]Department of Engineering Chemistry, Adichunchanagiri Institute of Technology, Jyothinagara, Chikkamagaluru - 577102, Karnataka, ., India, and
[d]IOE, Vijnana Bhavana, University of Mysore, Mysore - 570006, Karnataka, India
***Email:** bnlphysics@gmail.com*

The single-crystal X-ray diffraction study of the compound 4-Amino-N-(3-chloropyrazin-2-yl)benzene-1-sulfonamide showed that, it was crystallized into a orthorhombic crystal system with the space group of Pbca having the precise unit- cell parameters of a=11.5260 (19) Å, b= 9.6270 (16) Å, c=22.099 (5) Å, Z=8 and V=2452.1 (8) Å 3 . After subsequent cycles of refinement, finally the structure was converged to the Good-ness of Fit (S) = 1.33. The nitrogen atom (N) of a pyrazine ring have exhibited trifurcated intra-molecular relations through C—H···N, N···C and N···O incorporating S(5), S(6) and S(7) ring motifs respectively to the structure. The inter and intra-molecular interactions were analyzed and their percentage of contribution towards crystal packing was computed by using Hirshfeld surface analysis. Apart from these, interaction energies between the pairs of molecules were obtained using the energy model of B3LYP/6–31 G(d,p), analyzed and visualized.









Parameters	Values
CCDC	1945988
Chemical formula and Formula weight	$C_{10}H_9ClN_4O_2S$ and 284.72
Temperature (K) & Wavelength (Å)	293 & 0.71073
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions (Å,)	a=11.5260(19), b=9.6270 (16), c= 22.099 (5), α=β=γ=90
Cell volume (Å 3) and Cell formula units Z	2452.2 (8) and 8
Calculated Density (Mg/m) and F (000)	1.543 and 1168
Crystal size (mm)	0.34 × 0.30 × 0.27
Theta range for data collection (˚)	1.8, 27.8
Limiting indices	h=-15→15, k=-12→12, l=-29→29
No. of measured, independent and observed [I > 2σ(I)] reflections	15483, 2902, 2900
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1278 / 0 / 163
R Value and Goodness of Fit on F^2	0.083 and 1.24
Largest diff. peak and hole (e. $Å^3$)	0.29, -0.43

References:

1. G. G. Dubinina, M. O. Platanov and S. M. Golovach et. al, Eur. J. Med. Chem. 41, 727-737 (2006).
2. L. E. Seitz, W. J. Suling and R. C. Reynolds, J. Med. Chem. 45, 5604-5606 (2002).
3. C. Jr. Temple, J. D. Rose and J. A. Motgomery, J. Med. Chem. 13, 1234-1235 (1970).
4. X. H. Du and D. J. Gustin et. al, Bioorg. Med. Chem. Lett., 19, 5200-5204 (2009).
5. M. Yu. Shchelkanov and V. A. Shibnev et. al. Vopr. Virusol 59(2), 37-40 (2014).
6. M. U Anwar, A. Al-Harrasi, et. al, Dalton Trans. 47, 2511-2521 (2018).
7. A. Coskun, M. Banaszak, et. al, Chem . Soc. Rev., 41, 19-30 (2012).
8. M. T. Albelda J. C., Frias et. al., Chem. Soc. Rev. 41, 3859-3877 (2012).
9. APEX2 Bruker, SAINT-Plus and SADABS, Bruker AXS Inc., Wisconsin, Madison, USA, (2004).

10. G. M. Sheldrick, Acta Cryst. A64, 112–122 (2008)
11. A. L. Spek, Acta Cryst. D65, 148–155 (2009)
12. C. F. Macrae, I. J. Bruno and J. A. Chisholm et. al. J. Appl. Cryst. 41, 466 (2008).
13. S. K. Wolff, D.J. Grimwood, J.J. McKinnon, M.J. Turner, D. Jayatilaka, M.A. Spackman, CrystalExplorer
14. (Version 3.1), University of Western Australia, (2012)
15. J.J. McKinnon , M.A. Spackman , A.S. Mitchell , Acta Cryst. B60 (2004) 627–668 .
16. T. Srinivasan, V. Kalpana, P. Rajakumar and D. Velmurugan Acta Cryst. E69, o611, (2013)

****

PP-32

Linear magnetoresistance in $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ topological insulator single crystals

Gopi G and *Anandha Babu G

Department of Physics, SSN College of Engineering, Kalavakkam- 603110, Tamilnadu, India
Email: *gopig@ssn.edu.in; *anandhababug@ssn.edu.in*

We report synthesis, structural details and magneto-transport properties of $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ topological insulator single crystal. Single crystalline samples of $Bi_{1.5}Sb_{0.5}Te_{1.7}Se_{1.3}$ are obtained from high temperature (1123 K) melt growth. Single crystals of the above said samples are crushed into fine powders and subjected to powder X-ray diffraction analysis. The crystals belong to the rhombohedral cell with $R\bar{3}m$ space group. Electrical resistivity shows a metallic trend for both 0 and 15 T with a fluctuation at temperature region 50 -150 K. Hall measurements evince non-linear carrier concentration of n = 5.5×10^{17} cm^{-3} at 3 K. MR value increases at low temperatures due to the impurity band of the bulk carriers with MR reaching 23% at 4.2 K and 15 T.

****

PP-33

Spin-glass behavoiur in nanocrystalline $ZnFe_2O_4$ spinel ferrite

S.Thilagavathi, Praveen Shanker N and C.Venkateswaran*

Department of Nuclear Physics, University of Madras, Guindy campus, Chennai-600 025, India.
Department of Science and Humanities, M.Kumarasamy College of Engineering, Karur, Tamil Nadu- 639113, India.
__Email:__ cvunom@hotmail.com

The spinel zinc ferrite ($ZnFe_2O_4$) nanocrystalline material was synthesized by using high energy ball milling method. The samples were investigated for their structural and magnetic characterizations. X-ray diffraction study confirmed the well formation of $ZnFe_2O_4$ spinel ferrite crystal structure with space group fd-3m. The surface morphology of the sample was studied with

Scanning Electron Microscope (SEM). The valence state and the chemical composition of the $ZnFe_2O_4$ prepared sample, Zn 2p, Fe 2p and O 1s core level spectra were determined by using X-ray photoelectron spectroscopy (XPS). The XPS result proved the existence of Fe in double oxidation state of +2 and +3 at the tetrahedral and octahedral sites respectively. Magnetization measurements were carried out using a vibrating sample magnetometer at room temperature. Room temperature MH curve shows the ferrimagnetic nature of the sample arising from the various oxidation state of Fe ions. Low temperature VSM (showed in Figure 1) studies gives the information of transition from ferri to anti-ferro magnetic behavior and it shows the spin glass transition of $ZnFe_2O_4$ prepared sample at temperature around 290 K.

***Keywords*:** Spinel ferrites, High energy ball milling, Spin-glass transition

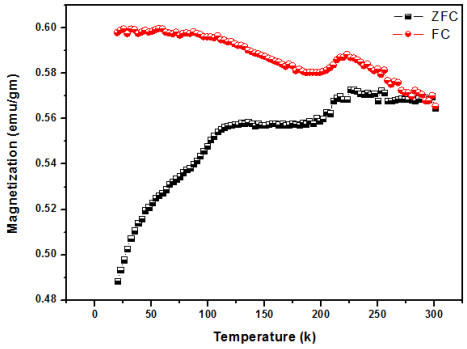


Figure 1: FC and ZFC magnetization of the $ZnFe_2O_4$ ferrite at H=1000 Oe.

****

PP-34

Geometrical Parameters, Atomic charges and electrostatic properties of dodecahydro-2H,2'H-2,2'-bi(cyclopenta) [b] thiphene by AIM Theory

S. Palanisamy[a], P. Srinivasan[b] and K. Selvaraju[a]*

[a]Department of Physics, Kandaswami Kandar's College, Velur-638182, Namakkal (Dt) India
[b]Department of Physics, Chikkaiah Naicker College, Erode-638004, Erode (Dt), India
***Email:** physicsselvaraj@gmail.com*

The effect of Au metal electrodes and the electric field in the insulating molecule entire computational work has been carried out with density functional theory coupled with Bader's AIM theory. A combination of B3LYP hybrid functions have been used for the whole calculation with LANL2DZ basis set while using G09 package. The characteristic of the geometrical parameters (bond length, bond angle and torsion angle), electrostatic and transport properties of the terminal Au-S and S-C bonds as well as all bonds have been analyzed. The variation of MPA and NPA atomic charges have been compared for various applied electric fields. The spatial redistribution of the molecular orbital for the zero and the maximum applied electric fields for dodecahydro-2H,2'H-2,2'-bi(cyclopenta) [b] thiphene molecule of HOMO-LUMO gap and these values are almost equal to the Density of states spectrum. The HLG from zero bias 2.313 eV, as the field increases the gap rapidly decreases from 0.218 eV. This small HLG exists in the molecular system; there is no delocalization of molecular orbital. Hence, the electrical conductivity is found to be

very less. The applied electric field polarizes the molecule, in consequence of that the dipole moment of the molecule increases from 3.56 to 7.32 Debye. The small increase of dipole moment shows that the molecule exhibits smaller conductivity.

***Keywords*:** Metal electrodes, MPA, NPA, HLG

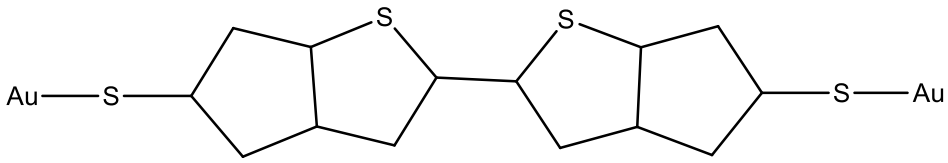


Figure: shows the Au and thiol substituted dodecahydro-2H,2'H-2,2'-bi(cyclopenta) [b] thiphene

****

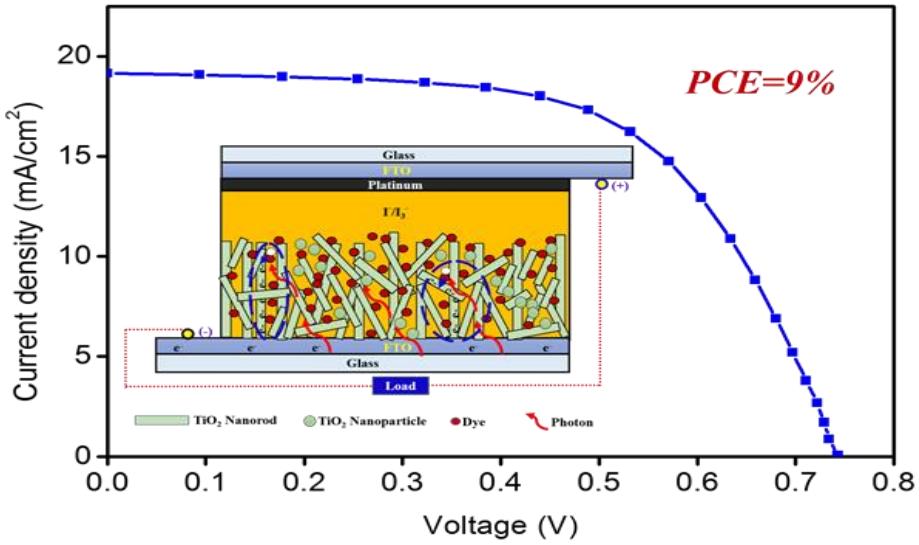
PP-35

Fabrication of Stable DSSC Using Hydrothermally Synthesized TiO_2 Nanostructures based photoanode

R. Govindaraj* and P. Ramasamy

SSN Research Centre, Department of Physics, SSN College of Engineering, Kalavakkam, Chennai, India
***Email:** govindarajr@ssn.edu.in*

In recent years, the nanocrystalline based dye-sensitized solar cells (DSSCs) have received much attention owing to their low-cost and high-power conversion efficiency (PCE). In the traditional fabrication process, nanocrystalline-TiO_2 nanoparticles have been widely used as the scaffold layer to support the dye molecules. One-dimensional (1D) nanomaterials have shown a significant advantage for the energy conversion applications. Aligned 1D nanostructures have been studied to improve electron transport properties in DSSC. However, such aligned 1D structure suffers from inefficient dye loading due to the lower surface area than traditional 20 nm size nanoparticles [1-6]. Therefore, a careful synthesis strategy is needed to synthesize TiO_2 materials, which is still a challenging task. In this approach, a novel TiO_2 nanorods/nanoparticles (NRs/NPs) were prepared via different hydrothermal conditions.



The crystallographic information of the prepared materials was confirmed by powder X-ray diffraction, which shows larger fraction of crystalline anatase phase of TiO_2. From the electron microscopy analysis, the formation of NRs/NPs is clearly found. Several solar cells have been fabricated and their performances were evaluated under illumination of 100 mW/cm^2. The high power conversion efficiency of 9 % has been achieved with NRs/NPs employed device.

References

1. B. O'Regan and M. Graetzel, Nature, 353 (1991), 737
2. K. Kakiage, Y. Aoyama, T. Yano, K. Oya, J-i Fujisawa and M. Hanaya, Chemical Communications, 51 (2015), 15894
3. S. K. Park and Y. S. Han, Solar Energy, 110 (2014), 260
4. Y. M. Liu, M. L. Zhang, Y. Jiang, Y. Xia, W. W. Sun and X. Z. Zhao, Electrochimica Acta, 173 (2015), 483
5. J. Lin, Y.-U. Heo, A. Nattestad, Z. Sun, L. Wang, J. H. Kim and S. X. Dou, Scientific Reports, 4 (2014), 5769
6. C. Xiang, C. A. Okonkwo, Q. Xiong, L. Wang, L. Jia, Solar Energy, 134 (2016), 461

****

PP-36

Growth and Characterization of 4-Aminopyridinium 4-Nitrophenolate 4-Nitrophenol (4AP4N) Single Crystal for Nonlinear Optical (NLO) Applications

T. Kamalesh[1 (a)], P. Karuppasamy[1], Muthu Senthil Pandian[1], P. Ramasamy[1], Sunil Verma[2, 3], A. K. Karnal[2, 3]

[1]SSN Research Centre, SSN College of Engineering, Chennai-603110, Tamil Nadu, India
[2]Laser Materials Development and Devices Division, RRCAT, Indore-452013, Madhya Pradesh
[3]Homi Bhabha National Institute (HBNA), Anushakti Nagar, Mumbai-400094, Maharashtra
[(a)]Email: *kamaleshkamal918@gmail.com;*

The good quality and bulk size organic nonlinear optical 4-aminopyridinium 4-nitrophenolate 4-nitrophenol (4AP4N) single crystals were grown by slow evaporation solution technique (SEST) using methanol as a solvent. The lattice parameters of the grown crystal were analyzed by single crystal X-ray diffraction (SXRD) analysis. The optical quality of the grown crystal was analyzed by UV-Vis NIR spectral analysis. The photoconductivity studies revealed that the 4AP4N crystal has negative photoconductivity nature. The laser damage threshold (LDT) was studied for the 4AP4N crystal by using Nd: YAG laser (532 nm). The second harmonic generation (SHG) efficiency of 4AP4N crystal was studied by Kurtz-Perry powder technique.

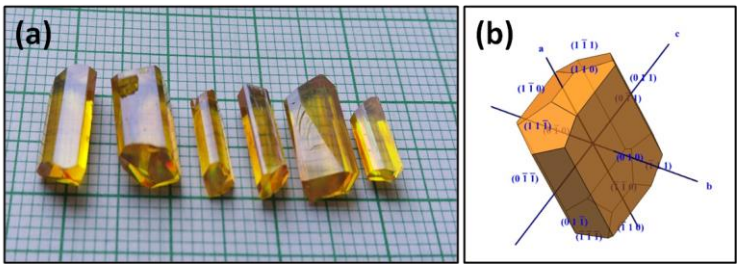


Figure 1. (a) As grown 4AP4N crystals and (b) its morphology

****

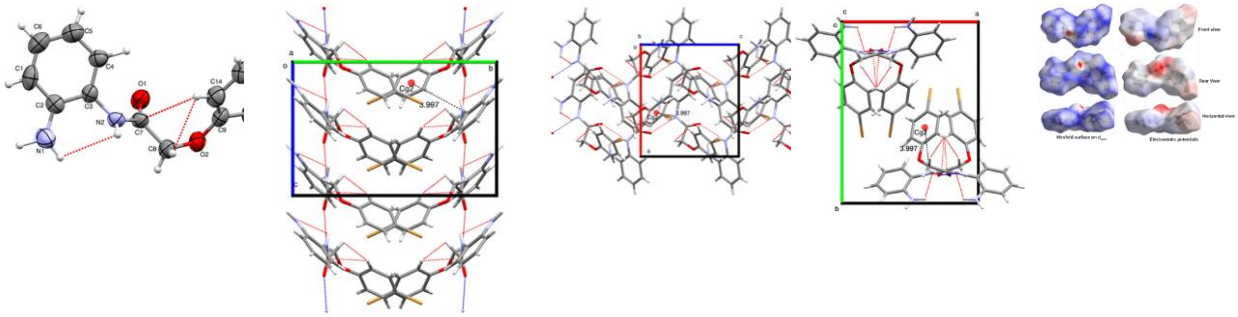
PP-37

Structure and Hirshfeld computation study of N-(2-Aminophenyl)-2-(4-bromophenoxy)acetamide

S. N. Chandana [a], Fares Hezam Al-Ostoot [b,c], Yasser Hussein Eissa Mohammed [d], Tareq N.AlRamadneh [e], Shaukath Ara Khanum [b], N. R. Sreenatha [a], P. Kumaradhas [f] and B.N. Lakshminarayana [a,*]

[a]Department of Engineering Physics, Adichunchanagiri Institute of Technology, Jyothinagara, Chikkamagaluru - 577 102, Karnataka, India
[b]Department of Chemistry, Yuvaraja's College, University of Mysore, Mysuru, India
[c]Department of Biochemistry, Faculty of Education & Science, Al-Baydha University, Yemen.
[d] Department of Biochemistry, Faculty of Applied Science, University of Hajjah, Yemen
[e] Department of Basic Science, Biology Unit, Deanship of Preparatory Year and Supporting studies, Imam Abdulrahman Bin Faisal University, P. O. Box 1982, Dammam 34212, Saudi Arabia
[f] Department of Physics, Periyar University, Salem, Tamil Nadu, India
***Email:** bnlphysics@gmail.com*

The XRD results showed that the title compound N-(2-aminophenyl)-2-(4bromophenoxy) acetamide was crystallized into an orthorhombic crystal system with the space group of $Pca2_1$ having the precise unit- cell parameters of a=10.426(3)Å, b= 13.904(4) Å, c= 9.123(2)Å, Z=4 and V= 1322.5(6) $Å^3$. The structure was solved by direct method and refined by full matrix least square method based on F^2 and reduced to R=1.04. In the crystal, molecules are inter-connected via N-H. . . O interactions and exhibited independent one-dimensional polymeric chain propagating infinitely along crystallographic a & b axes while layer stack of molecular units along c axis. The structure also exhibits C-N. . . Cg interactions. The intermolecular interactions were computed by Hirshfeld surface analysis. It showed that the H. . . H and H. . . C interactions taken the major role towards crystal packing.



Parameters	Values
CCDC	1956950
Chemical formula and Formula weight	$C_{14}H_{13}BrN_2O_2$ and 321.17
Temperature (K) & Wavelength (Å)	296 & 0.7107Å
Crystal system, space group	Orthorhombic,P $ca2_1$
Unit cell dimensions (Å, °)	*a*=10.426(3), b=13.904(4), c=9.123(2)

Cell volume (Å ^{3}) and Cell formula units Z	1322.5(6), 4
F (000)	648
Crystal size (mm)	0.22x0.17x0.10
Theta range for data collection (°)	2.4 to 28.3
Limiting indices	h=-13→13 k=-18→17 l=-8→12
No. of measured, independent and observed [I > 2σ(I)] reflections	11923 & 2048
Refinement method	Full matrix -least squares on F^2
Data / restraints / parameters	2871/1/224
R Value and Goodness of Fit on F^2	0.034 and 1.03
Δρ max , Δρ min eÅ $^{-3}$	0.26, -0.26

***References*:**

[1] G. Sharma, S. Anthal, D. V. Geetha, F. H. Al-Ostoot, Y. Hussein Eissa Mohammed, S. Ara Khanum, M. A. Sridhar, and R. Kant. Synthesis, structure and molecular docking analysis of an anticancer drug of n-(2-aminophenyl)-2-(2-isopropylphenoxy) acetamide. Molecular Crystals and Liquid Crystals, 675(1):85–95, 2018.

[2] Y. H. Mohammed, V. H. Malojirao, P. Thirusangu, M. Al-Ghorbani, B. T. Prabhakar, and S. A. Khanum. The novel 4-phenyl-2-phenoxyacetamide thiazoles modulates the tumor hypoxia leading tothe crackdown of neoangiogenesis and evoking the cell death. European journal of medicinal chemistry, 1(143):1826–1839, 2018.

[3] J. Lee, J. S. Shim, S. A. Jung, S. T. Lee, and H. J. Kwon. N-hydroxy-2-(naphthalene-2-ylsulfanyl)-acetamide, a novel hydroxamic acid-based inhibitor of aminopeptidase n and its anti-angiogenic activity. Bioorganic & medicinal chemistry letters, 15(1):181–183, 2005.

[4] A. Caruso, S. Marzocco, B. Nicolaus, C. Palladino, A. Pinto, A. Popolo, M. S. Sinicropi, G. Tommonaro, and C. Saturnino. Acetamide derivatives with antioxidant activity and potential anti-inflammatory activity. Molecules, 15(3):2028–2038, 2010.

[5] G. M Sheldrick. Acta Cryst, A64(2):112–122, 2008.

[6] A. L Spek. Acta Cryst, D65(2):148–155, 2009.

[7]M. A Spackman and J. J McKinnon. Cryst. Eng. Commun., 4:378–392, 2002.

****

PP-38

Growth and characterization of 4-Nitrobenzaldehyde – Phenylhydrazone Single Crystal

R. Gnanadeepam[a] and A. Senthil [a*]

[a]Department of physics, SRM Institute of Science and technology, Ramapuram Campus, Chennai-600089, India
***Email:** tasenthil@gmai.com*

4-Nitrobenzaldehyde – Phenylhydrazone single crystal was grown by slow evaporation solution growth method. The title compound synthesized using 4-Nitrobenzaldehyde and Phenylhydrazine HCl in the ratio of 1: 1 and dissolved in ethanol. The saturated solution was allowed for slow evaporation at room temperature. After the period of 15 days needle shaped crystal was obtained. The single crystal X-ray diffraction study reveals that 4NBP crystal belongs to the Tetragonal crystal system with space group P. The calculated cell parameter values are a=7.72 Å, b=17.47 Å, c= 17.49 Å, α = 89.89 º , β = 89.64 º, γ =89.93 º , V=2360 Å$^{3.}$ The SHG output for 4NBP for KDP and urea samples were found to be 80 mV and 270 mV, respectively.

***Keywords*:** Single crystal, solution growth, XRD, SHG.

****

PP-39

Growth of 1, 3, 5-Triphenylbenzene Single-crystal by modified Vertical Bridgman method and its Characterization for optical and Scintillation application

M. Manikandan, P. Rajesh*, P. Ramasamy

Centre for Crystal Growth, Department of Physics, SSN College of Engineering, Kalavakkam, Tamilnadu - 603 110.
***Email:** mani.3m333@gmail.com; rajeshp@ssn.edu.in**
***Mobile:** +91-8144333843, +91-9445434893**

The organic crystals play a crucial role in different potential applications such as frequency generation, optical fiber communication, and scintillation application. The 1, 3, 5-triphenylbenzene (TPB) single crystal successfully grown for the first time (length of 100 mm and diameter 10 of mm) by the modified vertical Bridgman technique (VBT). Physical, optical and scintillation properties such as crystalline nature, thermal stability, transmittance, radioluminescence and lifetime were investigated. Single crystal X-ray diffraction confirms that the grown crystal belongs to the orthorhombic structure with non-centrosymmetric space group $Pna2_1$. The crystallinity of the grown crystal was estimated by powder X-ray diffraction studies. The polished TPB sample has good transmission in the wavelength range between 300-1500 nm. Measurements of refractive index at five different wavelengths in the range between 407 to 1551 nm were carried out and birefringence properties of TPB crystal were analyzed using the prism coupling method. Birefringence study reveals that the grown crystal has good optical homogeneity.

Scintillation properties such as radioluminescence light yield using Sr-90 as a source and decay time were also investigated. Third-order nonlinear optical properties and related parameters were determined using the Z-scan technique. The TPB crystal proves its suitability for the optical, scintillation applications and optoelectronic device fabrications.

****

PP-40

Structure Assembly and The Biological Behaviour of 2-Amino-4, 6-Dimethyl Pyrimidine with Gallic Acid and Pimelic Acid

R.Mekala[a], R.Mathammal[b*]

[a] Sona College of Technology (Autonomous), Salem-636 005, Tamilnadu, India.
[b]Sri Sarada College for Women (Autonomous), Salem-636 016, Tamilnadu, India.

Reaction of 2-amino-4, 6- dimethyl pyrimidine with carboxylic acid such as gallic acid and pimelic acid, yielded a salt and co-crystal, respectively. The new crystal forms were obtained from slow evaporation technique. The crystal structure and hydrogen bond interaction of the two crystals were determined by single X-ray diffraction analysis. Inter molecular interactions of the compounds were investigated using the 3D Hirshfeld surfaces and the associated 2D fingerprint plots. The functional groups were identified by the FTIR and FT-Raman spectral studies. The presence of carbon and hydrogen in the two samples were identified by the ^{1}H and ^{13}C NMR analysis. The excited energy was observed using UV-Visible spectral analysis. The fluorescence spectra revealed the emission state of the two samples. The thermal behaviour and stability of the two compounds were evaluated by the TGA-DSC analysis. The enhanced pharmacological behaviour was studied by the anti-oxidant, anti-microbial and anti-cancer activities.

****

PP-41

Growth and characterization studies of L-cysteine hydrochloride monohydrate single crystal for Nonlinear Optical applications

Sudha Yadav[1,2*], Mukesh Jewariya[2], Girija Moona[2], N. Vijayan[2] , Manju Kumari[1,2], Debabrata Nayak[1,2] and Rina Sharma[2]

[1] Academy of Science and Innovative Research, New Delhi-110012, India
[2] CSIR-National Physical Laboratory, Dr. K.S. Krishnan Marg, New Delhi-110012, India
***Email:** sudhayadav1435@gmail.com*

Recent days, nonlinear optical materials are getting attention because of its potential applications in the area of lasers, optical sensing and terahertz etc. A good quality organic nonlinear optical single crystal of L-cysteine hydrochloride monohydrate (LCHCL) was grown by slow evaporation solution technique (SEST) using deionized water as a solvent. The above said single crystal was grown with the time span of 25 days and the grown single crystal was analyzed by different characterization techniques. Powder X-ray diffraction (PXRD) was carried out to estimate the lattice parameters and the structural information of LCHCL. It was found that the

grown crystal is non-centrosymmetric and belongs to orthorhombic crystal system having space group of $P2_12_12_1$. The different functional groups and vibrational bonds were identified using Fourier transform Infrared (FTIR) and Raman spectroscopic studies. To study the optical properties UV-Vis transmission spectrum was recorded. It was observed that the single crystal have a high value of transmission over a long range of wavelength. The obtained results of these investigations will be presented in detail.

****

PP-42

Study on Third Order Nonlinear behaviour of Bulk Iminodiacetic acid Single crystal for Optical limiting Application

Debabrata Nayak[1, 2*], N. Vijayan[1, 2], Manju Kumari[1, 2], R.P. Pant[1, 2]

[1] Academy of Scientific and Innovative Research CSIR – National Physical Laboratory, New Delhi – 110012, India

[2] CSIR – National Physical Laboratory, Dr. K.S. Krishnan Road, New Delhi – 110012, India

***Email:** debabratanayak254@gmail.com*

The single crystalline materials are having enormous applications in the field of photonics, optical limiting, self-focusing and self-defocusing device growth of nonlinear optical (NLO) crystals has been the core interest for the researchers community. Presence of conjugate π-electrons, Van-der waal and hydrogen bonds in the organic molecules play an important role for the enhancement of NLO responses of the materials. A single crystal of Iminodiacetic acid (IMDA) with dimensions 47mm×9mm×6mm was grown using slow evaporation solution growth technique (SEST) to study its third order nonlinearity using a femto second laser as a source. The structural confirmation of the ingot has been carried out through single crystal XRD and powder XRD. The crystalline perfection was assessed by high resolution X-ray diffraction and it has been found the crystal possess interstitial type defects. The wide range of transmission and optical band gap of the titled compound has been examined by using UV-visible spectroscopy. The luminescence behavior of the grown ingot was assessed by photoluminescence measurement. The open and closed aperture Z-scan measurement has been carried out in order to determine the nonlinear absorption co-efficient (β) and nonlinear refractive index (n_2) respectively. The positive value of β and n_2 suggest that IMDA single crystal can be used in optical limiting devices. The results will be presented in detail.

***Keywords*:** X-ray analysis, Optical studies, Third Harmonic generation (THG)

****

PP-43

Studies on Synthesis, Growth and characterization of Nonlinear Optical Single Crystal: Sodium Acid Phthalate

Manju Kumari[1, 2 *], N.Vijayan[2], Debabrata Nayak[1, 2] and R.P.Pant[1, 2]

[1,2]Academy of Scientific and Innovative Research, CSIR – National Physical Laboratory, New Delhi 110012, India
[2]CSIR – National Physical Laboratory, Dr K.S. Krishnan Road, New Delhi 110012, India
***Email:** manjukumari1794@gmail.com*

In the last few decades, much progress has been made in development of nonlinear optical (NLO) materials which play an important role in optical and many industrial applications. A good quality and potential nonlinear optical material of sodium acid phthalate (NaAP) was synthesized and the single crystal was grown using slow evaporation solution growth technique (SEST) at controlled atmosphere. The phase identification and lattice dimensions were evaluated using powder X-ray diffraction (PXRD) analysis and data refined using Rietveld analysis. The crystalline perfection of the grown ingot was confirmed using the high resolution X-ray diffraction (HRXRD) study. The UV-Vis study reveals that harvested single crystal have wide range of transparency and there is no absorption in the entire visible region. The photoluminescence (PL), Time resolved PL (TRPL) studies were performed to know about the defects concentration and decay time of the transition respectively. The acquired results will be presented in detail.

***Keywords*:** Nonlinear optics, NaAP, SEST, Photoluminescence, TRPL

****

PP-44

Structural, optical, thermal, and SHG studies on new organic NLO Co-crystal: 4-Pyridone succinic acid

M. Subha[2], K. Anitha[1*]

[1]School of Physics, Madurai Kamaraj University, Madurai-625021.
[2]Arulmigu Palaniandavar College of Arts and Culture, Palani
***Email:** singlecrystalxrd@gmail.com*

The molecular adduct of 4-pyridone succinic acid (4PSU) co-crystal is synthesized by slow evaporation solution growth technique at room temperature and good quality three dimensional single crystals of 4PSU are obtained. The complex formation of 4PSU single crystal is primarily confirmed by the density of the grown crystal by floatation method. The molecular structure of the grown crystal is found by single crystal X-ray diffraction analysis that elucidates the non-centro symmetric nature of the crystal and the space group as $Pna2_1$. The cut-off wavelength and the energy band gap values are found to be 338 nm and 4.4 ev respectively. The UV-Vis NIR spectrum analysis reveals that the grown crystal is more suitable for the optoelectronic applications. The SHG efficiency suggests that the 4PSU will be a promising material for the NLO applications. The thermal studies confirm the melting and decomposing point of the grown crystal and it infers that

the grown crystal melts at 257˚C. Thus it is highly recommended its usage for high-temperature applications. Hirshfeld surface analysis of 4PSU crystal expresses all the interactions. From the Hirshfeld analysis of 4PSU, it is concluded that the O···H is more prominent interaction and it is good acknowledgement for the crystal packing stabilization of 4PSU.

****

PP-45

Recovering Resources from the End-of-Life PV Modules

Nagarajan S G, Srinivasan M, and Ramasamy P[a)]

SSN Research Centre, SSN College of Engineering, Chennai
[a)]Email: *ramasamyp@ssn.edu.in*

The market of the PV (Photo-voltaic) industries has continuously increased due to its application in clean energy generation. Due to shortage of fossil fuels the PV modules get more attention and the Indian government funding on solar electricity has also increased incessantly. The country's solar installed capacity reached 30 GW as of 2019. India expects to install about 100 GW by 2022. Normally the life time of the PV modules is 20-25 years, hence more wastes will be generated in coming decades, so we need an optimal way to handle this End-of-Life PV modules. The burying of PV modules under the ground causes many environmental hazards because the PV modules contain risky components, so it causes serious illness to human because of their toxicity. Along with this the disposal of huge PV modules makes considerable economical needs. Therefore, the waste PV modules should be recycled for environment and economic benefits. To recycle the end-of-life PV module, the parts of the module (glass, back-sheet, silicon solar cell, electrodes) should be separated by proper thermal or chemical methods. Here we have carried out thermal pyrolysis process for part separation by which the silicon solar cell would be separated from the module. We have carried out chemical etching process to get the refined silicon wafers from the recovered silicon solar cells. The purity and quality of the reclaimed wafers sere ensured by EDS and minority carrier life-time measurement. The broken reclaimed wafers can be used as feedstock material for growing multi-crystalline silicon ingots and the unbroken wafers can be used for making solar cells with better efficiency.

****

PP-46

GROWTH AND CHARACTERIZATION OF PURE AND CERIUM DOPED KDP CRYSTALS GROWN BY GEL MEDIUM

Vinu Barathi.M and T.Asaithambi

P.G.& Research Department of Physics, Alagappa Govt. Arts College, Karaikudi - 630003
Email: *tkthambi@gmail.com* ***Mobile No.:*** *9487112437*

Crystals are the unacknowledged pillars of modern technology. Without crystals, there would be no electronic industry, no photonic industry and no fiber optic communications. Crystals growth is an interdisciplinary subject covering physics, chemistry, material science, chemical engineering, metallurgy, crystallography, mineralogy, etc. in past few decades, there has been a grow in interest on crystal growth processes, particularly in view of the increasing demand of materials for technological applications. Optically good quality pure and metal doped KDP crystals have been grown by microbial free gel growth method at room temperature and their characterization have been studied. Gel method is a very simple method and can be utilized to synthesize crystals which are having low solubility. Potassium dihydrogen orthophosphate KH_2PO_4 (KDP) continues to be an interesting material both academically and industrially. KDP is a representative hydrogen bonded materials which possess very good electro optic and nonlinear optical properties in addition to interesting electrical properties. Due to this interesting properties, we made an attempt to grow pure and cerium doped KDP crystals in various concentration (0.002, 0.004, 0.006, 0.008and 0.010) using gel method. The grown crystals were collected after 20 days with good quality and shaped. The dc electrical conductivity (resistance, capacitance, and dielectric constant) values were measured at two different frequencies (100Kz and 1KHz) of pure and cerium added crystal with a temperature range of 50^{o} C to 130^{o} C using simple two probe setup with Q band digital LCR meter present on our lab. The electrical conductivity increases with increase of temperature. The dielectric constant of cerium doped KDP crystals were slightly decreased compared to pure KDP crystals. The optical band gap was calculated from the UV-visible spectra. The structural and crystalline size measurements were carried out using XRD spectral analyses. Magnetic susceptibility and SEM analyses also done. Results were discussed in detail.

****

PP-47

Enhancing the SHG effect of Zinc Chloride doped DAST single crystal: A new potential material for nonlinear optical device applications

Thirumuruganantham Sivakumar, Jeyaperumal Kalyana Sundar[*]
Materials Science Laboratory, Department of Physics, Periyar University, Salem, Tamil Nadu - 636011, India.
[*] ***Email:*** *jksundar50@gmail.com*

The ionic organic salts of (4-dimethylamino-N-methyl-4-stilbazoliumtosylate (DAST)) single crystal, hold the predominant place on potential organic non-linear crystal materials and electrooptic applications. In the present work, we have reported the synthesis and growth of $ZnCl_2$ doped DAST single crystal with different concentrations. The crystal grown by the slow

evaporation technique at room temperature. A structural and lattice constants of the grown crystal were determined the powder X-ray diffraction (PXRD), and furthermore confirm along with SXRD. Using FTIR studies were affirm to the presence of different vibrational modes of assignments and identify the presence of elements in the grown crystal by EDAX study. The linear optical properties are confirmed by UV-Vis absorption studies and, the calculated bandgap energies for pure 2.19 eV and dopants have 3.46, 3.41 and 3.36 eV for suitable materials for insulating and semiconductor. The SHG output received from the pure and doped DAST crystal with applied input laser energy is 1.1 mJ/pulse using by Kurtz Perry powder technique. The produced SHG efficiency for 0.01 mol ratio dopants have slightly less than the pure is 0.96, and 0.03, 0.05 mol, has 1.20 and 1.80 times greater than that of Zinc Chloride DAST. Hence the results reveal that the doped crystal are optoelectronic and terahertz applications.

***Keywords*:** Slow evaporation technique; Refractive index; SHG; Terahertz; DAST;

****

PP-48

Synthesis, growth and characterization of semi-organic single crystal: p-Toluidinium nitrate for nonlinear optical application

S. Suresh[a], C. Amirthakumar[a], B. Valarmathi[a] and R. Mohan Kumar [a*]

[a]Department of Physics, Presidency College, Chennai-600 005, India
***Email:** mohan66@hotmail.com*

Semi-organic nonlinear optical material: p-Toluidinium nitrate (PTN) was grown by slow solvent evaporation technique. Single XRD analysis reveals that the PTN crystal belongs to monoclinic system with space group $P2_1/c$. UV-Visible transmission spectral study reveals that the PTN crystal has good transmittance (72%) in the entire visible region and lower cut-off wavelength (299 nm). The dielectric constant (ε') and dielectric loss (tan δ) as a function of frequency were measured for the grown crystal. The third-order nonlinear optical parameters were estimated for grown crystal by Z-scan technique using 532 nm diode pumped CW Nd:YAG Laser.

Figure: Photograph of as grown p-Toluidinium nitrate crystal

****

PP-49

Effects of 2-amino-4,6-dimethoxypyrimidine *on* PVDF/KI/I_2 based solid polymer electrolytes for dye sensitized solar cell application

Kannadhasan Sundaramoorthy*, Senthil Pandian Muthu, and Ramasamy Perumalsamy

SSN Research Centre, SSN College of Engineering, Chennai-603110, Tamil Nadu, India
***Email:** skannadhasanssn@gmail.com*

In this work, we have investigated the effects of 2-amino-4,6-dimethoxypyrimidine on polyvinylidene fluoride/ potassium iodide/ iodine (PVDF/KI/I_2) in dye-sensitized solar cell (DSSC). Different weight ratios (0%, 10%, 20%, 30%, 40% and 50%) of 2-amino-4,6-dimethoxypyrimidine doped PVDF/KI/I_2 based solid polymer electrolytes (SPEs) were prepared by solution casting method. The prepared 2-amino-4,6-dimethoxypyrimidine doped PVDF/KI/I_2 based SPEs were characterized by the powder X-ray diffraction (PXRD) analysis, AC-impedance analysis and scanning electron microscopy (SEM) analysis. The crystallinity of 2-amino-4,6-dimethoxypyrimidine doped PVDF/KI/I_2 based SPEs was confirmed by PXRD measurement. The ionic conductivity of 2-amino-4,6-dimethoxypyrimidine doped PVDF/KI/I_2 based SPEs was calculated by using AC-impedance analysis. The ionic conductivity values of different weight ratios (0%, 10%, 20%, 30%, 40% and 50%) of 2-amino-4,6-dimethoxypyrimidine doped PVDF/KI/I_2 based SPEs are 5.50×10^{-6} Scm^{-1}, 1.74×10^{-5} Scm^{-1}, 4.91×10^{-5} Scm^{-1}, 2.04×10^{-5} Scm^{-1}, 1.58×10^{-5} Scm^{-1} and 1.04×10^{-5} Scm^{-1}, respectively. Ionic conductivity studies revealed that the 20% of 2-amino-4,6-dimethoxypyrimidine doped PVDF/KI/I_2 based SPE showed the highest ionic conductivity value. The SEM images showed the surface morphology of 2-amino-4,6-dimethoxypyrimidine doped PVDF/KI/I_2 based SPEs. The power conversion efficiency (PCE) of different weight ratios (0%, 10%, 20%, 30%, 40% and 50%) of 2-amino-4,6-dimethoxypyrimidine doped PVDF/KI/I_2 based SPEs used DSSCs are 1.4%, 2.0%, 2.5%, 2.3%, 1.9% and 1.6%, respectively. These results revealed that the 20% of 2-amino-4,6-dimethoxypyrimidine doped PVDF/KI/I_2 based SPE used DSSC exhibited the highest PCE.

***Keywords*:** Powder X-ray diffraction; Ionic conductivity; Solid polymer electrolyte; *2-amino-4,6-dimethoxypyrimidine*; Crystalline nature.

****

PP-50

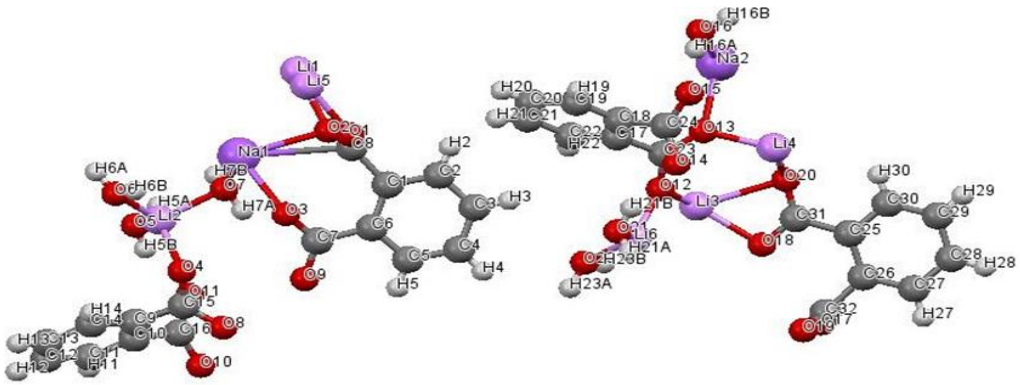
Crystal Growth and Optical Properties of Lithium Sodium Acid Phthalate (LiNaP) Single Crystal

Elavarasi[a], S. Mugundan[a*], C.Senthilkumar [b,*], M.Srinivasan[c]

[a]Department of Physics, Sri Vijay Vidyalaya College of Arts and Science, Dharmapuri-636807.
[b]Department of Physics, Government Arts and Science College, Hosur, Tamilnadu- 635110
[c]Department of Physics, SSN College of Engineering, Kalavakkam, India- 603 110
***Email:** mugugum@gmail.com*

Lithium sodium acid phthalate crystal was grown by slow evaporation method. Single-crystal X-ray diffraction shows that the grown crystal has a triclinic crystal structure. LiNaP has

three-dimensional network of O⋯⋯H---O hydrogen bonds. It has a positive coefficient solubility. The functional groups were identified by FTIR spectroscopy. The UV–Vis-IR absorption spectrum was analysed. The UV-VIS-NIR study was carried out from 200nm to 1100 nm.



****

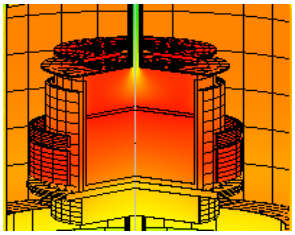
PP-51

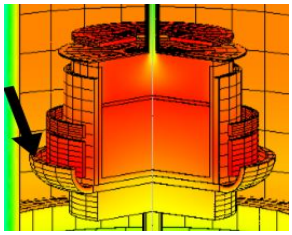
Modified Hot-Zone DS System to enhance the mc-Si ingot quality

Aravindan G*, Srinivasan M and Ramasamy P

SSN Research Center, SSN College of Engineering, Chennai.
**Email: aravindanvpt@gmail.com*

Silicon is the predominant material in PV markets and it has been second abundant material on earth. mc-Si solar cells occupy 60 % of PV markets. Most of the mc-Si wafers are produced by DS process, because of its relatively simple operating process, low purity feed stock material, mass production, lower wastage during the cell processing and low cost**.** During the DS process what happens inside the furnace is very complicated, numerical simulation is the best tool to answer the "what happens inside the furnace?". From the simulation we can save the money and time, we get information about the heat transfer characteristics inside the DS furnace during the solidification and cooling time. Multi-crystalline Silicon (mc-Si) ingot was grown by directional solidification (DS) process for photo voltaic (PV) application. Efficiency of mc-Si wafer is less than the mono-Si wafers but it has low cost, simple operating process and high mass production compared to mono-Si wafer production. During the mc-Si growth process stress and dislocation reduction is important because it will affect the conversion efficiency of mc-Si wafer solar cells.We have improved the mc-Si ingot quality by adding an additional layer at the hot-zone of DS furnace. We have simulated both modified and conventional DS process and compared the temperature distribution, growth rate and stress distribution of both systems. The modified DS system significantly increases the mc-Si ingot quality compared to the conventional DS process grown mc-Si ingot. With the modified DS system, we have prevented the wall growth during the initial casting process. Fig. 1 shows the 3D hot-zone view of DS furnace, fig. 1A is conventional DS furnace and 1B is modified DS furnace.





A

Figure: 1 3D hot-zone view of DS furnace. A is conventional and B is modified.

****

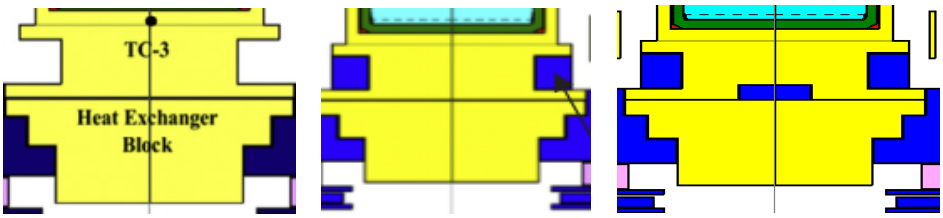
PP-52

Optimization of thermal properties by using different heat exchanger blocks in directional solidification furnace and experimental verification

Kesavan V*, Nagarajan S.G, Srinivasan M and Ramasamy P

SSN Research Center, SSN College of Engineering, Chennai.
***Email:** ectamilkesavan@gmail.com*

Directional solidification (DS) process is the main process for producing the multi-crystalline silicon ingots. This solidification process needs some efforts to reduce the dislocation and von Mises stress. It is economically beneficial to grow the good quality mc-Si ingots with lower power consumption. Here we have carried out numerical simulation for analyzing the impact of using high or/and low density graphite blocks in different places in the Heat Exchanger Block (HEB) on the DS process. The result is experimentally compared and analyzed. The effect of different density graphite blocks on the von Mises stress, dislocation and temperature difference are analyzed. The simulation has been made for G1-DS (first generation DS process) without side block (D1); G1-DS without grooved-HEB (D2); G1-DS with grooved-HEB with groove filled with the lower density graphite (LDG) block (D3); G1-DS with grooved-HEB with side gap filled with the higher density graphite (HDG) block (D4); G1-DS with grooved-HEB with groove filled with the LDG and side gap filled with HDG (D5). It is concluded from the comparison results with using different density graphite blocks that the minimum von Mises stress can prevent the multiplication of dislocations and D5 gives good quality ingots. Some basic heat transfer properties are understood in the G1-DS furnace through the simulation results. Fig. 1 shows the high or/and low density graphite blocks used in different places in the HEB.



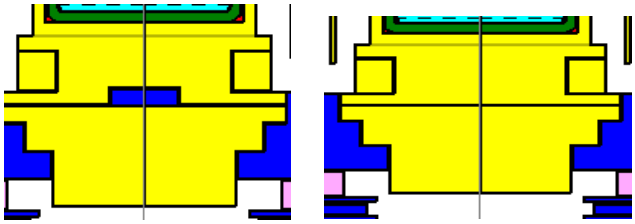


Figure 1: shows the different modifications of the Heat Exchanger Block (HEB).

****

PP-53

Studies on the synthesis and characterization of semiorganic Lithium bis(2-methyllactato) borate monohydrate crystal

G.Gokila and C.Ramachandra Raja*

Government Arts College (Autonomous), Kumbakonam 612002, Tamilnadu, India
***Email:** crrajaphy@gmail.com*

Semiorganic Lithium bis(2-methyllactato) borate monohydrate (LiMB) crystal was developed from solution growth solvent evaporation method. Powder X-ray diffraction pattern reveals the good crystalline nature of grow crystals through the observed sharp peaks. The lower cutoff wavelength is observed at 220 nm and the crystal is transparent upto 1100 nm. Vibrations of various functional groups present in the crystal structure is established through Fourier transform infrared and Fourier transform Raman spectral analyses. Molecular structure of LiMB crystal is confirmed through ^{1}H and ^{13}C Nuclear magnetic resonance spectroscopy. The intermolecular interactions present in the crystal structure is confirmed through the observed chemical shifts. The third order nonlinear susceptibility ($\chi 3$) is found to be 4.5517 X 10^{-5} esu and this is due to the presence of electron delocalization and intermolecular interaction present in the crystal structure. The self-defocussing and reverse saturable absorption behavior made LiMB crystal a potential candidate for Q-switching, optical pulse shorteners and optical energy limiters applications.

****

PP-54

Synthesis, Growth and Spectral characterization of halogen substituted Schiff base materials

S. Leela, Afrin Banu, U. Poomalai

Department of Physics, Ethiraj College for Women, Chennai – 08
***Email:** leelabeena@gmail.com*

Organic materials are increasingly being recognized as the “materials of the future” because their molecular environment combined with the versatility of synthetic chemistry can be used to alter and optimize their molecular structure in order to maximize their nonlinear optical

properties. The design and synthesis of organic molecules showing nonlinear optical properties have received tremendous interest recently due to their applications in areas like optical communication, optical computing, data storage, dynamic holography, harmonic generators, frequency mixing, optical switching and optical limiting. One of the organic materials is Schiff base derivative 5-bromo-4-methoxy salicylidene aniline were prepared by condensation reaction of p-methoxy aniline with 5-bromo-2-hydroxybenzaldehyde. The synthesized compound 5-bromo-4-methoxy salicylidene aniline was crystallized by ethyl acetate. The harvested crystal was 0.4mm*0.2mm*0.2mm by solvent evaporation method. The spectral properties revealed by FTIR and NMR techniques. Functional group of our compound was identified by FTIR spectrum. From NMR spectrum we observed the placement of the hydrogen atom of our compound. Absorbance of 5-bromo-4-methoxy salicylidene aniline compound observed by UV-VIS spectrum.

References:

1) Yonggang Yanga, Hongsheng Zhaia , Yang Liua , Xueli Jiaa , Yuanyuan Hea , Qianfei Maa , Kai Jiangb , Yufang Liua, Journal of Luminescence, 216, 116736 (2019)
2) Jiun-WeiHu, Hsing-YangTsai, Sin-KaiFang, Chia-WeiChang, Li-ChingWang, Kew-YuChen, Dyes and Pigments, 145, 493 (2013)

****

PP-55

Growth of sodium selenite doped Potassium Dihydrogen Phosphate single crystals by SR method and its Characterization

[1]K.Usha and [2]N.Joseph John

[1]Department of Physics, Sethupathy Government Arts College, Ramanathapuram, Tamilnadu-623502, India

[2]Department of Physics, Kamarajar Government Arts College, Surandai, Thenkasi District, Tamilnadu-627859, India
Email: *ushakk12486@gmail.com*

Single crystals of sodium selenite doped potassium dihdrogen phosphate (KDP) single crystals were grown by SR method, a novel solution growth technique gives unidirectional crystals with good quality from solution. The entire quantity of the solute was converted into crystal and thus achieving a solute–crystal conversion efficiency of 100%. Microbial contamination of the solution may also be controlled fairly from this method. The same crystals were grown by slow evaporation technique also. The grown samples were characterized by SXRD, PXRD, FTIR, UV and thermal. Dielectric studies were carried for the grown samples in two frequencies for various temperatures. Good crystalline perfections were found for the crystals grown by SR method. The details will be presented.

****

PP-56

Preparation and Characterization of Undoped and Samarium doped SnO_2 thin films by Spray Pyrolysis method

K.Radhidevi[a], G.Selvan[b], M.Karunakaran[c], K.Kasirajan[c], G.Rajeshkanna[d]

[a]Department of Physics, Sethupathy Govt. Arts College,Ramanathapuram-623502, India.
[b]Department of Physics ,Thanthai Hans Roever College, Perambalur-621220, India.
[c]Department of Physics, Alagappa Govt.Atrs College, Karaikudi-630003, India.
[d]Department of Electronics, Government Atrs College for Women, Ramanathapuram-623502, India.

The undoped and Samarium (Sm) doped tin oxide (SnO_2) thin films were successfully synthesized by nebulizer spray pyrolysis method. The prepared samples were characterized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) with EDAX, Photoluminescence (PL) and optical absorption (UV-Vis) studies. The XRD results showed that tetragonal structure for both pure and Sm doped thin films. From the SEM studies, the grains and voids are uniformly distributed and the particles are in tetragonal shape. Energy Dispersive spectroscopic analysis confirmed the presence of Sn, O and Sm elements. The optical spectra showed 80% transmittance for pure and Sm doped films and it was more suitable for fabrication of solar cells.

****

PP-57

Synthesis and Characterization of Undoped and Lanthanum doped SnO_2 thin films by Spray Pyrolysis method

K.Radhidevi[a], G.Selvan[b], M.Karunakaran[c],K.Kasirajan[c], G.Rajeshkanna[d]

[a]Department of Physics, Sethupathy Govt. Arts College, Ramanathapuram-623502, India.
[b]Department of Physics, Thanthai Hans Roever College, Perambalur-621220, India.
[c]Department of Physics, Alagappa Govt.Atrs College, Karaikudi-630003, India.
[d]Department of Electronics, Government Atrs College for Women, Ramanathapuram-623502, India.

The undoped and Lanthanum (La) doped tin oxide (SnO_2) thin films were successfully synthesized by nebulizer spray pyrolysis method. The prepared samples were characterized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) with EDAX, Photoluminescence (PL) and optical absorption (UV-Vis) studies. The XRD results showed that tetragonal structure with crystalline size found to be 35.8nm and 34.17nm for pure and La doped SnO2 thin films respectively. The films doped with La exhibit a change in the surface morphology. Energy Dispersive spectroscopic analysis confirmed the presence of Sn, O and La elements.

****

PP-58

VSM STUDIES ON SOME UNDOPED AND DOPED SINGLE CRSTALS

Ayarine G. Dhas[1] and N. Joseph John[2]

[1]Department of Physics, Government Arts College, Udhagamandalam – 643 002, The Nilgiris, Tamilnadu, India.
[2]Department of Physics, Kamarajar Government Arts College, Surandai – 627 859, Tenkasi District, Tamilnadu, India.
Email: *ayarine123@gmail.com*

Undoped and one mole% amino acids L-cystaine, L-asparagine, L-glutamic acid, L-leucine and L-methionine have been grown from aqueous solution by slow evaporation technique at room temperature. High quality transparent single crystals were harvested within fifteen days. The grown samples were characterized by SXRD, PXRD and FTIR. From single crystal XRD studies, the crystal structure and diffracting planes of the grown crystals have been identified. All the grown crystals of this work were found to crystallize in monoclinic structure. The unit cell parameters were found out using PXRD. Various functional groups such as NH_3^+, OH, C=O, C-N, SO_4^{2-}, PO_4^{3-} etc of the grown undoped and amino acids doped TGS crystals were identified from FTIR spectra. Since the concentration of l-asparagine, l-cysteine, l-glutamic acid, l-leucine and l-methionine dopants incorporated into TGS crystals are low, no characteristic absorption peaks due to the presence of dopants were noticed. VSM studies revels coercivity decreases with doping amino acid, L- asparagines, L- cysteine, L-glutamic acid, L- leucine and L-methionine. The details will be presented.

****

PP-59

Synthesis, crystal growth and characterization of an organic nonlinear Material: L- Alanine Mandelic acid single Crystal

V. Sudarvizhi, M. Sathish and T. Balakrishnan*

**Crystal Growth Laboratory, PG & Research Department of Physics, Periyar EVR College (Autonomous)*
Tiruchirappalli – 620 023, Tamil Nadu, India.
Email: *balacrystalgrowth@gmail.com*

An organic conjugated chromospheres L - Alanine Mandelic acid (LALM) single crystal was synthesized and successfully grown by slow evaporation technique at room temperature. The Lattice parameters were assessed from single crystal X-ray diffraction analysis. The single crystal X-ray diffraction study proclaimed that the LALMA crystal crystallized in monoclinic single and powder XRD confirmed the crystalline nature and the lattice parameters identified that the grown crystal. FTIR and FT-Raman spectral studies were carried out to confirm functional groups present in the crystal. Optical properties were analysed using UV-Vis-NIR spectrum. The optical band gap of the crystal was calculated, and it is 2.5 eV. The second harmonic generation (SHG) efficiency was measured by the Kurtz and Perry powder method. The SHG efficiency of LALMA is found to be 0.09 times greater that of KDP.

PP-60

Experimental Investigations on Bromoanilinium malonate

P. Yogheshwari[a], M. Tamil Elakkiya[a], S. Suresh Kumar[a], K. Anitha[a*]

[a] *School of Physics, Madurai Kamaraj University, Madurai-625021, Tamil Nadu, India.*
Email: *singlecrystalxrd@gmail.com*

Bromoanilinium Malonate (BAMAL) single crystals are grown by slow evaporation solution growth technique. The crystal structure is established with single crystal X-ray diffraction analysis. The present crystal belongs to monoclinic crystal system with $P2_1/c$ space group. In this structure one bromoanilinium cation is binded with three malonate anions via two two-centered and one three-centered N-H...O hydrogen bonds and thus forming a hanging bridge like structure running along b-axis. The UV-Visible absorption spectrum of the BAMAL compound shows an absorption peak at 265nm which contributes to $\pi \rightarrow \pi^*$ transition. The transmission spectrum of BAMAL shows about 90% transparency in the visible region with lower cutoff wavelength. Luminescence spectrum shows a peak at 387nm which indicates there is no defect in the crystal structure. Thermal properties of BAMAL are evaluated with thermogravimetric, differential thermal and differential scanning calorimetric analyses.

***Keywords*:** Single crystal, Slow evaporation technique, UV-Vis, PL, Thermal studies

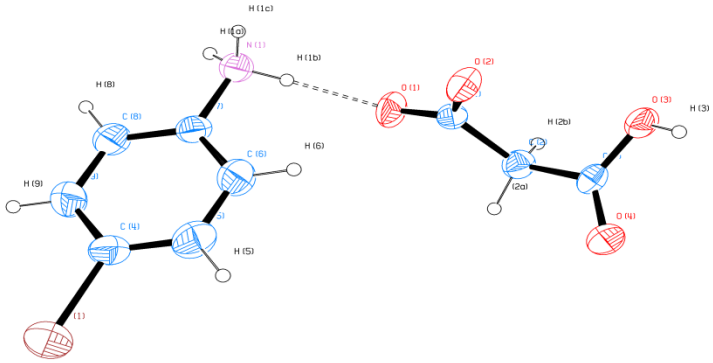


Figure 1: Ortep diagram of BAMAL

****

PP-61

Exploring the Effect of π-spacers on D-D-π-A Based Triphenylamine Dyes for Dye Sensitized Solar Cell Applications – Computational Approach

P. Pounraj, M. Senthil Pandian, P. Ramasamy*

SSN Research Centre, SSN College of Engineering, Kalavakkam, Chennai-603110, Tamilnadu, India.
***Email:** ramasamyp@ssn.edu.in*

The effect of different π spacers in D-D-π-A based triphenylamine sensitizers is studied computationally for DSSC application. Tetrahydroquinoline and triphenylamine groups are chosen as electron donor groups. The ground state structure, HOMO-LUMO energy studies, Local minimum energy, dipole moment and linear polarizability of the D-D-π-A based triphenylamine dyes are analysed by Density functional theory (DFT). The spectroscopic properties of triphenylamine based dyes are analysed by Time dependent density functional theory (TD-DFT). The free energy studies of electron injection and dye regeneration are also calculated based on the DFT and TD-DFT results. The computational results show that the number and position of the π-spacers largely affect the electronic, optical and spectroscopic properties. The calculated results of the D-D-π-A based triphenylamine sensitizer show that, the THQ-TPA-6 is more efficient compared to other sensitizers for DSSC application.

****

PP-62

Synthesis and Characterization of Disc-Shaped Thiophene Based Zn-Porphyrin for Organic Solar Cells Application

M. Muthu, P. Pounraj, N. Santhosh, M. Senthil Pandian, P. Ramasamy*

SSN Research Centre, SSN College of Engineering, Kalavakkam, Chennai-603110, Tamilnadu, India.
***Email:** ramasamyp@ssn.edu.in*

Disc-shaped thiophene donor-based Zn-porphyrin complex is designed and synthesized by Alder's two step method for organic solar cells application. The theoretical analysis is used to study the HOMO-LUMO and band gap energies. The synthesized porphyrin (THPY) and Zn-porphyrin complex (THPY-Zn) were characterized by Ultra Violet-Visible (UV-Visible), photoluminescence (PL), Fourier Transform Infra-Red (FTIR) spectroscopic methods. The experimental Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies are analysed by Cyclic Voltammetry (CV) and it is compared with theoretical HOMO and LUMO energies. THPY-Zn has red shifted absorption spectrum than corresponding THPY compound because of metallization. The synthesized THPY and THPY-Zn complex have strong absorption at visible region. The electronic and optical properties of the synthesized disc shaped porphyrin and Zn-porphyrin complex are investigated for organic solar cells application.

PP-63

Organic methyl 4-aminobenzoate (MAB) single crystal grown by Bridgman-Stockbarger method: A potential candidate for optical applications

K. Ramachandran*, A. Raja, Muthu Senthil Pandian, P. Ramasamy

SSN Research Centre, SSN College of Engineering, Chennai - 603 110, Tamilnadu.
***Email:** ramphy18@gmail.com*

Methyl 4-aminobenzoate (MAB) single crystal has been grown from Bridgman-Stockbarger method with the size of 1.8 cm diameter. The phase confirmation of organic MAB single crystal has been identified using single crystal X-ray diffraction analysis and its exposes the monoclinic system with centrosymmetry space group of C2/c. The presence of methyl and amine group of MAB material was carried out using Fourier transform infrared spectral study. Optical properties such as optical transmittance, cut off wavelength was evaluated from the UV-Visible NIR spectrum analysis and these results are used to calculate the optical absorption coefficient, bandgap, reflectance, refractive index and extinction coefficient. Thermal stability of MAB single crystal was obtained upto 150℃ (there is no weight loss), which is measured from the thermogravimetric (TG) analysis. Sharp endothermic and exothermic peaks were measured at 114℃ and 103℃, respectively and it reveals the melting and freezing point of the MAB single crystal. The laser damage threshold value was found to be 1.25 GW/cm^2, which is measured from the laser damage threshold study. The closed aperture curve represents the negative nonlinear refractive index ($n_{2<0}$) and the value was found to be -9.019×10^{-9} cm^2/W and it also exhibits the self-defocusing effect. The open aperture curve indicates the reverse saturation absorption and the value was found to be 0.25×10^{-4} cm/W. Third order nonlinear optical susceptibility of MAB crystal value was calculated at 2.01×10^{-6} esu.

****

PP-64

Photophysical-chemical properties of ethylenediamine ditartrate dihydrate acentric single crystal for nonlinear optical application

K. Sudhakar[1, 2] and P. Murugakoothan[2]*

PG and Research Department of Physics, Pachaiyappa's College, Chennai-600 030, Tamilnadu, India.
Department of Physics, C. Kandaswami Naidu College for Men, Chennai – 600 102, Tamilnadu, India.
***Email:** murugakoothan03@yahoo.co.in* ***Tel:** +91 944 444 7586*

An efficient organic nonlinear optical single crystal of ethylenediamine ditartrate dihydrate (EDADTDH) was grown by slow evaporation solution growth technique (SEST) at ambient condition using deionized water as solvent. The X-ray diffraction analysis was carried out to confirm the cell parameters, crystalline nature and structural perfection of EDADTDH crystal. Optical behaviour was determined using UV-vis-NIR transmittance study. The blue emission of the crystal was identified by photoluminescence and CIE studies. The SHG efficiency was found

using Kurtz-Perry powder technique. Mechanical stability of the crystal was analysed using Vickers microhardness measurement. The dielectric behaviour was established through dielectric study. Electromechanical behaviour was observed using piezoelectric coefficient analysis.

****

PP-65

Enhancement in ferroelectric, pyroelectric and photoluminescence properties in Lithium Lactate doped TGS crystals

P. G. Praveen[1], Ayarine G. Dhas[1] and N. Joseph John[2]

[1]Department of Physics, Government Arts College, Udhagamandalam – 643 002, The Nilgiris, Tamilnadu, India.
[2]Department of Physics, Kamarajar Government Arts College, Surandai – 627 859, Tenkasi District, Tamilnadu, India.
Email: *praveenphy2@gmail.com*

Pure and lithium lactate doped five different molar concentrations in Triglycine Sulfate (TGS) single crystals were grown by slow evaporation technique. XRD and FT-IR studies confirmed the lithium lactate doping. Decrease in dielectric constant and increase in Curie temperature (Tc) were observed with increasing doping concentration. Low absorption cutoff (298nm) and high optical transparency (89%) resulting in large band gap was observed in UV–VIS studies. In addition, strong hyper- luminescent emission bands at 470 and 565 nm were observed in which the relative intensity were found to be reversed as a result of doping. In P–E hysteresis loop studies, a higher curie temperature and an improved and more uniform figure of merit over a large region of the ferroelectric phase were observed. The improved dielectric, optical and ferroelectric / pyroelectric properties make the lithium lactate doped TGS single crystals better candidate for various opto- and piezo- electronics applications. The results will be presented.

****

PP-66

Growth and characterization of organometallic Calcium Lactate added L-Asparagine cadmium chloride single crystal by slow evaporation technique

R. Rakesh[1], Ayarine G. Dhas[2], Joseph John N[3]

[1]Department of Physics, Sethupathy Govrnment Arts College, Ramanathapuram-623502, Tamilnadu, India.
[2]Department of Physics, Government Arts College, Udhagamandalam, The Nilgiris – 643 002, Tamilnadu, India.
[3]Department of Physics, Kamarajar Government Arts College, Surandai – 627 859, Tenkasi District, Tamilnadu, India.
***Email:** rakeshragavan128@gmail.com*

Single crystals of Calcium Lactate L-Asparagine cadmium chloride (CLLACC), an organometallic nonlinear optical material, have been grown by the slow evaporation technique. The grown crystals were subjected to various characterization techniques, such as single crystal and powder XRD, FTIR, UV–vis and TGA-DTA. The mechanical properties of the crystals show that this material belongs to the category of hard materials. Second harmonic generation was confirmed by the Kurtz and Perry powder technique. Electrical parameters, such as dielectric constant, dielectric loss, ac and dc conductivity and their corresponding activation energies have been studied. The low dielectric constant and dielectric loss suggest that this material is a good candidate for micro-electronic applications. The details will be presented.

****

PP-67

Structural and Electrical Properties of (1-x)$Bi_{1/2}Na_{1/2}TiO_3$ –x$BaTiO_3$ single crystals across the morphotropic phase boundary by TSSG method

M. William Carry*, Muthu Senthil Pandian, P. Ramasamy

SSN Research Centre, SSN College of Engineering, Chennai, Tamilnadu, India.
***Email:** carrywilliam5234@gmail.com*

The solid solution of 0.94($Na_{0.5}Bi_{0.5}$) TiO_3-0.06$BaTiO_3$ NBBT94/6 is a promising material to replace Pb based piezoelectric materials. The bulk NBBT 94/6 single crystal was successfully grown by the top-seeded solution growth (TSSG) method. Lead-free piezoelectric NBBT single crystals with a composition across the morphotropic phase boundary (MPB) have been grown by the top-seeded solution growth (TSSG) method. NBT-xBT single crystal, encompassing the rhombohedral to largely monoclinic phase covering the morphotropic phase boundary (MPB) region were grown by the TSSG method. The crystal structure and its electrical properties were investigated. The Laue diffraction pattern confirms that the grown crystal is a single crystal. Rietveld refinement studies disclose the existence of a phase boundary between monoclinic (Cc) and Rhombohedral (R3c) phases near the MPB. The depolarization temperature (T_d), piezoelectric coefficient (d_{33}) and ferroelectric properties were enhanced at MPB.

PP-68

Effects of ZnO substitution on dielectric properties of $CaCu_3Ti_4O_{12}$ ceramics by a solid-state reaction method

M. Chinnathambi, R. Robert*

PG and Research Department of Physics, Government Arts College for Men, Krishnagiri, Tamil Nadu, India
***Email:** roberthosur@yahoo.co.in*

This work presents the results of ZnO doping of a $CaCu_3Ti_4O_{12}$ ceramic sample prepared by a solid-state reaction method. The samples were studied by X-ray diffraction (XRD) and scanning electron microscopy (SEM); dielectric measurements were measured in the 1 Hz - 1 MHz frequency range at room temperature; and the nonlinear behavior of all samples was measured. The doping of ZnO resulted in an increase in the dielectric constant of $CaCu_3Ti_4O_{12}$ but decreased the stability of the frequency dependence. Increasing concentrations of ZnO resulted in decreasing nonlinear coefficients.

***Keywords*:** $CaCu_3Ti_4O_{12}$ ceramics, Sol-gel method, Powder X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Dielectric properties.

****

PP-69

Highly efficient visible light photocatalytic activity and inherent property of pure & polymer capped SnO_2 nanoparticles by chemical precipitation method.

A.Sabarinathan, R.Robert*

PG and Research Department of Physics, Government Arts College for Men, Krishnagiri
*** Email:** roberthosur@yahoo.co.in*

In present investigation pure and polymer capped tin dioxide nanoparticles successfully synthesized by precipitation method. The polymer material CTAB is a vital role in the presence of the synthesis procedure. The role of CTAB is not produced any structural change apart from the particle size which is the advantageous part of the surfactant based synthesis. The particle sizes from X-ray diffraction (XRD) analysis were found that there is a decrease in particle size from 48 to 27 nm. The firmness of the SnO_2 nanoparticles was characterized by UV- vis, Fourier Transformer infrared (FT-IR) and morphology studies. The results from the UV-Vis study for prepared nanoparticles the bandgap energy values increased from 3.65 eV to 3.87 eV due to using of surfactant. From the FT-IR study confirms the Metal – Oxygen bond and several function groups especially methyl group C-H was observed due to using of CTAB surfactant. TEM results show spherical with stacked rod morphology. EDAX confirmed the presence of all the elements with high purity. The photocatalytic activity is investigated on CTAB based SnO_2 nanoparticles as catalyst under UV irradiation. The degradation of Methyl blue dye is 93 % degraded in the presence of ultra-violet radiation.

***Keywords*:** CTAB polymer, particle size, SnO_2.

PP-70

Role of Coupling Divalent Metal Ion of Tin on Structural and Magnetic Properties of $NiFe_2O_4$Nanoparticles

V.Mowlika[1], C.S. Naveen[2], A.R.Phani[2], R.Robert[1*]

[1] PG and Research Department of Physics, Government Arts College for Men, Krishnagiri, Tamil Nadu, India
[2]Innovative Nano and Micro Technologies Private Limited, Bangalore, Karnataka, India - 560 059
**** Email:** roberthosur@yahoo.co.in*

The present paper provides a simplistic way to understand the role of coupling divalent metal ions Tin (Sn) on the structural and magnetic properties of $NiFe_2O_4$Nanoparticles (NF NPs). A series on nanocrystalline Nickel ferrites ($Ni_{(1-x)}Sn_{(x)}$ Fe_2O_4) with composition x= 0.0, 0.2, 0.4,0.6,0.8 are synthesized by co-precipitation method. The synthesized product is characterized by powder X-ray diffractometer (PXRD), scanning electron microscopy (SEM) and vibrating sample magnetometer (VSM) respectively. PXRD graph provides the phase formation of $NiFe_2O_4$as well as with respect to Sn concentration, the lattice parameter, and cell volume is increased. SEM images describe that the surface morphology details and size of the particles. VSM studies are felicitated that saturation magnetization (Ms) of soft super-paramagnetic nature is reduced with respect to the variation of Sn concentration.

***Keywords*:** $SnNiFe_2O_4$ NPs, Divalent metals, Structural properties, Magneticproperties

****

PP-71

Growth and characterization of sodium nitrate doped L-Histidine hydrochloride monohydrate single crystals

Sweatha L, Robert R*

PG and Research Department of Physics, Government Arts College for Men, Krishnagiri, Tamil Nadu, India
** **Email:** roberthosur@yahoo.co.in*

Nonlinear optical materials (NLO) have attracted much attention because of their potential applications in emerging optoelectronic technologies. Recently, amino acids are displaying high NLO properties due to its zwitterionic nature. Many authors have grown and reported the properties of NLO crystals by adding amino acids with inorganic compounds. The amino acid L-Histidine having an imidazole group, as well as amino carboxylate groups were grown can display high NLO properties. In the present work, we report the growth of sodium nitrate doped L-Histidine hydrochloride monohydrate single crystals by slow evaporation technique at room temperature. The grown crystals were characterized by powder x-ray diffraction, FTIR, UV-Vis, microhardness, dielectric, thermal properties and SHG efficiency. Powder X-ray diffraction analysis ensures that the grown crystal is in the $P2_12_12_1$ space group and orthorhombic system.

FTIR Spectral analyses were performed to identify the presence of various functional groups in the crystal. UV-Vis spectral analysis has been carried out to find the transparency of the grown crystal. The dielectric constant and dielectric loss of the crystal were studied as a function of frequency and the results are discussed. The thermal behaviors of the material were studied by thermogravimetric and differential thermal plots. Microhardness studies were carried out to assess mechanical properties. The second harmonic generation conversion efficiency was found by Kurtz and Perry powder technique. The electrical properties were investigated by impedance analysis and the results of various studies of grown crystal are discussed.

***Keywords*:** L-histidine hydrochloride monohydrate, sodium nitrate, slow evaporation method, powder x-ray diffraction, mechanical, optical and thermal studies.

PP-72

Structural, Optical and Thermal Properties of Hg^{2+} Doped L-Alanine Tartarate Single Crystals

Silviya M, Robert R*

PG and Research Department of Physics, Government Arts College for Men, Krishnagiri, Tamil Nadu, India
***Email:** roberthosur@yahoo.co.in*

Crystals belonging to amino acids are promising candidates for NLO applications due to their chiral symmetry and non-centrosymmetric space groups. The L-Alanine molecule exists as a zwitterion, where the carboxyl group is dissociated and the amino group is protonated and if it is mixed with different organic and inorganic acids to form novel materials it is expected to get improved NLO properties. Group II B metals (Zn, Cd & Hg) compounds have high transparency in the UV region, because of their closed d10 shell. Transparent single crystals of Zn^{2+} doped L-Alanine Tartarate have been grown from slow evaporation technique. XRD analysis confirms the crystallinity of the grown crystal. FT-IR analysis illustrates the functional groups present in the grown crystal. The UV-Visible analysis shows the transparency of the grown crystal which reveals the fact that the dopant could increase the transparency of the parent material. TGA/DTA analysis describes that the metal dopant has not altered the thermal stability of molecules.

Keywords: Zn^{2+}, L-Alanine Tartrate, Slow evaporation, TGA/DTA.

****

PP-73

Growth and characterization of DSTMS Crystal for nonlinear optical applications

D.Bharath[1], S. Kalainathan[2], D. Anbuselvi[3]

[1]Department of Physics, MVJ College of Engineering (autonomous), Bengaluru-560067, Karnataka, India
[2]Centre for Crystal Growth, VIT University, Vellore-632014, Tamil Nadu,
[3]Muthayammal Engineering College (autonomous), Rasipuram-637408,
***Email:** dbhaarath@gmail.com*

4-N, N-dimethylamino-4'-N'-methyl-stilbazolium 2, 4, 6-trimethylbenzenesulfonate (DSTMS) terahertz organic material has been synthesized by the knoevenagel condensation method. DSTMS single crystals were grown in methanol by slow-cooling method. The linear optical property of DSTMS crystal has been studied using UV-VIS-NIR spectroscopy in the wavelength range 190 nm-1100 nm and optical constants are calculated theoretically. The magnitude of nonlinear refractive index (10^{-10} m ^{2}/W), nonlinear absorption (10^{-3} m /W) and third order nonlinear susceptibility (10^{-4} esu) has been studied using Z-scan technique. Dielectric property of DSTMS crystal has been studied at frequency range 50Hz to 5MHz. The electronic properties such as valence electron plasma energy, Penn gap, fermi energy, electronic polarization, electric susceptibility of the grown crystal has been studied. Photoluminescence spectrum was recorded using xenon lamp in the range of 450-700nm. Laser optical damage threshold of DSTMS crystal was calculated (0.744GW/cm^2) using pulsed Nd-YAG laser (1064nm) of repetition rate 10ns.The refractive index of the crystal (1.571) has been measured using Abbe's Refractometer. The optical limiting behaviour of DSTMS crystal has been studied using Nd-YAG laser. The response time (τ) of optical limiting power for the crystals is 10^{-11}s.

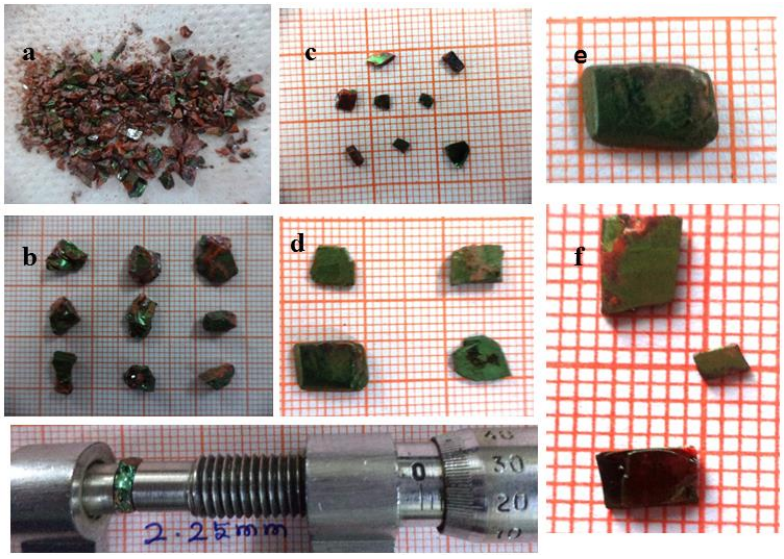


Figure: DSTMS crystals grown in methanol

****

PP-74

Studies on growth and characterization of nonlinear optical L-tartaric acid–nicotinamide single crystal

P. Rameshkumar*, P. Surendran, S. Sakthy Priya, A. Lakshmanan, S. Pushpalatha

PG and Research Department of Physics, Periyar E.V.R College (Autonomous), Tiruchirappalli-23, Tamilnadu, India.

Email: *rameshkumarevr@gmail.com*

Nonlinear optical (NLO) single crystal of L-tartaric acid–nicotinamide (LTN) has been grown by slow evaporation solution technique as shown in Fig 1. The grown crystals were subjected to various characterization techniques in order to examine their suitability for various applications. Powder X-ray diffraction (PXRD) analysis revealed that the compound is formed without any impurities. Functional groups and formation of the title compound were confirmed using FTIR analysis. Optical behavior of the material was examined using UV–Vis NIR spectrum and optical band gap energy were calculated. Microhardness, dielectric and piezoelectric studies have been carried out at ambient conditions. Electronic properties such as valence electron plasma energy, Penn gap, Fermi energy and electronic polarizability were calculated by Clausius–Mossotti relation. Photoluminescence analysis was carried out to study the luminescence nature of the crystal and its defect states. In addition photoconductivity, and powder Kurtz and Perry second harmonic generation (SHG) test were carried out.

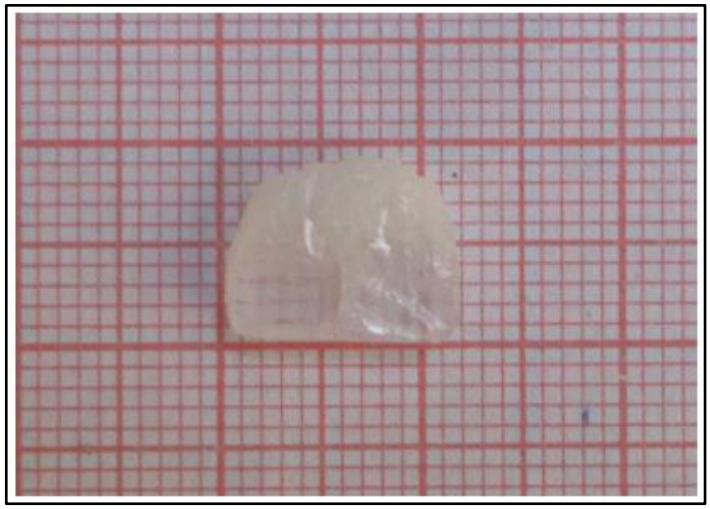


Figure 1: As grown LTN single crystal

****

PP-75

Crystal Structure and Hirshfeld Surfaces Analysis of Biologically Important Piperidine Derivative

P.Periyannan, M.Beemarao and K.Ravichandran,*

Department of Physics, Kandaswami Kandar's College, Velur (PO), Namakkal-638 182.
***Email:** kravichandran05@gmail.com*

Nitrogen-containing heterocyclic piperidine compounds are used as structural components in pharmaceuticals and agrochemicals due to their high functional activities [1]. The compounds possessing an amide bond linkage have a wide range of biological activities such as antimicrobial, anti-inflammatory, antiviral, antimalarial and general anesthetics [2]. The data for Piperidine compound *N*-Acetyl-t-3-Isopropyl-r-2,c-6-diphenylpiperidine were collected using Bruker AXS SMART APEX-II single crystal diffractometer. The structure was solved by direct methods and refined by full-matrix least-squares procedures to a final R-value of 0.0591. The molecule crystallizes in monoclinic system of space group P $2_1/n$. In the molecule piperidine ring adopts chair conformation [3]. The two phenyl rings are approximately perpendicular to each other with a dihedral angle of 56.04(9)°. The crystal packing is stabilized by C-H...O types of intra and intermolecular interactions. The Hirshfeld surfaces can be mapped with different properties namely, dnorm, electrostatic potential, shape-index and curvedness. They indicate that intermolecular H···H contacts provide the largest contribution (74.2%) to the Hirshfeld surface and the percentage contributions of the other interactions are C···H/H···C = 18.7%, O···H/H···O = 7.0% and N···H/H···N =0.1%. The large number of H···H, H···C/C···H, H···O/O···H and H···N/N···H interactions suggest that hydrogen bonding and van der Waals interactions play the major roles in the crystal packing.

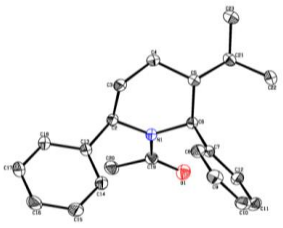


Figure 1

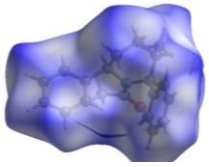


Figure 2

Figure 1: Perspective view of the molecule ***Figure 2:***.Hirshfeld surfaces mapped of the title compound.

Keywords: crystal structure, biological activities, Hirshfeld surfaces.

References:

1. Aridoss, G., Parthiban, P., Ramachandran, R., Prakash, M., Kabilan, S. & Jeong, Y. T. (2009). *Eur. J. Med. Chem.* 44,577–592.
2. Mobio, I. G., Soldatenkov, A. T., Federov, V. O., Ageev, E. A., Sergeeva, N. D., Lin, S., Stashenku, E., Prostakov, E & Andreeva, E. L. (1989). *Khim. Farm. Zh.* 23, 421–427.
3. Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* 97, 1354–1358.

PP-76

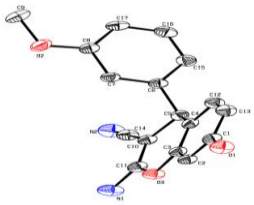
Crystal Structure and HOMO – LUMO Analysis of Pyran Derivative

M.Beemarao, P.Periyannan and K.Ravichandran*

Department of Physics, Kandaswami Kandar's College, Velur (PO), Namakkal-638 182.
***Email:** kravichandran05@gmail.com*

The pyran is an oxygen-containing heterocyclic moiety, which exhibits an array of pharmacological properties. The pyran is an important pharmacophore which shows antitumor, antibiotic, antibacterial, antiallergic, hypolipidemic and immunomodulating activities [1] [2]. The development of drug resistance to clinically used agents has increased the demand for discovery of new chemical scaffolds with antimicrobial activity. The data for pyran compound (2-amino-3-cyano-7-hydroxy-4-(3-methoxybenzaldehyde)-4*H*-benzo[1,2-*b*]pyran) were collected using Bruker AXS SMART APEX-II single crystal diffractometer. The structure was solved by direct methods and refined by full-matrix least-squares procedures to a final R-value of 0.0782. X-ray analysis confirms the molecular structure and atom connectivity. The molecule crystallizes in triclinic system of space group P-1. The HOMO and the LUMO are called Frontier Molecular Orbitals (FMOs) as they lie at the outermost boundaries of the electrons of the molecules. The HOMO–LUMO behaviour was elucidated to determine the energy gap. The HOMO/LUMO and energy gap energies have been calculated using B3LYP/6-311++G(d,p) level are -7.925 eV/ -4.202 eV and 3.723 eV, respectively. A molecule with a small frontier orbital gap is generally associated with high chemical reactivity and low kinetic stability.

***Keywords*:** Crystal structure, X-ray diffractometer, HOMO – LUMO analysis.



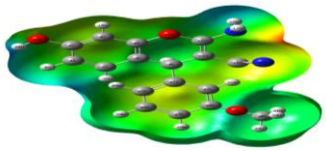


Figure: Perspective view of the molecule Molecular Electrostatic Potential (MEP)

***References*:**

1. Bonsignore, L., Loy G., Secci D, and Calignano. A., "Synthesis and pharmacological activity of 2-oxo-(2H) 1-benzopyran-3-carboxamide derivatives," European Journal of Medicinal Chemistry, vol. 28, no. 6, pp. 517–520, 1993.
2. Kumar, D., Reddy V.B., Sharad S.; Dube, U., Suman K A., Eur. J. Med. Chem., 2009, 44, 3805.

****

PP-77

Synthesis, Growth and Characterization of 2-Amino-5-Nitropyridine 4-Chlorobenzoic Acid (1:1): A New Organic Single Crystal for Third-Order Nonlinear Optical (NLO) Applications

V. Sivasubramani, Muthu Senthil Pandian*, P. Ramasamy
SSN Research Centre, SSN College of Engineering, Kalavakkam-603110, Chennai, Tamil Nadu
Email: *sivasubramaniv1989@gmail.com; senthilpandianm@ssn.edu.in*
Mobile: *+91-9791802135; +91-9944294169*

Organic nonlinear optical (NLO) 2-amino-5-nitropyridine 4-chlorobenzoic acid (1:1) (2A5NP4CB) single crystals have been grown by slow evaporation solution technique (SEST) for the first time in literature. The structural properties of the grown crystal have been determined by single crystal X-ray diffraction (SXRD) analysis. The results reveal that the grown crystal belongs to monoclinic crystal system with the centrosymmetric space group $P2_{1/n}$. The molecular weight and the density of 2A5NP4CB crystal have been found to be 295.68 g/mol and 1.538 Mg/m^3, respectively. The presence of functional groups and its molecular structure have been confirmed by FTIR and NMR spectrum analysis, respectively. By employing unidirectional Sankaranarayanan-Ramasamy (SR) method, optically transparent 2A5NP4CB single crystal has been grown with the size of about 30 mm length and 10 mm diameter over a period of 60 days. The comparative investigations of 2A5NP4CB crystals grown by SEST and unidirectional SR method have been carried out by HRXRD, UV-Vis NIR, chemical etching, Vickers microhardness and laser damage threshold analyses. The overall results show that the crystal grown by unidirectional SR method possesses high quality compared to conventional SEST grown crystals. Third-order nonlinear behavior of the grown crystal was studied using Z-scan technique by employing He-Ne laser of wavelength 532 nm and it reveals that the grown 2A5NP4CB crystal can serve as a promising candidate for NLO device applications. The optical limiting behavior was studied under He-Ne laser with the wavelength of 532 nm and the limiting threshold of the grown crystal was found to be 7.4 mW/cm^2. The optimized molecular structure, frontier molecular orbitals (FMOs), linear polarizability, first-order hyperpolarizability and natural bond orbital (NBO) of 2A5NP4CB molecule were performed by density functional theory (DFT).

Figure 1. (a) ORTEP view of 2A5NP4CB with the atom numbering scheme, (b) SEST grown 2A5NP4CB single crystals and (c) SR method grown 2A5NP4CB single crystal

****

PP-78

Growth difficulties and growth of crack free Eu^{2+} activated KSr_2I_5 scintillator single crystal by vertical Bridgman-Stockbarger technique for radiation detection applications

Arumugam Raja* and P. Ramasamy

SSN Research Centre, Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam – 603110, India.

***Email:** rajaphy014@gmail.com*

The parent compound of Strontium Iodide (SrI_2), Potassium Iodide (KI) and Europium Iodide (EuI_2) was purified by homemade Zone-refinement experimental set-up. Insoluble impurities were filtered by specially designed dual chamber quartz ampoule with frit filter method. The Europium activated potassium strontium iodide ($KSr_2I_5:Eu^{2+}$) compound melt was filtered by frit filtering method. Steep temperature profile of this growth furnace is also measured to growth a quality single crystal of $KSr_2I_5:Eu^{2+}$. The $KSr_2I_5:Eu^{2+}$ single crystal was grown by homemade vertical transparent Bridgman-Stockbarger technique. The photoluminescence excitation and emission spectra indicated the typical 4f 5d – 4f transition. The broad emission peak was at 443 nm. The X-ray excited radioluminescence broad emission was observed at 452 nm. The scintillation properties of the grown crystal were tested by gamma ray spectrometer. The energy resolution of the $KSr_2I_5:Eu^{2+}$ crystal was found to be 4.1% at 662 KeV under ^{137}Cs sealed gamma source and scintillation decay time was also determined and calculated value is 1.25 μs.

***Keywords*:** Bridgman-Stockbarger technique; Single crystal; Radioluminescence; Scintillator; Radiation detector; Gamma ray spectrometer

****

PP-79

Temperature-dependent index of refraction, type I and type II phase-matching angle of monoclinic imidazolium L-tartrate single crystal

S. Chinnasami [a], Rajesh Paulraj [a]*, Rajeev Bhatt [b,c], Indranil Bhaumik [b,c], P. Ramasamy [a], A. K. Karnal [b,c]

Centre for Crystal Growth, Department of Physics, SSN College of Engineering, Kalavakkam, Tamilnadu-603 110.
b Crystal Growth Laboratory, Laser Materials Section, Raja Ramanna Centre for Advanced Technology, Indore-452013.
c Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai-400094.
Email: *chinnatamil3264@gmail.com; rajeshp@ssn.edu.in*
Mobile: *+91-8524873264; +91-9445434893*

The temperature-dependent refractive index along crystallographic (001), (010) and a direction perpendicular to (010) (⊥bc) plane for monoclinic phase Imidazolium L-tartrate (IMLT) single crystals have been grown by slow cooling seed rotation technique. Refractive index (RI) measurements confirmed IMLT crystal is negative biaxial crystal. Also, the Sellmeier equation for wavelengths, in the range of 0.407–1.551 μm is formulated at different temperatures in the range of 30–125 °C. The thermal coefficient of the refractive index in the above-specified range is $\sim 10^{-5}$ °C. The temperature-dependent refractive index (RI) measurements depicted a negative thermo-optic coefficient (TOC) for RI. An important set of relations between TOC and wavelength (407–1551 nm) has been established which is useful for estimating TOC in the temperature range of 30–125 °C. Also, type I and type II phase-matching angle of XY and XZ ($\theta<\Omega$) plane calculated.

****

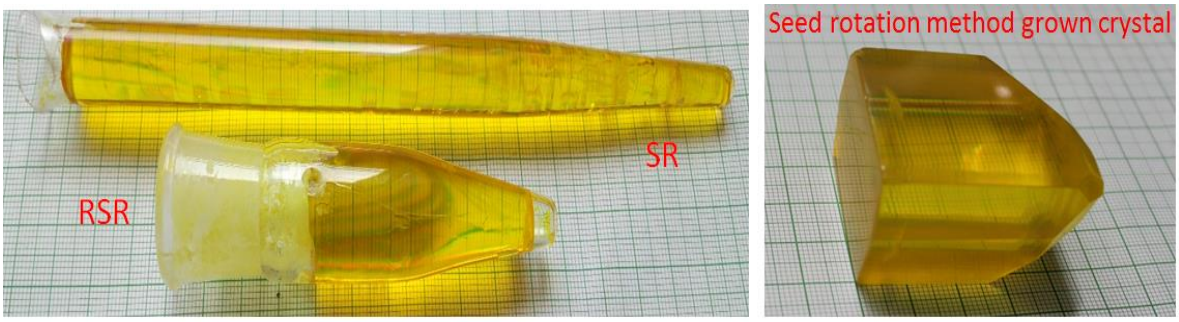
PP-80

Growth of High Quality Organic 2AP4N Single Crystal by Sr, RSR, RT-SR and Point Seed Rotation Methods: Fabrication of Type-I And Type-II Phase Matching Elements for NLO Applications

P. Karuppasamy,*[1] T. Kamalesh,[1] Muthu Senthil Pandian,[1] P. Ramasamy,[1] Sunil Verma,[2,3]

[1]SSN Research Centre, SSN College of Engineering, Chennai-603110, Tamil Nadu,
[2]Laser Materials Development and Devices Division, Raja Ramanna Centre for Advanced Technology (RRCAT), Department of Atomic Energy (DAE), Indore-452013, Madhya Pradesh,
[3]Homi Bhabha National Institute (HBNI), Anushakti Nagar, Mumbai - 400094, Maharashtra,
***E-mail:** karuppasamyp75@gmail.com ; karuppasamyp@ssn.edu.in; **Tel:** +91-9791552297*

The optically high quality 2-aminopyridinium 4-nitrophenolate 4-nitrophenol (2AP4N) single crystals have been grown by (i) Sankaranarayanan–Ramasamy (SR) method and (ii) Rotational Sankaranarayanan–Ramasamy (RSR) method, (iii) Roto-translation Sankaranarayanan–Ramasamy (RT-SR) and (iv) Point seed rotation method. The effect of rotation on unidirectional crystal growth method (RSR, RT-SR) have been reported for the first time. The apparatus was specially designed and developed for the growth of high quality crystals by slow cooling under several rotational conditions. The high-quality crystals have been achieved under forced convection and the quality of the crystal is high compared to the crystals grown under free convection conditions. The crystal structure was analyzed by single crystal X-ray diffraction (SXRD) measurement. The grown crystal was subjected to the powder X-ray diffraction (PXRD) analysis to confirm the growth plane along (001) plane. The optical quality of the grown crystals has been analyzed by UV-Vis NIR spectrophotometer. The photoluminescence behaviour was recorded. The grown crystal has less dislocation densities as confirmed by chemical etching analysis. The mechanical strength of the grown crystals was investigated. The frequency dependent dielectric properties (permittivity and loss) of the crystals were carried out. The laser damage threshold (LDT) was measured for the grown crystals. The full-width at half maximum (FWHM) of high-resolution X-ray diffraction (HRXRD) curves indicate that the RSR method grown crystal has high crystalline perfection. The second harmonic generation (SHG) of 2AP4N was analyzed by Kurtz-Perry powder technique. The SHG efficiency was found to be 4.5 times that of reference KDP material. Refractive index measurement was carried out with different wavelength using prism coupling method. The phase matching angle of 2AP4N was find out by fitting Sellmeier equation. Based on the phase matching angle, the grown 2AP4N crystal was cut and the type-I and type-II SHG elements were fabricated.



SR, RSR and Seed rotation method grown 2AP4N single crystals

****

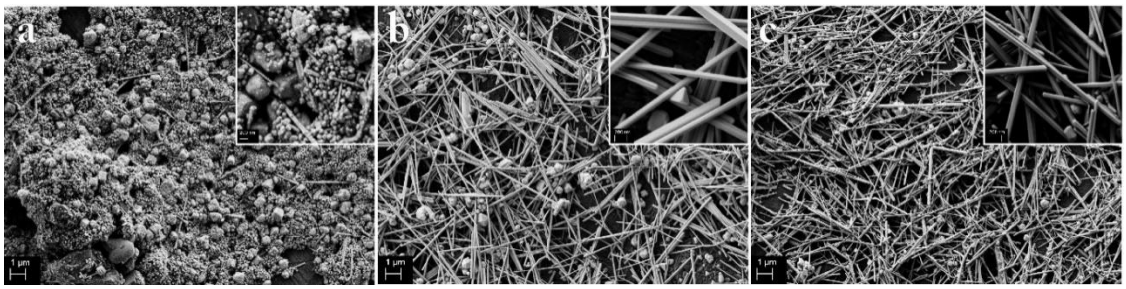
PP-81

Synthesis and characterization of Silver nanowires for optoelectronic applications

Mathew K Francis*, P. Balaji Bhargav, Nafis Ahmed, Balaji C

SSN Research Centre, SSN College of Engineering, Kalavakkam-603110, Chennai, Tamil Nadu
Email: *mathewfrancis@ssn.edu.in*

Transparent conducting electrode (TCE) is considered as a vital component in various optoelectronic devices such solar cells and touch screens. Due to the constant development in the field of opto-electronics, there is a need to develop alternate TCE materials at low cost and low processing temperature. Among various alternate TCEs, silver nanowires (AgNWs) occupy special place due to their superior opto-electronic properties. In the current work, AgNWs are grown using hydrothermal method. During the synthesis, PVP:AgNO3 ratio is kept constant. Morphological analysis is carried out using FESEM imaging. Microstructural properties are analyzed using TEM analysis. Lattice parameter and d spacing are obtained using the SAED pattern. The optical properties of synthesized nanowire are studied by UV-Vis NIR spectroscopy. The absorption peak around 352 nm confirms the formation of AgNWs.



****

PP-82

Growth and characterization of bisglycine cobalt dichloride dihydrate semiorganic single crystal

P.Revathi, M. Sathish and T. Balakrishnan*

**Crystal Growth Laboratory, PG & Research Department of Physics, Periyar EVR College (Autonomous), Tiruchirappalli – 620 023, Tamil Nadu, India.*
***Email:** balacrystalgrowth@gmail.com*

Single crystals of potential semiorganic third order nonlinear optical material of bisglycine cobalt dichloride dihydrate (BGCDC) were grown by slow evaporation technique at room temperature. The single crystal X – ray diffraction of BGCDC reveals that the crystal belongs to monoclinic system with centrosymmetric space group. The reflection planes of the sample were confirmed by the powder X – ray diffraction analysis and the peaks were indexed. Fourier transform infrared (FT – IR) and FT – Raman spectral analysis was used to confirm the presence of various functional groups in the grown crystal. UV – Vis – NIR spectral analysis of BGCDC crystal is transparent between the wavelengths 300 nm to 1100 nm. Vickers microhardness study reveals that the grown crystal belongs to soft material category. Dielectric constant and dielectric loss of BGCDC crystal were measured in the frequency range of 50 Hz to 2 MHz at different temperature.

****

PP-83

Synthesis and characterization of CZTS Thin Films by SILAR method for Solar Cells application

Ganesh Kumar K, Balaji Bhargav P*

SSN Research Centre, SSN College of Engineering, Kalavakkam, Tamilnadu, India, 603110.
***Email:** balajibhargavp@ssn.edu.in*

Cu_2ZnSnS_4 (CZTS) is considered to be a good absorber material for thin film solar cell applications. In the present study, CZTS thin films are successfully deposited on to the glass substrates using by SILAR method. Structural, morphological, optical and electrical properties of the deposited CZTS thin films are analysed. X-ray diffraction analysis confirms the formation of tetragonal structure of the deposited thin films. The defects are reduced by annealing the films in Ar atmosphere as observed from FESEM. Microstructure analysis is carried out using HRTEM and. Functional groups present in the film are analysed by FTIR studies. The Raman spectra is used to study the vibration mode of CZTS thin film. Binding energy values calculated from X-ray photoelectron spectroscopy (XPS) spectra. Band gaps values of CZTS film are calculated using Tauc's plot, these results are found to be suitable absorbing materials for solar cell applications.

***Keywords*:** SILAR, XRD, FESEM, HRTEM, XPS, Uv-Vis spectroscopy

***References*:**

1. N. Kamoun, H. Bouzouita , B. Rezig Fabricaition and characterization of Cu_2ZnSnS_4 thin films deposited by spray pyrolysis technique. Thin Solid Film vol.515 (2007) 5949-5952.
2. Min-Yen Yeh, Po-Hsun Lei, Shao-Hsein Lin, Chyi-Da Yang Copper-Zinc-Tin-Sulfur Thin Film Using Spin- Coating Materials 2016, 9, 526.

****

PP-84

Crystal Growth of Indium Monoselenide for Photovoltaic Applications

Teena Mathew[1], Bibin John[2] and A G Kunjomana[2*]

[1] Department of Physics, St. Thomas College, Palai - 686 574, Kerala
[2] Department of Physics and Electronics, CHRIST (Deemed to be University)
Bangalore -560 029, Karnataka
***Email:** kunjomana.ag@christuniversity.in, **Mobile No:** 9449645957*

Group III-VI chalcogenide semiconductor, indium monoselenide (InSe), serves as a benchmark material in the photovoltaic arena, owing to its inherent attributes such as direct transition, non-hazardous nature, optimum band gap, high absorption coefficient, etc. Melt solidification methods are often featured by high growth yield and controlled diameter adaptable for device structures. Of the various melt growth processes, the versatile Bridgman-Stockbarger method has been employed in a controlled environment, such that nearly perfect stoichiometric InSe crystals were grown and subjected for characterization. The degree of supercooling was optimized by controlling temperature gradient and translation rate of the ampoule. Prior to crystallization, the compound was prepared from high pure (99.999%) elements (In and Se) by vacuum fusion in a quartz ampoule with the aid of muffle furnace and rotation mechanism. Slow heating and periodic agitation resulted in uniform composition throughout the ingot length. The prepared compound was melted in a tapered ampoule under high vacuum (~ 10^{-6} Torr) for a period of 48 h and slowly translated down with respect to the temperature profile. By controlling the rate of cooling and growth parameters, crystalline samples were obtained in monophase corresponding to hexagonal system, with lattice constants, a = 4.005 Å and c = 16.643 Å. The harvested crystals of length 30 mm and diameter 10 mm were cleaved at liquid nitrogen temperature and the surfaces were examined to explore the microstructural development. Defect creation due to thermal stress was eliminated systematically, which promoted the extension of a single nucleus with minimum disorder than other conventional melt methods. Energy dispersive analysis by X-rays and diffraction experiments were carried out to confirm the chemical composition and phase of crystals. Spreading and piling up of different layers were observed using a scanning electron microscope on the cleaved planes, indicating layer growth mechanism. The microhardness values of InSe crystals were initially increased with load and further remained constant, limiting the slip due to plastic deformation. The grown crystals, devoid of polymorphism, were found to be mechanically stable with improved carrier concentration, energy band gap and resistivity compared to those prepared from non-stoichiometric melt, which indicate that they are reliable for photovoltaic energy conversion applications.

****

PP-85

Microstructural Characteristics and Mechanical Properties of Melt Grown SnTe Crystals

A G Kunjomana[1*], Bibin John[1], Teena Mathew[2] and Athira Rose Chittilappilly[1]

[1] *Department of Physics and Electronics, CHRIST (Deemed to be University) Bangalore - 560 029, Karnataka*
[2] *Department of Physics, St. Thomas College, Palai - 686 574, Kerala*
***Email:** kunjomana.ag@christuniversity.in, **Mobile No:** 9449645957*

The fascinating art of crystal growth stems from the formation of a tiny stable nucleus and its progressive evolution so as to obtain periodic solids with well-defined symmetry. In the recent years, extensive efforts have been carried out to explore novel semiconducting crystals for diverse applications. The design of group IV-VI binary chalcogenide materials has attained special attention due to their unique physical characteristics. Hence, tin telluride (SnTe) crystals have been engineered by Bridgman-Stockbarger technique, utilizing a cost-effective vertical gradient furnace with precise judgment of growth parameters. This method deeply concerns with the fundamental aspects of growth kinetics, heat flow and the transport of liquid-solid interface. As such, special care was taken to avoid these challenges by keeping the host charge in the molten state for 24 h and allowed to solidify very slowly to the cold zone at the rate of 2 mm/h, 5 mm/h and 7 mm/h using an indigenously fabricated translational mechanism. Specific control on the movement of liquid-solid interface so as to facilitate unidirectional solidification has produced single crystals with good cleavage faces bearing minimum structural deformations. The crystal surfaces were subjected to Powder X-ray Diffraction (PXRD) and Energy Dispersive Analysis by X-rays (EDAX) for the identification of phase and chemical composition. The lattice constant and density of the crystalline core-pieces were found to be a = 6.317 Å and 6.479 g/cm^3 respectively. The quantitative estimation of elemental constituents showed the composition of Sn and Te in the ratio 50.56:49.44, justifying the right stoichiometry and chemical purity. The microstructural features of the surface were examined by utilizing optical and electron microscopes, which disclosed the transition from polycrystalline to crystalline form, devoid of grain boundaries. Microindentation studies were carried out to assess the hardness and mechanical stability of the flat surfaces in response to external loads. The correlation between stoichiometric composition, processing conditions, microstructure and resulting mechanical properties propose the suitability of the grown samples for device applications.

****

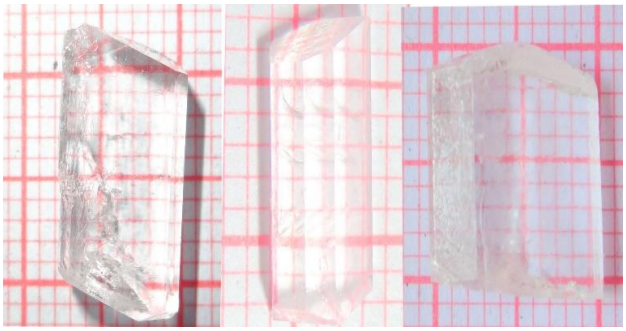
PP-86

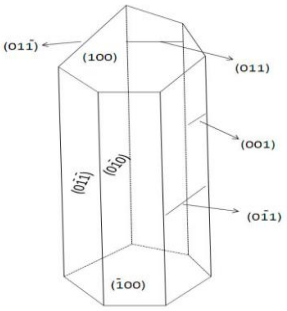
Crystal growth, structure, mechanical, thermal, spectral and optical properties of organometalic of L – Proline Strontium Bromide Tetrahydrate single crystal for nonlinear optical applications

M. Thairiyarajaa and S. Sathiskumar b,*

[a]PG and Research Department of Physics, Government Arts College, Ariyalur – 621 713 Tamil Nadu, India.
[b]Post Graduate Department of Physics, Srinivasan College of Arts and Science, Perambalur – 621 212, Tamil Nadu, India,
***Email:** sathiskumarphy@gmail.com*

Growth of organometalic nonlinear optical (NLO) L – Proline strontium bromide tetrahydrate (LPSBT) single crystals were reported for the first time by slow evaporation technique. Crystal structure was elucidated by single crystal X – ray diffraction analysis. Fourier transform infrared and FT - Raman spectroscopic studies were performed to indentify the various functional groups present in the grown crystal. Optical transmittance of the grown crystal was investigated by UV – Vis – NIR spectral studies. The lower cut off wavelength of the grown crystal is observed at 240 nm. The photoluminescence spectral study of the grown crystal showed an emission peak at 410 nm. Mechanical strength was assessed by Vickers microhardness measurements. The dielectric constant and dielectric loss were studied as a function of frequency at various temperatures. Thermal stability of the grown crystals was studied by thermogravimetric analysis, differential thermal analysis and differential scanning calorimetry. The laser induced surface damage threshold for the grown crystal was determined using Nd:YAG laser. The Kurtz powder second harmonic generation efficiency of grown LPSBT is about 0.8 times that of potassium dihydrogen orthophosphate.





References

1) S. Sathiskumar, T. Balakrishnan, K. Ramamurthi, S. Thamotharan, Acta Cryst. E71 (2015) 1199 –1202.
2) G. Anandha Babu, P. Ramasamy, Mater., Chem. Phys. 113 (2009) 727 – 733.
3) Z. Rzaczynska, R. Mrozek, T. Glowiak, J. Chem. Crystallogr. 27 (1997) 417 – 422.

****

PP-87

Influence of Si_3N_4 Coating Thickness on Multi-Crystalline Silicon Ingot: Oxygen Impurities

G. Anbu, G.Aravindan, M. Srinivasan[a)] and P. Ramasamy

SSN Research Centre, SSN College of Engineering, Kalavakkam, Chennai – 603110.
[a)]Email: *srinisastri@gmail.com*

Multi crystalline silicon (mc-Si) is an important substrate material for solar cells. The efficiency of the processed cells depends strongly on the concentrations of carbon and oxygen in the material. Oxygen related defects can reduce the minority carrier lifetime in solar cells. Multi crystalline silicon solar cell is usually made by using directional solidification grown mc-Si wafer. Si_3N_4 coated quartz crucible is used. The main concerns during solidification of multi-crystalline silicon are to avoid impurities entering the silicon from the crucible, to minimize the stresses that are created during solidification and the subsequent cooling which generate dislocations in the material. The main impurities in the silicon lattice are carbon, oxygen and nitrogen and metals which reduce the efficiency of the solar cells. The record lab cell efficiency is 26.7% for mono-crystalline and 22.3% for multi-crystalline silicon wafer-based technology. In this investigation, we simulate the directional solidification process with various Si_3N_4 thickness coated quartz crucible and analyses the oxygen impurity distribution in the melt during the various crystallization time and in the silicon ingot after end of the solidification. The effect of si_3N_4 coating thickness on grown mc-Si ingot was investigated by using the directional solidification process. The distribution of oxygen impurities in silicon melt at the various crystallization time and in the silicon ingot after the end of solidification was investigated. 200 micro meter Si_3N_4 coating thickness results in oxygen concentration 3.08E15, 7.44E15 and 4.53E15 atom/cm^3 at bottom, center and top of grown mc-Si ingot.

****

PP-88

Studies on growth and optical behaviour of L- Ornithine Monohydrochloride Single crystal for nonlinear applications

Nikhilesh Kumar Dilwaliya[1,*], N. Vijayan[2,3], M. A. Shah[1], Debabrata Nayak[2,3], Manju Kumari[2,3], Sudha Yadav[2,3], R.P. Pant[2,3]

[1] National Institute of Technology Srinagar, Hazratbal, Kashmir, 190006.
[2] Academy of Scientific and Innovative Research CSIR – National Physical Laboratory, New Delhi – 110012, India
[3] CSIR – National Physical Laboratory, Dr. K.S. Krishnan Road, New Delhi – 110012, India
Email: *nikhileshkumar988@gmail.com*

The excellent nonlinear and electro optical features of amino acid based grown single crystals have made them suitable for various scientific and technological applications. Organic amino acid single crystals have lower mechanical and thermal stability. This leads to development of hybrid single crystal growth which possesses more mechanical and thermal stability as

compared to organic and can be more suitable for nonlinear applications. In this work we have grown amino acid based hybrid single crystal of L – Ornithine using the conventional slow evaporation solution growth technique (SEST). The structural information and the lattice dimensions of unit cell of the ingot crystal was confirmed using powder X – ray diffraction analysis. The presence of strain was calculated using Wlliamson – Hall plot. The functional group and the existence of chemical bonds in the structure were identified by FTIR. The formed single crystal was characterized by UV – visible spectroscopy in order to find its transparency in visible region and was observed that crystal possesses wide significant transparency for the entire visible region with less absorption. The direct optical band gap of this ingot has also been determined using Tauc's plot. The wide optical band gap and transparency in visible region of the grown crystal makes it suitable for various nonlinear applications. Further photoluminescence was carried out for finding the emission wavelength of the material to find the appropriateness of crystal to work in visible region.

****

PP-89

Crystal growth, structural, piezoelectric, photoluminescence and HOMO-LUMO mechanism of guanidinium tetrafluoroborate single crystal

S. Nandhini[1], P. Murugakoothan[1,2]*

[1]MRDL, PG and Research Department of Physics, Pachaiyappa's College, Chennai – 600 030.
[1,2]Department of Physics, C. Kandaswami Naidu College for Men, Chennai – 600 102.

A semi-organic single crystal, guanidinium tetrafluoroborate (GFB) was successfully grown using slow evaporation solution growth technique. The present work explains the experimental and theoretical aspects of GFB crystal. The cell parameters of the grown titular crystal were confirmed using single crystal X-ray diffraction study. The solubility nature of the GFB single crystal was analyzed. Piezoelectric nature was confirmed by determining the piezoelectric charge coefficient (d_{33}). Emission property of grown crystal was characterized using photoluminescence study. The quantum chemical calculation of the title crystal was performed. The energy gap (E_g) of GFB was computed using HOMO-LUMO orbitals. The 3D-matrix of hyperpolarizability tensor components was computed to enumerate the NLO activity. These results reveal that the titular compound exhibit good optical and NLO properties.

***Keywords*:** NLO crystal; Solubility; Piezoelectric charge coefficient; Photoluminescence

****

PP-90

Compact discussions on the structural, morphological and optical properties of thiophenol capped cadmium sulphide (CdS) quantum dots

S. Muniyappan, P. Murugakoothan*

MRDL, PG and Research Department of Physics, Pachaiyappa's College, Chennai-600 030.
** **Email:** murugakoothan03@yahoo.co.in*

This article describes the synthesis of CdS quantum dots by conventional chemical precipitation technique using thiophenol as a stabilizer. Structural information, crystallite size, lattice strain and dislocation density were determined by powder XRD analysis. FESEM and TEM analyses were used to investigate the morphology, particle size, phase identification and particle size distribution of the CdS nanoparticles. EDX analysis gives the elemental composition of the title compound. UV-vis-NIR reflectance spectroscopy brings out the nano-regime nature and bandgap of the resultant CdS product. Photoluminescence analysis describes the various emission properties of CdS quantum dots. The emission spectrum was analyzed through Commission International de I'Eclairage (CIE) 1931 chromaticity diagram to explore the dominant emission from the CdS quantum dots. DLS analysis gives out the information regarding secondary particle size of CdS nanoparticles. This work may help to develop a better understanding of solution growth mechanism and stabilizing nature of nanoparticles through chemical synthesis technique. The CdS quantum dots are useful for the photovoltaic device applications.

***Keywords*:** Thiophenol, Blue shift, Reflectance, Photoluminescence.

****

PP-91

Electronic, Nonlinear Optical and Optical limiting properties of 2- Amino-3-(1H-imidazole-4-yl) Propanoic Tetrafluoroborate (2A3PT) Single Crystal

M.Madhangi1, P. Murugakoothan1, 2*

[1]MRDL, PG and Research Department of Physics, Pachaiyappa's College, Chennai – 600 030.
[2]Department of Physics, C. Kandaswami Naidu College for Men, Chennai- 600 102.
***Email**: murugakoothan03@yahoo.co.in* ***Tel:** +91 9444447586*

A semi-organic nonlinear optical (NLO) single crystal of 2-amino 3-(1H-imidazole-4-yl) propanoic tetrafluoroborate (2A3PT) was synthesized and grown by the slow evaporation solution technique (SEST) at room temperature by using millipore water as a solvent. The crystal system has been confirmed from the single crystal X-ray diffraction study. The title compound crystallizes in the monoclinic crystal system with non- centrosymmetric space group of P21. Dielectric properties such as dielectric constant and dielectric loss were studied as a function of temperature and frequency to find the charge distribution within the crystal. The nonlinear absorption coefficient, nonlinear refractive index and nonlinear optical susceptibility of the grown crystal

were determined using Z-scan technique. The optical limiting behavior of the 2A3PT crystal is found to saturate with threshold and amplitude of 15.48 mW/cm2 and 6.45 mW/cm2 respectively.

****

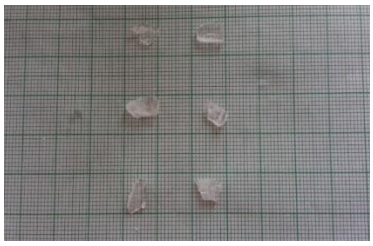
PP-92

Growth, Structure, Vibrational, Optical characterization of Imidazolium Glycine NLO Single Crystal

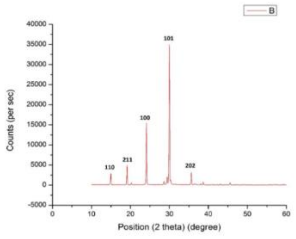
Author1[a] – S. Ranjith Priyan , Author2[b] R. Fathima Beebei

[a]Department of Physics-PG, K.S.Rangasamy College of Arts and Science (Autonomous), Tiruchengode – 637215
[b]Department of Physics-PG, K.S.Rangasamy College of Arts and Science (Autonomous), Tiruchengode - 637215
***Email:** fouziyafouzi373@gmail.com*

Crystal growth is one of the most important field of material science, which involves controlled phase transition. A nonlinear single crystal of Imidazolium glycine were grown by slow evaporation method at room temperature in universal solvent. The solution were prepared by mixing of Imidazole with glycine in 1:2 ratio. Optically clear and well-shaped crystals were grown. The characterisation of grown crystal by powder XRD, FT-IR, UV visible method which is used to know about functional groups, spectral analysis and identification of crystalline material. From the Powder X-Ray diffraction it is found that the Imidazolium Glysine crystal belongs to Monoclinic crystal system. The highest peak value is 30.0160˚ obtained. The FTIR analysis reveals C=C, C=N stretching frequencies and the carboxylic acid, amine, aromatic functional groups. The UV-Vis spectroscopic studies shows that the grown crystal have high transparency in entire visible region. The absence of strongly conjugated bonds leads to higher optical transparency in the visible and UV spectral regions. The lower cut off wavelength was observed at 220 nm and it shows around 95% transparency of the grown crystal.



Imidazolium Glycine Crystal image



Powder XRD pattern of crystal

****

PP-93

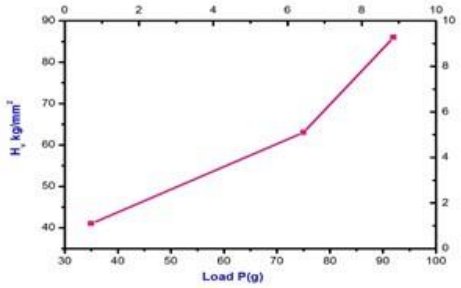
Growth & Structure of Inorganic Pottasium Penta Borate Tetra Hydrate (PPBTH) NLO Single Crystal

[a]C. Bavatharani, G. Suguna & G.Vanmathi , [b]R. Fathima Beebei

[a]Department of Physics-PG, K.S.Rangasamy College of Arts and Science (Autonomous), Tiruchengode - 637215
[b] Department of Physics-PG, K.S.Rangasamy College of Arts and Science (Autonomous), Tiruchengode – 637215
***Email:** fouziyafouzi373@gmail.com*

Crystal growth is a vital and fundamental part of materials science and engineering. The crystal of PPBTH were grown by slow evaporation method at room temperature. For this water taken as a solvent. The solution were prepared by mixing of Pottasium Hydroxide with Boric acid in the 1:3 ratio. Optically well clear and well-shaped crystals were grown. The grown crystal characterized by powder XRD, FT-IR, UV visible for identification of crystalline material, functional groups and spectral analysis and also the hardness of the material will be characterized. From the PXRD it is found that PPBTH crystal belongs to orthorhombic crystal system. The highest peak value is 15.5˚ obtained. FTIR analysis reveals C=C, C- H, N-H stretching frequencies. The UV-Vis spectroscopic studies shows that the grown crystal have high transparency in entire visible region. The UV-Visible absorption spectrum of title compound in the region from wavelength of 190-1100 nm. The lower cut-off wavelength of grown crystal is 210 nm. The strong absorption band corresponds to the presence of water molecules and luminescence nature of the sample. Vickers's hardness number for PPBTH crystal shows that the hardness increases with the increase of load.

Imidazolium Glycine Crystal image



Hardness pattern of crystal

****

PP-94

Effect of Cd/Ni inclusion on structural and magnetic properties of strontium hexaferrite

T. Jayakumar and C. Ramachandra Raja*

Government Arts College (Autonomous), Kumbakonam-612002, India
***Email:** crrajaphy@gmail.com*

Cd/Ni substituted strontium hexaferrite $SrFe_{12-2x}Cd_xNi_xO_{19}$ (for x=0.0,0.1 and 0.2) has been prepared via sol-gel method. The synthesized samples were sintered at 950 ˚C. Powder X-ray diffraction (XRD) results establishes the single-phase magnetoplumbite structure. Lattice parameters (a and c), cell volume (V_{cell}) and crystallite size (D) have been determined. The magnetic characteristics such as saturation magnetization (M_s), retentive magnetization (M_r), and coercive field (H_c) have also been determined from VSM data (hysteresis loop). The value of M_s Increases, M_r and H_c decreases with increase in dopant concentration. FT-IR and Raman analysis reveals that the metal-oxygen vibrations present in various sites. The result reveals that Cd/Ni substituted strontium hexaferrites are suitable candidates for microwave devices and recording media.

****

PP-95

Effects of Rb and Cs dopants on the structural and optical properties of potassium pentaborate crystal

A.N.Vigneshwaran[1] and C. Ramachandra Raja[2*]

[1]Department of Physics, Khadir Mohideen College, Adirampattinam-614 701, Tamilnadu.
[2]Government Arts College (Autonomous), Kumbakonam-612 002, Tamilnadu.
***Email:** crrajaphy@gmail.com*

In order to fulfill the need of the lasers for various sectors, it is important to develop the NLO crystals with better efficiency. Wide transparency in the electromagnetic spectrum is a peculiar property of borate crystals. Wide transparency of the potassium pentaborate (KB5) crystal even in the deep UV region which makes it as a prominent NLO crystal. Since it is a unique NLO crystal, it is important to analyse the KB5 crystal with the addition of dopants. In this work, growth and characterization of the Rb and Cs doped KB5 crystal are reported. From the UV-Vis-NIR spectrum of the crystal the cut-off wavelength is found out to be 230nm. Structural perfection and influence of dopants on crystal structure was analysed using HRXRD analysis. Second harmonic generation of the crystal is confirmed using Kurtz-Perry powder technique. Z-scan analysis is carried out to study the third order properties of the crystal using He-Ne laser of wavelength 632.8nm. It reveals the self-focusing and saturable absorption properties of the grown crystal.

****

PP-96

Effect of Annealing on Directionally Solidified Multi – Crystalline Silicon Ingot for Solar Cell Applications

S. Sanmugavel*, G. Aravindan, S. G. Nagarajan, V. Kesavan and P. Ramasamy

SSN College of Engineering, Kalavakkam, Chennai – 603 110.
***Email:** sanmugavels@hotmail.com*

Renewable energy is blooming now-a-days due to the shortage of fossil fuels and requirement of energy, in which, the solar energy is unlimited and free. That is why people are moving towards harvesting solar energy for their energy needs. Solar energy is being harvested in many ways but wafer-based silicon photovoltaic technology holds 95% of share of production. India has set a goal to produce 175 GW energy through renewable sources by 2022 in which 100GW power will be produced by solar photovoltaic and more than 26 GW of solar photovoltaic modules were installed already. There are many types of silicon cells and many ways are there to produce them. One of them is multi-crystalline silicon solar cell produced by directional solidification process. Even though the conversion efficiency of multi-crystalline silicon (22.3%) is less compared to the conversion efficiency of mono-crystalline silicon (26.7%), the mc-Si contributes 62% of production in wafer-based PV technology.

In this present work, two-dimensional numerical simulation on growth of multi-crystalline silicon (mc-Si) ingot using directional solidification has been carried out. Two mc-Si ingots were grown to study the effects of annealing on multi-crystalline silicon ingot using CGSim commercial software. First ingot is as grown and the latter one is annealed after growth process. The thermal field has been analysed in both the systems during and after growth process. The thermal stress and dislocation density of the grown ingots have been investigated. Based on the simulation results the experiment has been made to grow the high quality mc-Si ingot for PV applications. The different stages of growth process such as melting of silicon, solidification of melt and annealing of grown ingot have been discussed. The quality of the grown ingot has been investigated based on the minority carrier lifetime measurements. The results show that the ingot which has undergone annealing will be having less stress and dislocations, and will have more minority carrier lifetime. The results may be useful for the mass production of mc-Si ingots for PV applications.

****

PP-97

Anatase TiO_2 Nanospheres Synthesized Via Sol-Gel Process with High Light Scattering Effect for Dye-Sensitized Solar Cell Application

N. Santhosh*, K.R. Acchutharaman, R. Isaac Daniel, M. Senthil Pandian, P. Ramasamy

SSN Research Centre, SSN College of Engineering, Chennai-603 110, Tamilnadu, India
***Email:** santhosh.10409@gmail.com*

In this paper, anatase TiO_2 nanospheres were prepared by sol-gel process with cetyl-trimethylammonium bromide (CTAB) as surfactant and polyethylene glycol (PEG m.w. 20,000) as template. The synthesized TiO_2 nanospheres were analyzed by XRD, FESEM, Raman and UV-visible diffuse reflectance. The prepared TiO_2 nanospheres are have high crystallinity anatase phase with a diameter from 50 to 200 nm. The spherical morphology were formed through the aggregation of interconnected nanoparticles, which are provide the high specific surface area and high light scattering ability. The dye sensitized solar cells (DSSCs) based on the TiO_2 nanospheres demonstrated power conversion efficiency of 5.2% as against 2.7 % of commercial P25 photoanode under standard AM 1.5 G illumination (100 mW/cm^2), mainly due to the superior light scattering effect, dye loading capacity, crystal phase and inter and intra sphere connection. This work provides potential candidate to develop the photoanode material with magnificent photovoltaic performance.

****

PP-98

Investigation of Structural and Magnetic Phase Behaviour of Nickel Oxide Nano Particles under Shock Wave Recovery Experiment

A. Rita, A.Sivakumar, S.A.Martin Britto Dhas*

*Department of Physics, Abdul Kalam Research Centre, Sacred Heart College, Tirupattur, Tamilnadu, India-635 601 **Email:**: martinbritto@shctpt.edu **Mobile**: +91-8903101253*

In this current research article, nickel Oxide (NiO) nanoparticles were synthesised by hydrothermal process. The stability of structural and magnetic properties of NiO nanoparticles has been examined by shock wave loading experiment. In the present experiment, authors employed the shock waves with Mach Number 2.2 and different shock pulses such as 100 and 200 pulses were loaded on the test samples. The test sample's molecular and crystalline structure stabilities are scrutinized by FTIR and PXRD technique. SEM and VSM techniques are utilized to understand the surface and magnetic behaviour of NiO nanoparticles. The obtained crystallographic structure, molecular structure and surface changes are not showing any significant changes, but in magnetic properties the value of the saturated magnetization has gradually reduced by the impact of shock waves. The obtained results of NiO nanoparticles have stable crystalline properties against the impact of shock waves; hence the test material is suggested to the aerospace and military including high temperature and high pressure operation conditions.

Keywords: NiO nanoparticles, Shock waves, Structural stability.

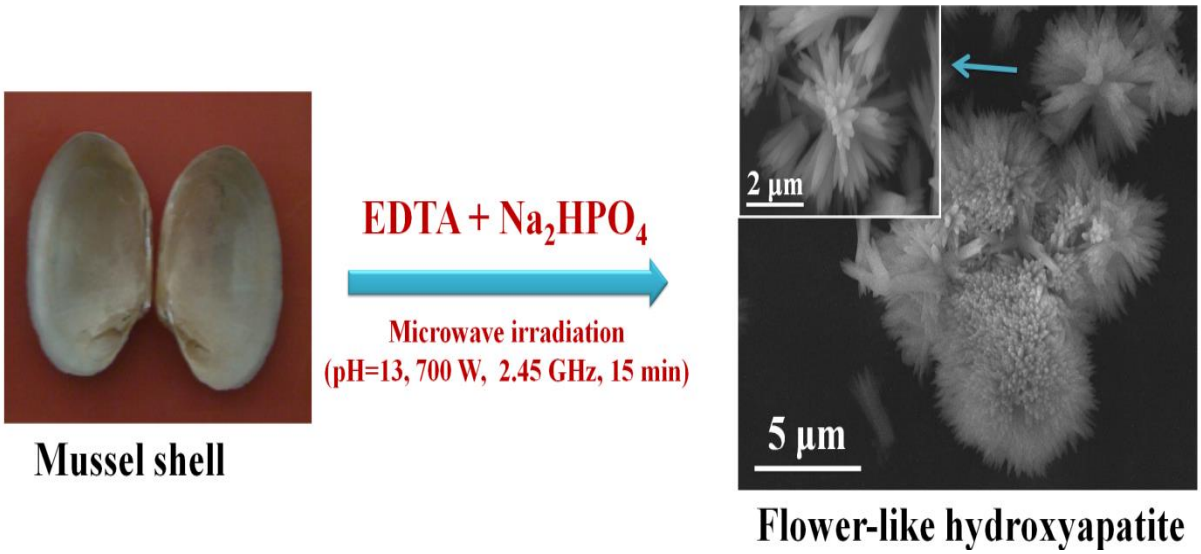
PP-99

One step method to synthesize flower-like hydroxyapatite architecture using mussel shell bio-waste as a calcium source

S. Mowniga*, G. Suresh Kumar*

Department of Physics, K.S. Rangasamy College of Arts and Science (Autonomous), Tiruchengode 637 215, Tamil Nadu, India.
***Email:** ksmowniga6598@gmail.com*

Mussel shell, a calcium-rich resource, is found plenty in nature. We have developed a novel and facile method to convert mussel shell bio-waste into hydroxyapatite (HAp) biomaterial using microwave irradiation with the aid of ethylenediaminetetraacetic acid (EDTA) as chelating agent. The obtained HAp had flower-like morphology which can be a potential candidate for developing biomaterial for orthopedic applications. Moreover, the developed method has the potential to recover the bio-waste and reduce environment pollution.



****

PP-100

Synthesis and characterization of hydroxyapatite nanocrystals for the developments of biological probes

R. Kirubakaran, M. Dhanasekar, G. Suresh Kumar*

Department of Physics, K.S. Rangasamy College of Arts and Science (Autonomous), Tiruchengode 637 215
**** Email:** gsureshkumar1986@gmail.com*

The development of novel biological probes has received much attention in biological staining and diagnostics. So far, several materials such as semiconductor quantum dots and rare earth elements have been widely investigated for this purpose. However, toxicity of these materials significantly prevents their biomedical applications. Biocompatible luminescent materials have received much attention for the development of novel bioprobes. In the present work, we have synthesized the flower-like hydroxyapatite (HA) nanostructure from eggshell biowaste via a simple and rapid microwave conversion process. The synthesized product is identified as Mg containing B-type carbonated HA. It showed an intense blue emission between 360 nm to 550 nm with maximum around 430 nm under UV light excitation (λ_{ex}= 344 nm). This blue emission might result from the carbonate related impurities present in the structure of HA and it can be a potential luminescent material for the development biocompatible probes.

****

PP-101

Morphology and size controlled synthesis of zinc oxide nanocrystals and their optical properties

S. Surendhar, G. Suresh Kumar*

Department of Physics, K.S. Rangasamy College of Arts and Science (Autonomous), Tiruchengode 637 215, Tamil Nadu, India.
**** Email:** gsureshkumar1986@gmail.com*

Zinc oxide (ZnO) is one of attractive II–VI compound semiconductor material due to its wide direct band gap (3.37 eV) and large excitonic binding energy (60 meV) at room temperature Owing to its unique chemical and physical characteristics, ZnO is widely used in various applications such as gas sensors, light emitting diodes, field effect transistors, ultraviolet lasers, photodetectors, solar cells, photocatalysts, and so on. We report the facile synthesis of zinc oxide (ZnO) nanostructures with different sizes and morphologies by a rapid microwave assisted synthesis using ethylenediamminetetraacetic acid (EDTA) and/or trisodium citrate as chelating agents and their characterization. The obtained ZnO nanostructures having hexagonal Wurtzite structure with different morphologies. With aid of EDTA and/or trisodium citrate, flowers, flakes, solid spheres and porous spheres were obtained by controlling the crystal growth habit and the concentration of ZnO growth units under microwave irradiation. The optical behaviour was

analyzed using UV-Visible spectroscopic technique which indicates that the prepared ZnO nanostructures exhibit band gap between 3.27-3.37 eV due to potential fluctuations in electronic band. Consequently, developed method can be potential method to obtain ZnO nanostructures for wide spectrum of applications.

****

PP-102

Study of Seed Layer Effect on ZnO Nanorods Growth on SiO_2 / Si by Hydrothermal Method

ManojkumarChellamuthu, Subramanian Senthilkumar,SivamKalaiyarasi*

Department of Physics, K.S . Rangasamy College of Arts and Science (Autonomous), Tiruchengode, Tamilnadu - 637 215, India.
* ***Email**: manojmuthu321@gmail.com, kalaiphysics.buc@gmail.com*

The proposed study is to prepare vertically aligned Zinc Oxide nanorods by hydrothermal method by using different seed layer deposited by RF sputtering over the SiO_2 / Si substrate. The surface morphology, structural and optical properties were analyzed by using X-ray Diffraction (XRD), Field Emission Scanning Electron Microscope (FESEM) and X-ray Photoelectron spectroscopy (XPS). It is observed that the seed layer thickness effects largely on the orientation of the nanorod, length of the nanorod and crystalline properties of the nanorod. The investigation can prove a new path electronics device compatible with advanced CMOS technology for different electronics optical and gas sensing application.

Keywords: ZnO nanorod, vertical growth, hydrothermal method, ZnO seed layer.

****

PP-103

Effect of Additives on Characterizations and Photocatalytic Activity of BiPO4-ZnO Nanocomposite Prepared via Wet chemical synthesis method

Prabhakaran Selvaraj, * Subramanian Senthilkumar

Department of Physics , K.S . Rangasamy College of Arts and Science (Autonomous), Tiruchengode, Tamilnadu - 637 215, India.
* ***Email:** prabhakaranselva26@gmail.com, senthil.phy10@gmail.com*

A systematic investigation on the structural, functional, optical and photocatalytic properties of $BiPO_4$-ZnO nanocomposites of different molar ratios were synthesized by wet chemical method, which is simple technique and cost effective. X-ray diffraction (XRD) analysis revealed that the presence of $BiPO_4$-ZnO nanocomposites with the particle size of 40-50nm. Raman analysis shows that the formation of wurtzite hexagonal phase of ZnO and $BiPO_4$ tetrahedron with high symmetry vibration. Optical studies shows that the blue shift in the absorption spectra with increasing the concentration of $BiPO_4$-ZnO nanocomposites.

Photoluminescence (PL) spectra indicates the presence of oxygen vacancy is the important factor for narrow band gap of ZnO. Methylene blue (MB) degradation of the prepared $BiPO_4$-ZnO nano composites were studied. Under UV irradiation, ZnO shows higher degradation efficiency (98%) than $BiPO_4$ (94%).From the results, the possible degradation due to the generation of actives species induced by the photo generated electrons.

Keywords: $BiPO_4$-ZnO nanocomposites; wet chemical method; XRD; UV; PL; Photo degradation; Methylene blue.

****

PP-104

EFFECT OF TEMPERATURE ON THE MECHANICAL, OPTICAL, ELECTRICAL AND MAGNETIC PROPERTIES OF NANO HYDROXYAPATITE BIOMEDICAL APPLICATIONS

Nikela Ramasamy * Subramanian Senthilkumar

Department of Physics, K.S . Rangasamy College of Arts and Science (Autonomous), Tiruchengode, Tamilnadu - 637 215, India.
** **Email:** nikilarubaniki@gmail.com, senthil.phy10@gmail.com*

Nano sized hydroxyapatite [$Ca_{10}(Po_4)_6(OH)_2$ or HA] was prepared by wet-chemical precipitation route using Calcium chloride di-hydrate $CaCl_2.2H_2O$ and di-Sodium hydrogen phosphate Na_2HPO_4. The thermal decomposition of the prepared sample was carried out by Thermogravimetric and Differential Scanning Calorimetry (TG/DSC) analysis upto 1000˚C, it showed that the sample was stable up to 919.2˚C. The phase formation, functional groups, morphology and magnetic property of as-prepared and annealed samples were characterized using X-ray diffraction (XRD), Fourier Transform Infrared (FTIR), micro Raman, Field Emission Scanning Electron Microscopy (FE-SEM), Transmission electron microscopy (TEM) and vibrating-sample magnetometer (VSM). By adopting Scherer method detailed structural analysis like the crystallite size, strain, dislocation density, lattice parameter, unit cell volume, surface area and fraction of crystallinity were calculated for as-prepared and annealed HA_P samples.

Keywords: Hydroxyapatite, Nanoparticles, XRD, FTIR, Raman spectra

****

PP-105

Eco-friendly Synthesis and characterization of Nanostructured SnO2 Thin films using Citrus aurantifolia peel extract by Spin coating MethodMegala

Devarasan , Subramanian Senthilkumar, Sivam Kalaiyarasi*

Department of Physics , K.S . Rangasamy College of Arts and Science (Autonomous), Tiruchengode, Tamilnadu - 637 215, India.
* ***Email:*** *megaladevarasan@gmail.com, kalaiphysics.buc@gmail.com*

The present study of reveals green synthesis of nanostructured SnO2 is becoming increasing importance as eco-friendly alternative to traditional production process because of its growing industrial applications. Thin film is produced using $SnCl_2.2H_2O$ solution which prepared in *citrus aurantifolia* peel extract and DH_2O. The solution which prepared in *citrus aurantifolia peel* extract by spin-Coating System fabricated. Thin film are annealed at 100˚C and 200˚C for one hour. The structural properties were studied using characterization such as XRD, FTIR, and UV-Visible, analyzed for synthesized SnO2 thin films.

Keywords: SnO2 nanoparticles, Green synthesis, Spin coating, citrus aurantifolia peel leaf extract

****

PP-106

Preparation and Characterization of Ni Added ZnO Thin film by Sol-Gel Spin Coating Techniques

Saranya Natarajan, Subramanian Senthilkumar, Sivam Kalaiyarasi*

Department of Physics, K.S . Rangasamy College of Arts and Science (Autonomous), Tiruchengode, Tamilnadu - 637 215, India.
* ***Email:*** *saranyanatarajan98@gmail.com, kalaiphysics.buc@gmail.com*

Pure and Ni added Zinc Oxide thin films were prepared by Sol-gel method using Spin – Coating technique on glass substrates. The influences of nickel on ZnO thin films are characterized by Powder X-ray diffraction study. Pure and Ni added are hexagonal wurtzite structure without any secondary phase in c-axis orientation. The SEM image of thin films show uniform sphere like particles covered completely on glass substrates. All the films exhibit transmittance of 85- 95% in the visible rang up 800 nm and cut-off wavelength observed at 394 nm corresponding to the fundamental absorption of ZnO. The Photoluminescence property for pure and Ni added Zno thin films has been studied and results are presented details.

Keywords*:* Sol-gel method, XRD, SEM, PL.,

****

PP-107

Phytosynthesis and Characterization of TiO2 Nanoparticles using Diospyros ebenum leaf extract and their Antibacterial and Photocatalytic Degradation of Crystal Violet

M.C.Satheesh, * Subramanian Senthilkumar

Department of Physics, K.S. Rangasamy College of Arts and Science (Autonomous), Tiruchengode, Tamilnadu - 637 215, India.
** **Email:** mcsatheeshk3@gmail.com, senthil.phy10@gmail.com*

Crystalline anatase titanium dioxide (TiO_2) nanoparticles (Nps) were prepared and green synthesis of Diospyros ebenum leaf extract as reducing agent and were the reported first time. The Crystallization nature, morphology of the particles, and stability of the nanoparticles were investigated at different calcinations temperatures. The Synthesized of TiO_2 nanoparticles were investigated for the performance of photodegradation of crystal violet under UV light irradiation. Effects of temperature on structural properties, Photocatalytic activity, and antibacterial activity of TiO_2 Np were evaluated. This study revealed that TiO_2Np synthesized at 600 C exhibited high photocatalytic efficiency excellent antibacterial activity.

***Keywords**:* Diospyros ebenum, TiO_2NPs, Photocatalytic, Crystal Violet, antibacterial activity

****

PP-108

Green synthesis of CeO2- TiO2 compound using Cleome chelidonii leaf extract for excellent photocatalytic activity

Rangasamy Mayilsamy, * Subramanian Senthilkumar

Department of Physics, K.S . Rangasamy College of Arts and Science (Autonomous), Tiruchengode, Tamilnadu - 637 215, India.
** **Email:** anbanamayil35@gmail.com, senthil.phy10@gmail.com*

A facile novel green synthesis of Cerium oxide doped titanium dioxide (CeO_2- TiO_2) nanocompound was prepared using *Cleome chelidonii* leaf extract as the reducing agent and was investigated for the photodegradation of dyes under UV light irradiation. The synthesized compounds are characterized by X-Ray Diffraction Raman spectroscopy, UV and FL spectroscopy, XPS, FESEM and TEM.The results signify that prepared materials show superior result compared to bare TiO_2 and CeO_2 particles due to alternation in the band gap, surface adsorption and enhanced photo responsive were played a virtal role in performing the degradation activity. In corporation of TiO_2 and CeO_2 controls the higher recombination of electron – hole and acting as electron supporter for creating more cation / anion and additionally, the higher amount of oxygen content in CeO_2 leads an advantage in degradation of dyes which shields the valency bands which reduce the recombination

***Keywords*:** *Cleome chelidonii* leaf extract, XRD, XPS, TEM

****

PP-109

Effective photocatalytic performance of CdS/TiO2 nanocomposite Synthesized under hydrothermal process

B. GomathiThanga Keerthana1, P. Murugakoothan1, 2*

1MRDL, PG and Research Department of Physics, Pachaiyappa's College, Chennai 600 030.
2Department of Physics, C. Kandaswami Naidu College for Men, Chennai 600 102.
**** Email:** murugakoothan03@yahoo.co.in, **Email:** bgtkeerthi@gmail.com*

CdS/TiO_2 nanocomposite was synthesized by hydrothermal method. The sample was calcined at 150°C for 2 hours. The as prepared sample was characterized by various techniques. The mixture of hexagonal wurtzite/ anatase phase formation of CdS/TiO_2 nanocomposite was identified from powder X-ray diffraction analysis. The transmission electron microscopy (TEM) images show that the CdS nanoparticles are intimately enwrapped over the TiO_2 nanotubes. The presence of functional groups in CdS/TiO_2 nanocomposite was identified using IR spectroscopy. The CdS/TiO_2 nanocomposite exhibited strong absorption in the visible region. Brauner, Emmett and Teller (BET) analysis used to determine the surface area of the sample is found to be 30.47 m^2/g and an average pore diameter is 23.61 nm. The ability of the sample to degrade methylene blue was investigated under solar irradiation.

Keywords: Hydrothermal method, CdS/TiO_2 nanocomposite, TEM, BET analysis.

****

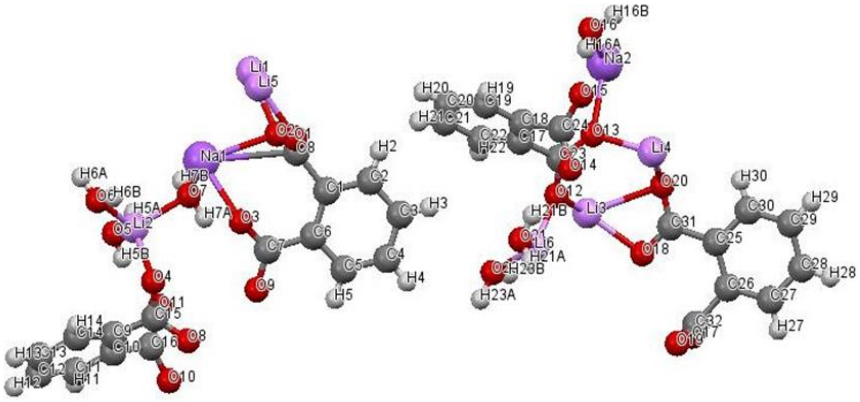
PP-110

Crystal Growth and Optical Properties of Lithium Sodium Acid Phthalate (LiNaP) Single Crystal

C. Elavarasia, S. Mugundanb,*, C.Senthilkumarc , M.Srinivasand

[a] Department of Physics, Sri Vijay Vidyalaya College of Arts and Science, Dharmapuri-636807
[b]Department of Physics, Sri Vijay Vidyalaya College of Arts and Science, Dharmapuri-636807
[c]Department of Physics, Government Arts and Science College, Hosur, Tamilnadu- 635110
[d]Department of Physics, SSN College of Engineering, Kalavakkam, India- 603 110
***Mail:** mugumam@gmail.com*

Lithium sodium acid phthalate crystal was grown by slow evaporation method. Single-crystal X-ray diffraction shows that the grown crystal has a triclinic crystal structure. LiNaP has three-dimensional network of O⋯⋯H---O hydrogen bonds. It has positive coefficient solubility. The functional groups were identified by FTIR spectroscopy. The UV–Vis-IR absorption spectrum was analyzed The UV-VIS-NIR study was carried out from 200nm to 1100 nm.



****

PP-111

EFFECTS OF AMINO ACIDS DOPED WITH KCL CRYSTAL BY SLOW EVAPORATION TECHNIQUES

T.R.K. Priyadarzini, S. Sharmila Ruth Ebenezar, R. Daphine

Department of Physics, The American College,Madurai

Email: *trkpriya@gmail.com*

Single crystal technology is one of the most important fields of material science and the mother of all the recent technologies and modern science. Now a day, crystal growth technology has rapid advancement in the development of nonlinear optical materials (NLO). The organic NLO materials have large nonlinear optical coefficients compared to inorganic material and it has excellent mechanical and thermal properties. Hence, an enormous work has been done in its growth and characterization. Potassium Chloride (KCL) is one of the well-known non-linear optical material. In this study, we attempt to synthesis amino acid doped potassium chloride by slow evaporation technique. The amino acids are doped with KCL and the grown crystals are characterized to know about its structure and interactions.

Keywords: Crystal growth, Amino acids, slow evaporation.

****

PP-112

An investigation on optical, mechanical and thermal properties of nickel sulphate hexahydrate single crystal – a UV band pass filter

J. Thirupathy, S.A. Martin Britto Dhas*

Department of Physics, Abraham Panampara Research Centre,
Sacred Heart College, Tirupattur- 635601, India
***Telephone:** +91-8903101253, **Email:** brittodhas@gmail.com*

Nickel sulphate hexahydrate (NSH) crystal is known to be an excellent material for UV light band-pass filter applications. In this research work, good quality and enhanced size of NSH single crystal has been effectively grown by implementing Sankaranarayanan – Ramasamy (SR) method. After a prolonged period of 185 days, a fine quality of transparent as well as improved size single crystal of NSH with dimension 220 mm in length and 12 mm in diameter has been successfully harvested. The grown crystal has been subjected to various characterizations as that of single crystal X-ray analysis to confirm the crystal system with unit cell parameters, UV-Vis analysis to know the transmission spectrum, FTIR spectral analysis to find out the functional groups and photoluminescence study to affirm the green emission of the crystal. NSH crystal falls into the category of soft material as identified by microhardness study and etching study confirms that it has good quality as the surfaces are almost free of defects. Photoacoustic spectroscopy has been utilized to find the thermophysical parameters. The resultant value of thermal diffusivity is compared with few other familiar nonlinear optical materials such that it is asserted by the observed superior value of NSH single crystal that it is an added advantage for band-pass filter and harmonic generation applications.

Keywords: NSH crystal, optical, mechanical properties, etching, photoacoustic spectroscopy

Figure: Photograph of as grown NSH single crystal

****

PP-113

Growth, Structural and Optoelectronic Properties of γ-glycine Single Crystals Using Nickel Chloride as an Additive

V.Vijayalakshmi[1], P.Dhanasekaran[2 *] and N.M.Ganesan[1]

[1] Crystal Growth Laboratory, Department of Physics, Erode Sengunthar Engineering College, Erode- 638057, India.
[2]Department of Physics, Bharathiar University Arts and Science College, Modakurichi- 638104, India.
Email: *dhanasekaranp1@gmail.com*

In this current investigation, we have successfully grown γ-glycine single crystals using nickel chloride as an additive by slow evaporation method at ambient conditions. Powder X-ray Diffraction study confirms γ-polymorph structure and it crystallizes into a hexagonal crystal system with a space group of $P3_1$. UV–Visible transmittance spectra was recorded for the grown crystal to analyse the transparency in visible and near infrared region (NIR). In Kurtz-Perry powder test, the SHG efficiency of grown crystal is found to be 1.88 times higher than reference KDP crystal. The dielectric constant and dielectric loss of nickel chloride added glycine was carried out as a function of frequency and the obtained results were discussed.

****

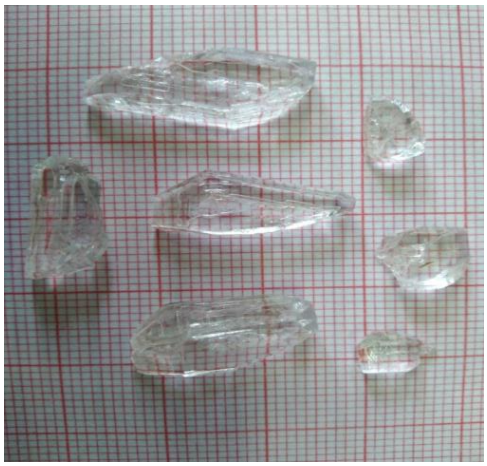
PP-114

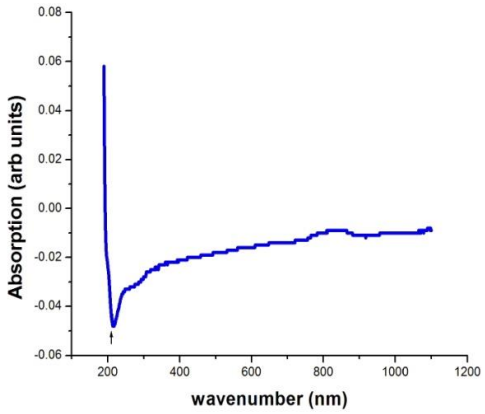
SYNTHESIS AND CHARACTERIZATION OF GLYCINE MAGNESIUM CHLORIDE

K. Karthika[*] and P. Srinivasan[*+]

** PG & Research Department of Physics, Chikkaiah Naicker College, Erode, Tamil Nadu, India*
*[*]**Email:** Dr. P Srinivasan (sriniscience@gmail.com)*

Glycine magnesium chloride semiorganic nonlinear optical single crystal has been successfully grown by using aqueous solution by slow evaporation method in room temperature. The grown crystals were colorless and transparent. The crystalline nature and purity of the grown crystals are confirmed by powder X-ray diffraction pattern. The FT-IR spectra recorded to identify the functional groups present in GMC crystals. The optical quality of the grown crystals has been analyzed by Ultra Violet (UV) visible studies and it confirms that grown crystals have lower cut off wavelength at 216 nm.





Keywords: Solution growth, FT-IR studies, UV-VIS

****

PP-115

Growth and Characterization of Histidine Phosphite Single Crystals

M. Arivumathi, C. Shobana and S. Shanmuga Sundari*

PSGR Krishnammal College for Women, Coimbatore – 641004, Tamil Nadu, India.
***Email:** shanmugi.s@gmail.com*

Great efforts have been devoted to the research and design of highly efficient nonlinear optical (NLO) materials due to their widespread applications such as high-speed information processing, optical communications, and optical data storage. Amino acids are widely utilized because they not only contain chiral carbon atoms directing the crystallization in non-centrosymmetric space group, but also possess zwitterionic nature favouring crystal hardness. In the design of novel materials for nonlinear optical applications, hydrogen bonding often acquires on an important role. In a hydrogen bonded organic crystals very large non-linear optical and electro optics responses have been obtained due to the delocalised π-electron systems. L- Histidine phosphite (HPI) crystallizes in non- centrosymmetric monoclinic system with space group P21. In the present work, slow evaporation technique has been adopted to grow the HPI single crystals. The grown crystals were characterized for its structural, optical and dielectric properties.

****

PP-116

SYNTHESIS AND CHARACTERIZATION OF COPPER SULPHATE DOPED CLUM LEAVES EXTRACT

R. Revathi[1]*, P. Manikandan[1] and V. Vinayagamoorthy[1]

[1]Department of Physics, Dr. N.G.P. Arts and Science College, Coimbatore- 641 048.
***Email:** rrevathi@drngpasc.ac.in*

The advancement of nanotechnology is increasing the interest of researchers towards synthesis of nanoparticles because nanoparticles have a rising application towards the medical field. Copper sulphate and their derivatives has been used for different medical purposes like to prevent asthma, cough, and gallbladder and used to test blood for anemia. An adaptable technique was implemented for the synthesis of copper nanoparticles using leaves extract of bamboo leaves extract; first we prepare leaves extract in distilled water. An appropriate amount of the extract is added with copper sulphate solution, and we observed the change in color of the solution from colorless to colored solution, this indicates that there is a formation of CuNPs. These green synthesis CuNPs were characterized with the help of ultraviolet visible spectroscopy, X-ray diffraction and Scanning Electron Microscope. It was observed that the bamboo leaf extract can reduce Cu ions into CuNPs within 8-10 minutes of reaction time. Thus, this method can be used for rapid and eco-friendly green synthesis of stable Cu NPs.

Keywords: Green synthesis, Structural properties, SEM and Medical application

****

PP-117

ROLE OF Sn ON STRUCTURAL AND OPTICAL PROPERTIES OF ZnO CHUNK SHAPED NANOSTRUCTURES

S.S. Kanmani[1*], K.R.N. Jaya Prasanth[1] and V. Gowthambabu [1]

[1]Department of Physics, Dr. N.G.P. Arts and Science College, Coimbatore- 641 048.
***Email:** kanmani@drngpasc.ac.in*

The undoped and Sn doped ZnO chunk shaped nanostructures were synthesised by simple and cost effective chemical method. Sn was doped in order to study the influence of structural and optical properties. X-ray diffraction revealed a hexagonal wurtzite ZnO structure with average crystallite size from 20-30nm. With increase of Sn doping, intensity of SnO_2 peak increases but the intensity of ZnO decreases. The chunk-shaped nanostructures comprised of regular arrangement of non-uniform sized spherical-shaped nanoparticles. The high magnification of SEM image shows that the size of the spherical shaped nanoparticles varies from 35-49 nm. The Uv-Vis-NIR spectroscopy revealed that absorbance spectra of pristine and Sn doped ZnO obtained in the range of 300-800nm and optical energy band gap of samples obtained from 2.9 to 3.2eV from Tauc's plot. UV excitonic emission of pure ZnO is red shifted from bulk ZnO excitons. On the other hand, Sn doping generates defects and also destroys the actual crystallinity (observed from XRD) and this is confirmed from the decrease of UV emission intensity with the increase of Sn

content in ZnO. The pristine and Sn doped ZnO chunk shaped nanostructures can be further act as metal oxide semiconductor layer for dye sensitized solar cell.

Keywords: Chunk shaped nanostructure, X-ray measurements, and Nanotechnology

****

PP-118

EFFECT OF Mg DOPING ON STRUCTURAL AND OPTICAL PROPERTIES OF ZnO CHUNK SHAPED NANOSTRUCTURES

V. Gowthambabu[*1] and S.S. Kanmani[1]

[1]Department of Physics, Dr. N.G.P. Arts and Science College, Coimbatore- 641 048.
***Email:** gowthambabu44@gmail.com*

The pristine and Mg doped ZnO chunk shaped nanostructures were synthesised by simple and cost effective chemical method. Mg was doped in order to study the influence of structural and optical properties. The structural properties of synthesized samples were analysed by Powder X-ray diffraction, scanning electron microscope and energy dispersive X-ray analysis. The optical properties were characterized by UV-Visible spectroscopy and photoluminescence spectroscopic techniques. X-ray diffraction reveals a hexagonal wurtzite ZnO structure with average crystallite size of 31nm. Mg-doped samples do not exhibit any additional diffraction peaks, which confirms the absence of any secondary phase formation. Highly magnified SEM image shows that the individual particles are distinctly spherical in nature but their regular arrangements finally appeared as rectangular chunk shaped nanostructures. Mg doping does not affect the actual morphology of ZnO. The Uv-Vis-NIR spectroscopy reveals that absorbance spectra of pristine and Mg doped ZnO obtained in the range of 300-800nm and optical energy band gap of samples obtained from 3.15 to 3.17eV from Tauc's plot. UV excitonic emission of pure ZnO is red shifted from bulk ZnO excitons. This excitonic emission energy from PL spectrum directly correlates with the UV spectral band gap. The doping of any dopant in ZnO lattice changes PL properties. NBE position undergoes slight blue shift upon increase of Mg dopant. It is a direct consequence of the band gap widening with Mg dopant as absorbed form UV-Vis absorption spectra. The analysed pristine and Mg doped ZnO chunk shaped nanostructures can be further used as metal oxide semiconductor layer for dye sensitized solar cell.

Keywords: Chunk shaped nanostructure, optical properties and solar cells

****

PP-119

GROWTH, CHARACTERIZATION AND NUCLEATION KINETICS OF L-GLUTAMINE BASED NON LINEAR OPTICAL CRYSTALS

Jebaraj P.G[a,c], Sivashankar.V[a], Helina.B[a] and Anuradha.G.V[b]

[a]Department of Physics, St.Xavier's College, Palayamkottai
[b]Department of Physics, Sri Parasakthi College for Women, Courtallam
[c]18231282131041, Manonmaniam Sundaranar University, Tirunelveli-12
***Email:** jebaraja@gmail.com*

Growth of amino acid based crystals is important because of their advantageous optical properties. Nonlinear Optical crystals are useful in the field of optoelectronics and photonics. In the present investigation, L-Glutamine Potassium Chloride, L-Glutamine Ammonium Chloride and L-Glutamine Barium Chloride crystals were grown with different molarity ratios by slow evaporation technique. Structural parameters were confirmed by powder X-ray diffraction. Functional groups present in the grown crystals were identified with the help of FTIR spectroscopy. Thermal stability was confirmed from the TGA/DTA studies. Metastable zone width and induction periods were determined experimentally. Transparency of the crystals were confirmed by UV-Vis spectroscopy. Nucleation kinetics of L-Glutamine based crystals were carried out. Nucleation parameters such as interfacial energy (γ), Gibbs free energy change (ΔG), nucleation rate (J) and radius of critical nucleus (r*) were calculated for optimizing the growth conditions by low temperature solution growth technique.

****

PP-120

SELECTIVE REVIEW OF RECENT RESEARCHES ON THE GROWTH AND CHARACTERIZATION OF TECHNOLOGICALLY SIGNIFICANT CRYSTALS BY S-R METHOD

Jebaraj.P.G[a,c], Sivashankar.V[a], Helina.B[a] and AnuradhaG.V[b]

[a]Department of Physics, St.Xavier's College, Palayamkottai
[b]Department of Physics, Sri Parasakthi College for Women, Courtallam
[c]18231282131041, Manonmaniam Sundaranar University, Tirunelveli-12
***Email:** jebaraja@gmail.com*

For any research, the Review of Literature is important. It is the preparatory work for taking up a futuristic research in a particular field. It enables a Researcher to become an expert in the selected field. It also provide foundation of knowledge on the research field of interest. Sankaranarayanan-Ramasamy (SR) method was discovered in the year 2005. It is a novel method to grow large size crystals. By this growth method, single crystals shall be grown in a particular controlled orientation by achieving higher crystallization rate. Many research papers have been appeared in International Peer Reviewed Journals. Several laboratories in India and Abroad are growing crystals by SR method. Positive, Negative, High, Moderate and Low solubility materials

shall be grown by SR method. Modified SR Method, Vacuum Assisted SR Method are the different types of SR Method. The Rotational SR Method (RSR) is the latest modification in SR Method.

In this Review, Twenty selected recent researches on SR Method which were published between the year 2010 and 2019 were reviewed. The Growth and Characterization of technologically significant crystals such as L-Glutaminium P-Toluene sulfonate, Phase matching KDP single crystal, 4-Hydroxy l-Proline (HLP), [1 1 0] Ammonium nickel sulfate crystal, L-alaninium p-toluenesulfonate, Ammonium D,L-Tartrate (AMT), Transition metal doped l-cysteine hydrochloride monohydrate, Bisthiourea Zinc Chloride (BTZC), Tris (glycine) Calcium (II) dichloride (TGCC), 1,3,5-Triphenylbenzene, Bis (hydrogen L-malate) hexahydrate, Pure and L-Lysine added ADP, <001>Triglycine Zinc Chloride(TGZC), Lithium Sulphanilate Hydrate (LS), Ninhydrin, L-Arginine phosphate monohydrate, [001] α-Nickel sulphate hexahydrate, Potassium dihydrogen orthophosphate. KDP (KH_2PO_4), β-alanine doped glycine phosphite (β-alanine-GPI), Bisthiourea zinc chloride were reviewed, analysed and chronologically arranged.

Keywords: Review, Crystal Growth, Significant Crystals, S-R Method

****

PP-121

Investigation on dielectric and mechanical properties of guanidinium p-toluenesulfonate single crystal

Paavai. Era[a], P. Murugakoothan[a,b]*

[a]MRDL, PG and Research Department of Physics, Pachaiyappa's College, Chennai–600 030.
[b]C. Kandaswami Naidu College for Men, Chennai–600 102.
***Email:** murugakoothan03@yahoo.co.in* ***Tel:** +91 9444447586

A promising third order nonlinear optical material, guanidinium p-toluenesulfonate (GPTS) was synthesized adopting slow evaporation solution growth technique (SEST) and the crystals were harvested from aqueous methanolic medium. Constitution of crystalline material was confirmed by single crystal X-ray diffraction study. The title compound crystallizes in the monoclinic crystal system with space group $P2_1/c$. The charge distribution within the crystal was found using dielectric property as a function of temperature and frequency. The low dielectric loss at higher frequency confirms that the grown crystal is of good quality with fewer defects. Anisotropy in the mechanical behavior of GPTS crystal was observed while measuring for individual planes. The experimental results ensure the optimum utilization of the material for device fabrication purpose.

Keywords: Bulk crystal, SEST, polarization, low dielectric loss, mechanical anisotropy.

****

PP-122

GROWTH, EXPERIMENTAL AND THEORETICAL INVESTIGATIONS ON PIPERAZINIUM BIS (5-CHLORO-2-HYDROXYBENZOATE) NONLINEAR OPTICAL MATERIAL

G. Parvathy, R. Kaliammal, G. Maheshwaran, K. Velsankar, S. Sudhahar*

Department of Physics, Alagappa University, Karaikudi-630 003
Email: *sudhahars@alagappauniversity.ac.in*

A novel report on piperazinium bis(5-chloro-2-hydroxybenzoate) organic crystal was grown by solution growth technique. P5C crystal has Monoclinic crystal structure with a centrosymmetric space group $P/2_1$ by a single crystal X-ray diffraction. The vibration modes and ^1H proton NMR were confirmed through FTIR and NMR spectral analysis. The optical studies of UV-Vis and PL spectrum showed cutoff wavelength at 380 nm and excitation wavelength at 350 nm. The thermal stability of P5C crystal is 175^oC was confirmed by TG-DSC analysis and the mechanical property was analyzed by Vickers microhardness tester. Second harmonic generation (SHG) efficiency was tested by the Kurtz-Perry powder technique. The theoretical calculations were analyzed by DFT B3LYP method 6-311++G(d,p) as a basis set. The crystal structure of P5C was optimized and the geometric parameters were compared. The charge transfer properties and hydrogen bonding interaction were analyzed by HOMO-LUMO and natural bond (NBO) analyses. The Mulliken charge, molecular electrostatic potential (MEP), polarizability and first order hyperpolarizability of the present molecule were theoretically analyzed.

****

PP-123

INVESTIGATION OF PIPERAZINIUM PHTHALATE SINGLE CRYSTAL WITH ITS MECHANICAL, THERMAL, STRUCTURAL AND MORPHOLOGICAL PROPERTIES FOR NON-LINEAR OPTICS

*G. Maheshwaran, K. Velsankar, G. Parvathy, R. Kaliammal, S. Sudhahar**
Department of Physics, Alagappa University, Karaikudi-630003.
***Email**: sudhahars@alagappauniversity.ac.in*

Good quality organic non-linear optical single crystal of piperazinium orthophthalate (PPA) was grown successfully by solution growth at room temperature by achieving the supersaturation state in slow evaporation method. The powder XRD analysis confirms the crystalline nature and structural parameters of the grown PPA crystal. The FTIR spectra confirm the existence of acid-base functional groups along with their vibrational mode exhibited, present in the grown PPA crystal. UV–Vis spectrum exhibits better transparency in the visible region with cut-off wavelength of 330 nm and the energy band gap (E_g) is analyzed to be 3.8 eV. Photoluminescence spectra shows good optical property with the excitation of 342 nm and two emission peaks in near edge UV band with blue emission at 364 and the energy transition in deep level defect states in crystals by exhibiting the green emission at 533 nm respectively. The thermal stability and the thermal absorption of the PPA crystal were identified by the TG - DTA analysis and obtained thermal stability was up to 88^oC. Vickers micro hardness test illustrates the

mechanical stability of the grown PPA crystal and it belong to soft category (n=4.6). Second harmonic generation study illustrates the grown PPA crystal (λ=532 nm) exhibit good nonlinear optical response.

****

PP-124

Dual approach on experimental and theoretical investigation of new single crystal from amino acid family

Radhakrishnan Anbarasan, Palaniyasan Eniya and Jeyaperumal Kalyana Sundar*

**Materials Science Laboratory, Department of Physics, Periyar University, Salem, India*
***Email:** jksundar50@gmail.com*

In current technological world, the need of efficient nonlinear optical material is a key role in material science for optoelectronic applications. A new non-centrosymmetric crystal L-Histidinium trichloro cadmium (HCC) was grown by slow evaporation method. The crystalline structure of the material was explored with single crystal X-ray diffraction analysis. The functional groups present in the molecule was confirmed by vibrational analysis. The material hold more than 80 % transmission in the entire visible region and the cut-off wavelength is 240 nm. The thermal decomposition and melting point were explored by thermal analysis and it reveals that the material is thermally stable upto 217 ^{o}C. The crystal gives 1.4 time greater second harmonic generation efficiency compared to typical KDP material. All the structural and optical results reveal that HCC crystal is prominent material for second harmonic generation applications.

****

PP-125

Molecular structure and Electron deisnty analysis of high energetic 2,4,6-Trinitropyridine N-oxide molecule via Quantum chemical calculations

L. Sathya[1], B. Gnanavel[1], A. David Stephen[2] and P. Srinivasan[1*]

[1] PG & Research Department of Physics, Chikkaiah Naicker College, Erode – 638 004
[2]Department of Physics, Sri Shakthi institute of Engineering Technology, Coimbatore – 641 062
***Email:** sriniscience@gmail.com*

The TNPyO molecule has been optimized using quantum chemical methods (B3LYP/Aug-cc-PVDZ) in order to find the potential HEDMs. The predicted optimized structural parameters are in good agreement with experimental value. This quantum chemical calculation reveals that, the TNPyO molecule C–NO_2 and N–O (N-oxide) bonds are weak, which confirms that these bonds are the weakest bonds in the molecule. The simulated TNPyO molecule reveals negative oxygen balance (-0.86%) and its energy gap is 3.45 eV. The calculated impact sensitivity and imbalance parameters show very good agreement with already known explosives. These computational studies are the viable pathway and helpful for the experimental characterization and production of some of high energetic nitrogen rich molecules.

***Keywords*:** Electron density, Explosives, Oxygen balance, Impact sensitivity and ESP

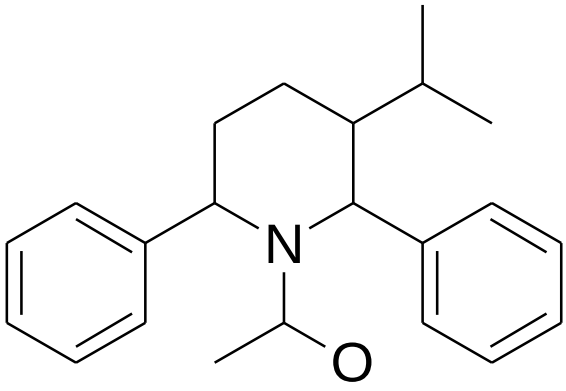
PP-126

Crystal structure, DFT and Hirshfeld surface analysis of *N*-Acetyl-t-3-Isopropyl-r-2,c-6-diphenylpiperidine (AIDP)

P.Periyannan,[a] M.Beemarao[a], K.Ravichandran[a]*

**Department of physics, Kandaswami Kandar's College, Velur, Namakkal 638182, India*
***Email:** kravichandran05@gmail.com*

The syntheses and crystal structure of *N*-Acetyl-t-3-Isopropyl-r-2,c-6-diphenylpiperidine, C_{22} H_{26} N O are described . The space group was deduced to be $P2_1/n$ and the crystal system is also monoclinic. The sum of bond angles around N1 atom in the molecule is 359.8° indicating sp^2 hybridized state. The planar phenyl rings at 2nd and 6th positions of the piperidine ring are occupy axial and equatorial orientation. The crystal packing is stabilized by C-H...O types of intra and intermolecular interactions, which link the molecules into a chain extending along *b-axis*. Geometrical parameters have been carried out by the computational density functional theory (DFT) B3LYP/6–311G (d,p) basis set . Further, Hirshfeld surface and electrostatic potential surface analysis were carried out to understand the intermolecular interactions along with their graphical visualization.



****

PP-127

Synthesis and Characterization of $Zn_{1-x}Yb_xO$ nanocrystals for thermoelectric applications

T.M.V.Murugu Thiruvalluvan[1], V.Natarajan[2], P.Anandan[3], M.Arivanandhan[4], R.Jayavel[4]

[1]Department of Physics, Manonmanium Sundaranar University, Tirunelveli
[2]Department of Physics, Dr.Sivanthi Aditanar College of Engineering, Tiruchedur
[3]Department of Physics, Thiru Kolanjiappar Govertment Arts College, Virudhachalam
[4]Centre for Nanoscience and Technology, Anna University, Chennai

Zinc Oxide (ZnO) is one of the promising II-VI semiconductors with wide bandgap and useful for many applications include solar cells, biological labeling, optoelectronics. The thermoelectric properties of ZnO have been extensively investigated. The thermoelectric performance of a material can be determined by the dimensionless figure of merit (ZT). The problem with ZnO is its high thermal conductivity at elevated temperature which results low ZT of the material. Nanostructuring the material is an effective way to control the phonon transport thereby thermal conductivity of the material. In the present work, $Zn_{1-x}Yb_xO$ nanocrystals were synthesised by sol-gel method with various Yb concentration in the precursor solution. The structural properties of the material was studied by X-ray diffraction analysis and it confirms the crystal structure of the material. The functional groups of the nanocrystals were analysed by Raman spectra. The morphology of the synthesized nanocrystals was studied by FE-SEM analysis. The thermoelectric properties of the nanostructured material was studied as a function of temperature and Yb concentration.

Keywords: Thermoelectric materials; Nanostructures; Figure of merit; ZnO

****

PP-128

Preparation and characterization of $Bi_xCo_{3-x}O_4$ nanocrystals for thermoelectric applications

A. S. Alagar Nedunchezhian[1], D.Sidharth[1], N. Yalini Devi[1], R.Rajkumar[2], G.Anbalagan[2], M. Arivanandhan[1]*, R. Jayavel[1]

[1]Centre for Nanoscience and Technology, Anna University, Chennai 25.
[2]Department of Nuclear Physics, University of Madras, Guindy Campus, Chennai-25.

Thermoelectrics is a promising technology to convert waste heat into electricity. The performance of a thermoelectric material can be determined by its figure of merit (ZT) which is directionally proportional to electrical conductivity and inversely proportional to thermal conductivity. Therefore a material should have high electrical conductivity and low thermal conductivity for better thermoelectric performance. Nanostructuring is one of the promising ways to control the thermal conductivity by enhancing the phonon scattering. The oxide thermoelectric material shows the promising improvement in recent years. Moreover, the oxide materials are non-toxic, environmental friendly and ease to process as a device. The cobalt oxide based

thermoelectric materials are more reliable and hence a series of $Bi_xCo_{3-x}O_4$ nanocrystals are synthesized. The structural, morphological and compositional properties of the prepared materials are studied by XRD SEM and EDS analysis. Thermoelectric properties of the synthesized materials are studied at various temperatures. The electrical conductivity is measured using the Hall measurement system and the seebeck coefficient is measured using indigenously fabricated Seebeck measurement system at various temperature. Using the measured data, the thermoelectric power factor ($S^2\sigma$, where S is seebeck coefficient and σ is electrical conductivity) is calculated for $Bi_xCo_{3-x}O_4$ samples (where x = 0, 0.025, 0.05, 0.1, and 0.2) and the results are discussed in detail.

Keywords: Thermoelectrics, cobalt oxide, nanosturcturing, oxide thermoelectrics.

****

PP-129

STRUCTURE DETERMINATION AND SPECTROSCOPIC ANALYSIS OF A NEW ACTIVE NLO AZO DERIVATIVE

P.SANGEETHA

Department of physics, Adhiyaman Arts and Science College for Women, Uthangarai – 635207, Krishnagiri, TN, India.
Email: *sanphysics87@gmail.com*

The Azo derivative compound was synthesized by slow evaporation method and the structure of the compound elucidated from single crystal XRD. The UV-visible absorption spectrum indicates cut off wavelength of the crystal is 360nm. The different modes of vibration present in crystal are identified by using FTIR analysis. Single crystal X – ray diffraction analysis reveals that the crystal belongs to monoclinic system. Thermo gravimetric and differential thermal analysis study was carried out to determine thermal properties of grown crystal. The SHG efficiency of azo derivative material is comparable higher than that of KDP.

Keywords: grown crystal, Azo derivative, single crystal XRD.

****

PP-130

HARDNESS AND DIELECTRIC BEHAVIOUR OF LITHIUM SULFATE MONOHYDRATE SODIUM IODIDE CRYSTAL

PREETHA P, CHELLAMMAL R, ANITHALAKSHMI M*

Department of Physics, Adhiyaman Arts and Science College for Women, Uthangarai, Tamilnadu, India, 635 207.
****Email:*** *manithalakshmi30@gmail.com*

Lithium sulfate monohydrate sodium iodide single crystal was grown from Lithium sulphate monohydrate and sodium iodide. The sample was synthesized and grown by slow evaporation technique at room temperature. The grown crystal were subjected to powder crystal

X-ray diffraction study and confirms the crystal nature of it, Fourier Transform Infrared Spectroscopy ensures the functional groups, the mechanical property of grown crystal was tested from Vicker's Micro Hardness analysis and dielectric studies used to analyze the electrical property of the grown sample.

***Keywords**:* Slow evaporation, FTIR, mechanical property, dielectric and electrical property.

****

PP-131

THERMAL CHARACTERISTICS OF SODIUM IODIDE DOPED LITHIUM SULFATE MONOHYDRATE SINGLE CRYSTAL

SARANYA N, ANITHALAKSHMI M*

Department of Physics, Adhiyaman Arts and Science College for Women, Uthangarai, Tamilnadu, India, 635 207.
***Email:** manithalakshmi30@gmail.com*

In this present work single crystals of Sodium Iodide doped lithium sulfate monohydrate (LSMH) have been grown by slow evaporation solution technique at room temperature. The crystalline quality of lithium sulfate monohydrate crystal would be improved by the metal dopant was incorporated into the pure crystals. The grown crystals are clear transparent metal. The powder X-ray diffraction study was carried out to ascertain lattice parameters and identify different phase nature. FT-IR and thermal analysis were carried out to investigate the functional group and thermal behavior of the grown crystals respectively. The grown crystals were found to be transparent in the entire visible region.

Keywords: Powder X-ray diffraction, FT-IR and thermal analysis, UV-visible analysis.

****

PP-132

GROWTH AND CHARACTERIZATION OF L-ALANINE CADMIUM IODIDE CRYSTAL FOR NONLINEAR OPTICAL APPLICATIONS.

S.THANGAVEL*, R.ASHOKKUMAR

PG and Research Dept of Physics, Thiruvalluvar Govt. Arts College,Rasipuram.
***Email:** thangavels1@gmail.com*

Cadmium iodide doped L-Alanine (LACI) semi organic crystal has been synthesized and grown by slow evaporation technique at room temperature. The grown crystal was subjected to single crystal X-ray diffraction analysis. Energy dispersive X-ray analysis (EDAX) reveals the presence of elements in the title compound. UV-Visible-NIR transmittance studies were carried out for the grown crystal. From the transmittance data, the optical bandgap as a function of photon energy was estimated and the different optical constants were calculated. The mechanical property of LACI crystal was investigated employing microhardness studies. A fluorescence study was

performed for the LACI crystal. The thermal property of the LACI crystal was analyzed by thermogravimetric and differential thermal analysis studies. The second harmonic generation (SHG) efficiency of the title crystal was investigated. The magnetic and electrical properties were estimated by VSM analysis and impedance study, respectively.

Keywords: X-ray diffraction, Fluorescence, Microhardness, Thermal analysis, Impedance, VSM.

****

PP-133

GROWTH AND OPTICAL PROPERTIES OF PURE AND METAL IONS DOPED SODIUM D-ISOASCORBATE MONOHYDRATE SINGLE CRYSTALS

R. Sathyaranayanan and M. Selvapandiyan*

Department of Physics, Periyar University PG Extension Centre, Dharmapuri 636 701
Email: Dr.M.Selvapandiyan,(mselvapandiyan@rediffmail.com)

Sodium D-isoascorbate monohydrate Crystal is among the most widely-used commercial NLO materials, characterized by good UV transmission, high damage threshold, and high birefringence, though their NLO coefficients are relatively low. Optically good quality single crystals of pure nickel and zinc doped sodium D-isoascorbate monohydrate will be grown from aqueous solution using slow evaporation technique. Structural characterization of the grown pure, nickel and zinc doped sodium D-isoascorbate monohydrate crystals will be carried out by powder X-ray diffraction analysis. The functional groups present in the grown crystals were ascertained using FT-IR spectroscopic analysis. The optical properties of the grown crystals have been investigated by using UV–visible spectra. The band gap energy for the doped sodium D-isoascorbate monohydrate crystals has been calculated from optical transmission spectrum. Second harmonic generation test was used to study the NLO properties of pure, nickel and zinc doped sodium D-isoascorbate monohydrate crystals. Powder second harmonic generation efficiency will be confirmed by Kurtz and Perry powder method. The various investigations indicate the changes in structural, optical and NLO properties of the sodium D-isoascorbate monohydrate crystal due to the incorporation of the nickel and zinc doped into the sodium D-isoascorbate monohydrate crystal lattice.

Keywords: Slow evaporation, X-ray, FT-IR, UV, TG-DTA, Z-Scan

****

PP-134

Preparation of 3D flower-like CuO/Co3O4/rGO heterostructure and high performance asymmetric hybrid supercapacitor

S. Prabhu[a], P. Maadeswaran[b], S. Sohila[c], R. Ramesh[a,d*]

[a]Department of Physics, Periyar University, Salem, 636011, Tamilnadu, India.
[b]Department of Energy Science, Periyar University, Salem, 636011, Tamilnadu, India.
[c] Department of Physics, Department of Physics, Shri Sakthikailassh Women's College, Tamil Nadu, India.
[d]Center for New and Renewable Energy Periyar University, Salem, India.
*[*]**Email:** rameshphys@gmail.com*

With increasing energy demand and rapid depletion of fossil fuels, the development of novel renewable and sustainable energy resource become one of the greatest challenges in the energy storage field. Supercapacitors are promising energy storage devices for flexible electronics because of their integration of lightweight, tiny volume and high flexibility. Herein, we described a facile hydrothermal method to synthesized 3D flower-like CuO/Co_3O_4/r-GO composites. Physical and chemical properties were studied by different characterization techniques. FE-SEM result revealed that Co_3O_4 nanoclusters was embroidered on 3D flower like CuO anchored homogeneously on the reduced graphene oxide (r-GO) nanosheets. The CuO/Co_3O_4/r-GO composites shows a high specific capacitance of 1458 F/g at a charge/discharge current density of 0.5 A/g in 3M KOH electrolyte solution. The asymmetric supercapacitor composed of 3D flower like CuO/Co_3O_4/r-GO and r-GO exhibited a specific capacitance of 198 F/g at 2 A/g. Moreover, excellent cycling stability with 97% of the 10000 cycles at 5 A/g both three and asymmetric hybrid supercapacitor system. These findings demonstrate that the CuO/Co_3O_4/r-GO composite material is a promising candidate for supercapacitor applications.

Keywords: CuO; Hydrothermal approach; Electrochemical study: Asymmetric supercapacitor.

****

PP-135

A theoretical interpretation and screening of perylene based metal-free organic dye sensitizers withdifferent lengths and functional groups of acceptors for DSSC's

D. Nicksonsebastin[1], M. Prasath[1,*]

[1] Department of Physics, Periyar University PG Extension Centre, Dharmapuri, 636701
***Email:** sanprasath2006@gmail.com (M. Prasath)*

Perylene based metal-free organic sensitizers are computed through Density functional theory (DFT) and Time-dependent density functional theory (TD-DFT) for the ground state and excited state geometries using 6-311G (d,p) basis set. In this present investigation, 2,5-dip-tolylperylene as an electron donor, phenylthiophene as a π-spacer, and four acceptors, it is named as A1-A4, which have various blends of lengthsand functional groups adjacent to the carboxyl

acid group. Accordingly, A1-A4 sensitizers systematically analyzed with the aid of the use of various parameters which include, Light-harvesting efficiency, Frontier molecular orbital,electron injection,Ultraviolet-visible absorption spectrum, Energized statelifetime (τ), and Non-linear optical properties. As an entire, the designed sensitizers, in particular,A3 has the lowest energy gap and exciton binding energy, highest molar extinction coefficient (ε), good planarity and negative electron injection (ΔG_{inject}) values compared to other designed sensitizers.Based on our result shows that A3 sensitizer is the better candidate for DSSC performances.

Keywords: Dye Sensitizer, DSSC, DFT, Excited state lifetime, Electron injection.

****

PP-136

Quantum mechanical, Spectroscopic and Molecular docking studies of Doxofylline by Density Functional Method

N. Mani and M.Prasath*

Department of Physics, Periyar University PG Extension centre, Dharmapuri-636701
***Email:** sanprasath2006@gmail.com*

The Doxofylline (C11H14N4O4) molecule was optimized using density functional theory (DFT) with B3LYP/6-311G(d,p) basis set. The vibrational frequencies and potential energy distribution (PED) of doxofylline molecule was computed and it shows excellent conformity with the experimental values. The vibrational spectroscopic analysis of anti lung cancer agent doxofylline was performed using Fourier-transform infrared (FT-IR) and Fourier-transform Raman (FT-Raman) spectra. The time-dependent DFT method was engaged to calculate the Frontier Molecular orbitals (FMOs) of the doxofylline molecule and their differences were compared with transitions of UV-absorption spectra. The reactivity and selectivity of the title compound be analyzed using parameters like MEP, global reactivity descriptors, Fukui function and NBO (Natural Bond Orbitals). The molecular orbital contributions were measured use the density of states. Mulliken atomic charges are calculated and interpreted. Thermodynamic properties of the title compound at various temperatures have been calculated, illuminating the correlations the heat capacity (C), entropy (S) and enthalpy (H) changes with temperatures. The doxofylline molecule exhibits good bioactive score and less toxicity. A molecular docking analysis of doxofylline was carried out with non-small cell lung cancer protein cell (EGFRm) and these results show that has lowest binding affinity with inhibition constant when present in the active site.

Keywords: DFT · FT-IR · FT-Raman · HOMO–LUMO , Fukui function , Molecular docking,

****

PP-137

Structure and intermolecular interactions of some benzodiazepine derivative molecules with GABA-A receptor: A molecular docking and quantum chemical analysis

M. Ramaraj and * M. Prasath

Department of Physics, Periyar University PG Extension centre, Dharmapuri-636701
***Email:** sanprasath2006@gmail.com*

Benzodiazepine is an antixylotic agent, induce and maintain sleep, reduce seizures, and induce conscious sedation. It acts as a positive allosteric modulator of gamma-aminobutyric acid-A (GABA-A) receptor. Here some of the benzodiazepine derivative molecules like Halazepam, Ketazolam and Medazepam were evaluated using theory models.

In this context, the molecular geometric parameters were predicted by DFT method and the gas phase is compared with active site. A molecular docking, HOMO-LUMO and dipole moment have been carried out to understand the conformational change in the active site of GABA-A receptor. The nearest neighbours, shortest intermolecular contacts between the molecules and GABA receptor and the lowest binding energy of the molecules have been analysed from the docking method. Further, the electrostatic properties of the molecule also determined. The electrostatic potential (ESP) map of the molecule allows identifying the nucleophilic and electrophilic regions of the molecules. Stability of the molecules arising from hyper conjugative interactions, charge delocalization has been analysed using natural bond orbital (NBO) analysis. The Entropy of the molecules are also performed at B3LYP/6-311G(d,p) levels of theory. In addition, the thermodynamic properties of the compounds were calculated at different temperatures and corresponding relations between the properties and temperature were also studied.

****

PP-138

Spectroscopic investigation (FTIR,FT-Raman), (RS)-N,N-bis(2-chloroethyl)-1,3,2 oxazaphosphinan -2-amine2-oxide an anti-cancer drug by HOMO-LUMO, ADMET and molecular docking evaluation

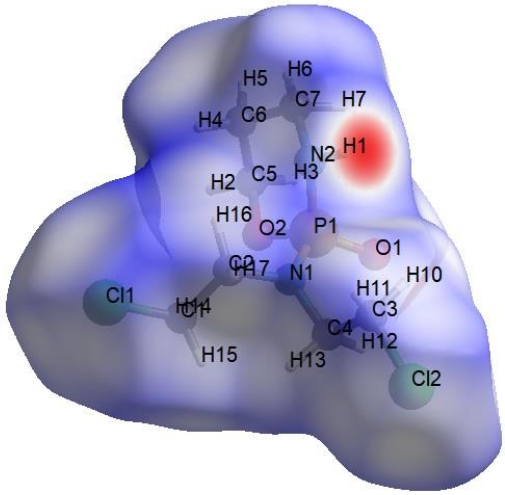
M.Govindammal[1] and M.Prasath[1*]

[1]Department of Physics, Periyar University PG Extension Centre, Dharmapuri-636701
**Email: sanprasath2006@gmail.com (9942922455).*

The Cyclophosphamide molecule was optimized utilizing DFT with B3LYP/6-311++G employing (d,p) basis sets. In the present work, a quantum chemical calculation was followed to study the vibrational frequencies and potential energy distribution (PED) of Cyclophosphamide molecule were calculated and compared with experimental calculations. The band gap energy obtained from the both HOMO-LUMO analysis, this acceptor-donor interaction of the NBO analysis and color code grid traced found the MEP map were analysis. The charge distribution and

Fukui function analysis were performed for the title compound. Intermolecular interaction of the title compound has been examined through Hrishfeld surface analysis. The evaluation of drug-likeness was performed on the basis Lipinski's rule of five and molecular descriptors were used to predict the absorption, distribution, metabolism, excretion and toxicity (ADMET) of the title compound. Biological activity of the title compound confirmed from the molecular docking study anti-cancer protein (PI3K inhibitor) and ligand Cyclophosphamide.

Keywords: DFT, Cyclophosphamide, Lung-cancer, PI3K inhibitor and molecular docking study



****

PP-139

Vibrational, electronic spectral analysis and molecular docking evaluation of Isowighteone as Neuraminidase inhibitor against influenza diseases using DFT simulations

B. Sathya and M. Prasath*

*Department of Physics, Periyar University PG Extension Centre, Dharmapuri – 636701 *Email: sathyacreator@gmail.com*

Influenza (flu) is an infectious viral disease which causes severe illness by RNA virus and capable for morbidity and mortality in annual epidemics. The flu affects the respiratory systems and damages the tissues easily. The elder people affected by flu virus and it causes leading sudden death. The flu unevenly spherical and embraced by a lipid membrane it contains two glycoproteins namely Hemagglutinin (HA) and Neuraminidase (NA) which are fundamental for flu viral disease. The simulation has turned into a purpose for the plan of anti-influenza drugs. The structure of Isowighteone molecule was optimized and their values are compared with experimentally available crystal XRD data. The experimental data of FT–IR, FT–Raman vibrational frequencies and UV-Vis electronic spectra was recorded and their values are in good agreement with the computational results. The title molecule obeys the properties of Lipinski's rule of five, hence the molecule exhibit good bioactive score. Therefore, the title molecule Isowighteone is taken for

further calculation. A molecular docking analysis of Isowighteone was carried out with neuraminidase enzyme. The docking result shows the lowest binding affinity and inhibition constant of the molecule present in the active site, which is considered to be a better inhibitor. The HOMO-LUMO reveals the good kinetic stability and less toxicity of the Isowighteone molecule. The dipole moment is an important molecular parameter to study the orientation of the dipole vector and intermolecular interactions of the molecule such as dipole-dipole interactions of non-bonded type. The molecular electrostatic potential (MEP) shows the chemical reactivity site in Isowighteone. This implies that the title molecule enhances the good candidate for anti- influenza drugs.

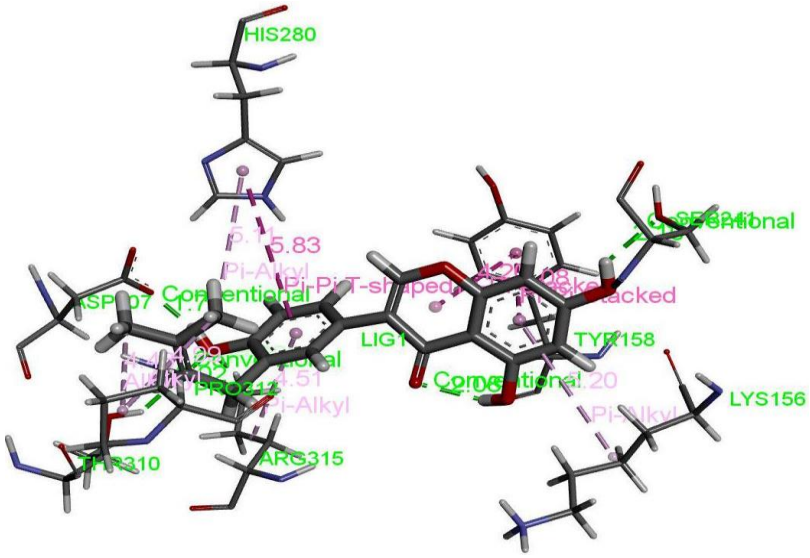


Figure: Intermolecular interactions of Isowighteone with NA enzyme.

****

PP-140

Fabrication of MoO_3/Ag_2S hybridized with graphitic-C_3N_4 for effective catalyst under visible-light exposed photocatalytic activity

Shanmugam Vignesh, Jeyaperumal Kalyana Sundar*

Materials Science Research Laboratory, Department of Physics, Periyar University, Salem - 636 011, Tamil Nadu, India

***Email:** jksundar50@gmail.com; vigneshattur1@gmail.com*

Herein, a novel graphitic carbon nitride (g-C_3N_4) was combined with Ag_2S and MoO_3 to fabricate g-C_3N_4/MoO_3/Ag_2S hybrid nanocomposites via facile calcination and hydrothermal method. And it as visible-light-induced photocatalysts for cationic dyes photodegradation such as RhB and MB. The structural, elemental, optical and chemical composition of fabricated samples were investigated. MoO_3/Ag_2S nanoparticles formed on g-C_3N_4 nanosheets remarkably exhibited the highest photocatalytic activity was 3.5 and 4.7 times higher than that of the pristine g-C_3N_4 in the removal of RhB and MB dyes respectively. The excessive upgrading in photocatalytic activity performance is mainly attributed to the MoO_3/Ag_2S nanoparticles formed on g-C_3N_4 nanosheets,

ensuing that can increase the interfacial charge transfer, effective suppression of recombination of photogenerated electron-hole pairs, and an increase of light absorption. A probable photocatalytic mechanism on the g-C_3N_4/ MoO_3/Ag_2S nanocomposites was proposed. Too, the stability of the nanocomposite was characterized through cyclic photocatalytic tests and enhanced antibacterial activities. The existing work exposes that the combination of the g-C_3N_4/ MoO_3/Ag_2S composite as a promising catalyst should be a good strategy to boost the visible-light exposed photocatalytic degradation of organic pollutants of semiconductor catalysts.

****

PP-141

Structural, spectroscopic, magnetic behaviour and DFT investigations of L-tyrosinato nickel (II) coordination polymer

G. Gayathri, V. Sasikala and J. Kalyana sundar

Material Science Laboratory, Department of Physics, Periyar University, Salem- 636501. Tamil Nadu, India.

1D-coordination polymer {[Ni(L-Tyr)2(μ-4,4'-bpy)].$4H_2O$}$_n$ (1) (L-Tyr = L-tyrosine, 4,4'-bpy = 4,40- bipyridine) is composed of L-tyrosinate anions chelated nickel(II) centres via N amino and O carboxylate atoms, whereas the apices of the elongated octahedral coordination sphere are occupied by the N atoms of 4,4'-bipyridine. Its molecular structure was determined by single-crystal X-ray diffraction and characterized using vibrational (FT-IR), Raman spectroscopy (FT-Raman), electronic (NIR-Vis-UV) and high field electron paramagnetic resonance (HF-EPR) spectroscopy and thermal (TG-DTA, DSC) and magnetic methods. The tetragonality distortion parameter (T) equals 0.945. The g_x, g_y and g_z parameters (HF-EPR spectra) are slightly temperature dependent and the set g_x = 2.178(5), g_y = 2.156(4), g_z = 2.19(1), D = -5.76(2) cm^{-1}, E = -0.41(1) cm^{-1} was found at 5 K. The analysis of the temperature and field dependent magnetization shows the weakness of magnetic interactions in 1.

****

PP-142

GROWTH AND CHARACTERIZATION OF SODIUM PENTA FLUORO ANTIMONATE CRYSTAL

Dr. C.BESKY JOB

Dept. of Physics, Scott Christian College (Autonomous), Nagercoil.

Sodium Penta Fluro Antimonate crystal has attracted the researchers for its superionic conductivity and its electro optic properties. It has been grown by the conventional slow evaporation technique. The single crystal XRD results confirms that the grown crystal belongs to Orthorhombic system with lattice parameters a=5.454 Å, b=8.006 Å, c=11.133 Å, α= β= γ=90^o and has the space group of $P2_12_12_1$. The FTIR spectrum analysis confirmed the functional groups present in the grown crystal, especially the Sb-F bond. UV-Vis spectral studies performed the lower cut off wavelength of the grown Na_2SbF_5 crystal as 311 nm in the UV region. The band gap

energy has been found to be 5.3 eV using Tauc's plot. The dielectric behavior of the grown crystal has been investigated with different frequencies at different temperatures. Activation energy for the migration of ions has been found out at 1KHz and 1 MHz are 0.0032 eV and 0.0026eV. The thermal properties of the grown crystals were studied by TGA-DTA analysis and the melting point has been found out as 472.12^{o}C. It is noticed that the SHG efficiency of the grown crystal is observed to be 0.265 times that of the KDP Crystal.

****

PP-143

Observation of Intermediate Band in $CuGaS_2$ thin films via Fe doping by using Chemical Spray Pyrolysis Technique

S. Suba Viveka and K. Sethuraman

School of Physics, Madurai Kamaraj University, Madurai.
Email: *sethuraman_33@yahoo.com*

We have experimentally studied the intermediate bands formation in the $CuGa_{1-x}Fe_xS_2$ chalcopyrite system.Pristine and Fe-doped $CuGaS_2$ of various compositions are deposited using facile chemical spray pyrolysis technique. The crystal structure, morphology and topography of the deposited thin films are examined using Powder X-ray Diffraction (PXRD), Scanning Electron Microscopy (SEM), and Atomic Force Microscopy (AFM), respectively. The binding energy and chemical composition of Fe doped $CuGaS_2$ thin filmare determined using X-ray Photoelectron Spectroscopy (XPS). The direct and sub-band optical responses have been probed through UV-Vis-NIR spectroscopy (190 nm – 1100 nm). Pristine $CuGaS_2$ (CGS) exhibits a direct band gap of 2.43 eV, with formation of intermediate bands in Fe-doped $CuGaS_2$at 1.82 eV, 1.75 eV, 1.54 eV and 1.49 eV with varying Fe atomic percentage. The highest photocurrent (1.1 mA) and electrical conductivity are obtained for Fe doped $CuGaS_2$ thin films as compared to pristine owed to sub-band optical response.

****

Crystal Display

CD-01

4-Nitrophenol derivative single crystals

T. Kamalesh and P. Karuppasamy

SSN College of Engineering, Kalavakkam, Chennai

Engineering of new nonlinear optical (NLO) materials, structures and devices with enhanced figures of merit has developed over the last two decades as a major force to help drive nonlinear optics from the laboratory to real applications. A lot of experimental and theoretical efforts are focused on the bulk NLO properties as well as their dependence on the first-order hyperpolarizabilities of molecules.

Second-order nonlinear optical (NLO) materials are interesting candidates for number of application like second harmonic frequency conversion, electro-optic modulation and optical parametric oscillation/amplification etc.

The new and efficient nonlinear optical (NLO) organic materials which can fulfill the essential requirements like high laser damage threshold, larges nonlinear figure of merit for frequency conversion, fast optical response time, architecture flexibility for molecular design and optical transparency. Even though organic nonlinear optical materials with aromatic ring have been attracting much attention because of their high nonlinearity, fast response and high optical damage threshold, their practical applications are limited due to poor mechanical, thermal stabilities and the inability to produce and process large crystals.

During the past decade, researchers have shown much interest in the nitrophenol family of crystals due to their high laser damage threshold, wide transparency windows, extended thermal stability and high NLO coefficient.

4-Nitrophenol is a classic dipolar NLO-phore and a typical one-dimensional (1D) donor-acceptor π system, and presence of proton transfer of the phenolic OH of 4-nitropherolate with various organic and inorganic bases results in an enhancement of the hyperpolarizability of both species. Therefore, many 4-nitrophenol derivative nonlinear optical (NLO) single crystals have been synthesized and investigated.

****

ipgi instruments

Technical Support for Electrochemistry, XRD , Polymer & Analytical Instruments.

Electrochemistry:-
Zahner Electrochemical workstation. CIMPS, IMVS,QE
All kinds of cell kits for Electro analytical , corrosion , Battery , high temperature c , Membrane permeation, etc. Custom designed cell kits.
Compact Mini Potentiostat.

Xe light Source – Solar Simulator:- Sciencetech – Canada`

150W ,300W ,1000W, 1600W Xe light source.

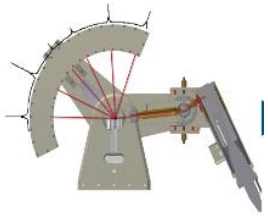
Solar Simulators.

IV testing System. DSSC , PV , Solar cell characterization

IPCE , EQE , IQE efficiency measurements.

Reactors: Customized Reactors , Bio reactors , etc

High Temperature reference electrode 0°C up to +800°C



Thermo - XRD, XPS,

EQUINOX FAMILY **X Ray Diffractometer** **Thermo Inel - France**

EQUINOX 100 : Stand Alone Benchtop X-Ray diffractometer

EQUINOX 1000 : Benchtop X-Ray diffractometer

EQUINOX 3000 : Powder X-Ray diffractometer

EQUINOX 5000 : High resolution X-Ray diffractometer

Chillers – Cold water circulator:-
Compact chillers, Imported chillers. Labtech -Italy
ipgi chillers from 0.5kw ~ 90kw. Temperature range -20oC ~ RT ~ 95°C.

Service Support:-
Service support to various analytical , lab equipment, polymer testing , Polymer Processing instruments , etc.AMC for various analytical , lab equipment , etc.

ipgi instruments , old No.15/1 , New No.46 , Naickamar street , West mambalam, Chennai – 600033 . Ph: 9444345824, 7358082134 , 94444168027, 9094966589. Tel.04443362589. Email: sales@ipgi.co.in, gbsubramani@ipgi.co.in, aanandharaj@ipgi.co.in **www.ipgi.co.in**

Advertisement matter:

With best compliments from

JAISURYA SCIENTIFIC CO

B-19,10TH CROSS
FURTHER WESTERN EXTN
THILLAINAGAR
TRICHY- 620018
PHONE – (0431)- 2740423
MOBILE – 9894054358
Whatsapp - 9894054358
EMAIL- citysury@yahoo.co.in

DEALER IN ALL KIND OF LABORATORY CHEMICALS, EQUIPMENTS, MICROSCOPES, MICROSCOPES- CAMERA, WEIGHING BALANCE, ETC

AUTHORISED DEALERS

CHEMICALS	**:**	**SIGMA-ALDRICH, ALFA, TCI-JAPAN, LOBA, SRL, MOLYCHEM,**
TEACHING KITS	**:**	**MEDOX BIOTECH**
GLASSWARES	**:**	**RIVIERA, BOROSILICATE GLASS**
POLYTHENEWARES:		**TARSONS , POLYLAB, KASABLANKA**
EQUIPMENTS	**:**	**SYSTRONICS, EQUIPTRONICS, BESTO, PICO, OSAW, ELTEK, INCO, MITTAL, SUPERFIT, NUCLEONIX BRANDED EQUIPMENTS**
ELECTROPHORESIS:		**BIOTECH YERCAUD & MEDOX BIOTECH**
MICROSCOPES	**:**	**LABOMED, OLYMPUS, WESWOX, GETNER**
DIGITAL BALANCES:		**SHIMADZU, INFRA BALANCE**