



One Day Theme Meeting on Recent Trends in Solid State Chemistry

April 6, 2024

DAE Convention Centre, Anushaktinagar, Mumbai-400094



Organized by Chemistry Division Bhabha Atomic Research Centre, Mumbai- 400 085

Supported by Society for Materials Chemistry (SMC) C/o Chemistry Division, BARC, Mumbai-400 085

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भारत सरकार Government of India निदेशक, भाभा परमाणु अनुसंधान केंद्र Director, Bhabha Atomic Research Centre सदस्य, परमाणु ऊर्जा आयोग Member, Atomic Energy Commission



MESSAGE

I am glad to know that a "One day Theme Meeting on Recent Trends in Solid State Chemistry (RTSSC)" is being organized on April 6, 2024 at DAE Convention Centre, Anushaktinagar, Mumbai by Chemistry Division, Bhabha Atomic Research Centre and Society for Materials Chemistry.

Solid State Chemistry plays a pivotal role in development of materials for a wide spectrum of applications. With the pace of time, there has been an unprecedented advancement in the synthesis and characterisation techniques, and that has bolstered the growth in this research arena. The role of solid-state chemistry has become even more indispensable with the energy scenario prevalent in the world with energy scarcity looming large upon us. In nuclear industry, the importance of solid-state chemistry cannot be over-emphasized. It is required at every step in the nuclear fuel cycle from mining to reactor applications of materials as well as for the back-end applications. In addition, the development of advanced nuclear technologies that are essential for the energy transition, requires invaluable inputs about better materials that can be provided by solid state chemistry. It is the dire need to understand the behaviour of materials to design novel and better materials for societal development.

In view of its significance, it is essential for the scientists to come together on a platform to discuss the recent development happening in various areas of materials and how solidstate chemistry can contribute in an effective way to the growth of the country and world as a whole.

It is indeed heartening to see the efforts of Chemistry Division to bring together eminent scientists and researchers for discussions on such a relevant theme. I congratulate the organizers for planning this wonderful event and wish an overwhelming success for this theme meeting.

(Vivek Bhasin)



03.04.2024

विवेक भसीन Vivek Bhasin



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भाभा परमाणु अनुसंधान केंद्र внавна атоміс RESEARCH CENTRE

भारत सरकार Government of India भाभा परमाणु अनुसंधान केंद्र BHABHA ATOMIC RESEARCH CENTRE Chemistry Group



I am delighted to know that "One day Theme meeting on Recent Trends in Solid State Chemistry (RTSSC)" is being organized on April 6, 2024 at DAE Convention Centre, Anushaktinagar, Mumbai.

MESSAGE

Today's era is the age of materials. Solid State Chemistry of materials plays a significant role in the development of new technologies. The field of solid-state chemistry comprises of synthesizing new and conventional materials, their characterisation by various techniques and understanding their structure and properties. Over the years, correlating the properties of materials with their crystal structures and microstructure has taken centre-stage as it helps in understanding the nuances of effect of structure on the functionalities exhibited by the material thereby providing keys to improvise the existing materials or designing newer ones. Over last few decades, solid state chemists have been able to develop smart materials having myriad applications in various fields such energy, medical and healthcare, electronics, catalysis, drug delivery etc. In view of the current energy scenario in the world as well as "Net zero resolution" of Government of India, the design and development of effective functional materials based on simple solid-state concepts that could be easily scaled up has become paramount.

I am glad to know that this event aims to discuss recent and contemporary trends in solid state chemistry of relevant functional materials. I am sure it will act as the breeding ground for various new ideas leading to exceptional research and useful technologies.

I heartily compliment the organisers for arranging the workshop on such a contemporary theme and I wish it a grand success.

(A. K. Tyagi)

Preface

Solid-state chemistry is an important research area with profound significance across various scientific disciplines and industrial applications. Advances in solid-state chemistry play pivotal role in the development of efficient and sustainable technologies. The basic principles of solid-state chemistry lay the foundations for the synthesis of new materials with tailored properties. In this context, a theme meeting on "Recent Trends in Solid State Chemistry" is being organized to highlight the current and upcoming developments in solid state research. Eminent scientists and academicians from reputed institutes will share their experiences and research results in this area. The discussions will cover various topics of solid-state chemistry including frontline research areas, structure-property relations, nano materials and low-dimensional solids, nuclear and functional materials, rational design of materials and materials for energy and health applications. The discussions will include, recent developments on fluoride-based materials for X-ray detection, imaging and therapeutic applications, unconventional synthesis routes, and rational design of materials based on structure-property correlation. Role of solid-state chemistry in nuclear power program, ranging from front end to the back end of nuclear fuel cycle, will be discussed. The deliberations will also cover recent developments on ferroelectric and multi-ferroic materials, materials for energy applications, frame-work materials, nanomaterials and metal free polymeric solids. A discussion on the gap between laboratory and market will also be presented.

More than 350 delegates from different Universities, IITs and Research Institutes will participate in this one-day theme meeting. We hope the discussions will enlighten the researchers and motivate them to take-up challenging and relevant research on material science. We wish all the participants a pleasant and fruitful meeting.

B. P. Mandal Vinita Grover Gupta S. N. Achary P. A. Hassan

One Day Theme Meeting on Recent Trends in Solid State Chemistry (RTSSC-2024)

April 06, 2024 (Saturday) DAE Convention Centre, Anushaktinagar, Mumbai – 400094

TECHNICAL PROGRAM OF RTSSC-2024				
09:00-9:30		Registration	DAE Convention Centre, Anushaktinagar	
09:30-10:00 Inauguration Chief Guest: Prof. A. K. Ganguli, Director, IISER, Berhampur				
	Plenary Session Chair: Prof. J. P. Mittal			
10:00-10:30	PL 1	Prof. A. K. Ganguli	Design of Nanomaterials for Medical Applications	
10:30-11:00	PL 2	Prof. A. K. Tyagi	Solid State Chemistry: Basic Concepts to Technologies	
11:00-11:15		H	ligh Tea	
		Tech Chair: P	unical Session-1 <mark>rof. Swapan K. Ghosh</mark>	
11:15-11:40	IT-1	Prof. A. Sundaresan	Magnetoelectric Properties of Chemical Ordering-Induced Pyroelectric Oxides	
11:40-12:05	IT-2	Prof. S. Uma	Targeting Functional Materials by Exploratory Solid State Chemistry Approach and by Rational Design	
12:05-12:30	IT-3	Prof. R. Murugavel	Molecular and Framework Metal Phosphates for Applications in Energy, Catalysis, and Magnetism	
12:30-12:55	IT-4	Prof. Shaikh M. Mobin	Design and Synthesis of Alkali Metals (Na and K) Based CP and MOF: Rare to Novel Topology and Solid-State Structural Transformation	
12:55-14:00	12:55-14:00 Lunch			
		Tech Chair: Pro	nical Session-2 of. Awadhesh Kumar	
14:00-14:25	IT-5	Prof. V. Grover	Solid State Chemistry of Nuclear materials	
14:25-14:50	IT-6	Prof. B. L. V. Prasad	A Chemist's Perspective on Nanomaterial Synthesis: How to Bridge the Gap Between Laboratory and Market?	
14:50-15:15	IT-7	Prof. Amreesh Chandra	Disrupting the Trends in Rechargeable Batteries: Re-Injectable Architectures for Aluminium Ion Full Cells	
15:15-15:30			Теа	
Technical Session-3 Chair: Prof. Niharendu Choudhury				
15:30-16:00	IT-8	Prof. Kulamani Parida	Graphitic Carbon Nitride: Strategies to Enhance its Photocatalytic Activity	
16:00-17:00		Valedio	ctory and Felicitation	
17:00-17:15 High Tea				

ALL ARE CORDIALLY INVITED

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Design of nanomaterials for medical applications

Ashok K Ganguli

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Abstract: Lanthanide-doped bismuth fluorides are emerging as a promising family of phosphor materials because of excellent luminescence efficiency, photostability, low phonon energy and low toxicity. $Yb^{3+}-Tm^{3+}$ doped NaBiF₄ based upconversion nanomaterials have been designed for bioimaging of cells (1). Methylene blue loaded K_{0.3}Bi_{0.7}F_{2.4}: Yb, Er upconversion nanoparticles have been designed for near-Infrared activated photodynamic therapy(2). We have also designed Ln³⁺ (Ln = Tb, Gd) ions doped NaBiF₄(NBF) and K_{0.3}Bi0.7F_{2.4} (KBF) nanoparticles as nanoscintillators for high resolution X- ray imaging (3). Further, we have fabricated flexible, large-area scintillator films for high-resolution XEOL imaging of numerous objects, including biological tissue and electronics chips. PMMA polymer mixed with NBF was used to fabricate the inorganic - organic composite films. Upon UV- visible and X-ray excitation, the NBF:Ln particles and the films show excellent radioluminescence capabilities and good photostability against long-time X-ray exposure. Our findings demonstrated the viability of using the NBF and polymer nanocomposite for X-ray detection and imaging applications. Apart from this we have also explored these bismuth-based host materials as UCNPs for NIR activated photodynamic therapy and bioimaging.

We also discuss design of spiky surface - modified silica nanoparticles in drug delivery enhancing drug loading, controlled release, and therapeutic efficacy. Our approach involves decorating the virusmimicking, spiky silica nanoparticles with MOFs (Metal-Organic Frameworks) like ZIF-8/ZIF-90, imparting pH-responsive properties which enables the selective release of payloads in appropriate environment. These SNP-ZIF-90 particles, exhibit exceptional loading capacity for drugs like Doxorubicin (Dox) and also superior cellular uptake when compared to pure ZIF-90 nanoparticles. Some results on SNP-ZIF for bacterial inhibition and mRNA delivery will also be discussed (4,5).

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	Prof. Ganguli is currently the Director and Professor of Chemical Sciences at			
	IISER Berhampur. He is on Lien from IIT Delhi where he is a Professor of			
- CO (201)	Chemistry. He was Deputy Director, IIT Delhi and was also the founding			
	Director of Institute of Nano Science and Technology (Mohali, India). He			
	studied in University of Delhi (BSc and MSc) and obtained his PhD from			
	SSCU, IISc Bangalore in 1990. He worked at Dupont R&D (USA) and Ames			
	Lab (Iowa, USA) before joining IIT Delhi in 1995. His main interest is in the			
	area of design of new materials, especially nanomaterials for energy conversion			
	and superconducting materials. He has published over 350 papers and has filed			
	five patents (two granted).			
	He is a recipient of the MRSI Medal, CRSI Silver & Bronze Medal & CRSI-			
	CNR Rao National Prize, National Award of Nano Science and			
	Nanotechnology (DST Govt. of India), Bangalore India Nano award			
	(Karnataka Govt) and Distinguished Materials Scientist of the Year Award			
	(2021), by the Materials Research Society of India, A V Rama Rao lecture			

Award and J N Mukherjee lecture award (Indian Chemical society). He is a
fellow of the Indian National Science Academy, Indian Academy of Sciences
and the National Academy of Sciences (India), Royal Society of Chemistry
(London) and the Asia-Pacific Association of Materials. Dr Ganguli was keenly
involved in the formation of Delhi S&T Cluster (DRIIV) part of the initiative
of PSA, Govt of India. Dr Ganguli has very keen interest to promote outreach
activities for underprivileged sections of society and has been to remotest
schools and colleges in several states in the country.

Solid state chemistry: Basic concepts to technologies

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Solid state chemistry is a legacy activity spanning more than 150 years. A thorough knowledge of various factors is essential to design new materials. New functional materials can be designed by interplay of synthesis and crystallographic structure. Unconventional synthetic routes play an important role in this direction as many of these new materials are metastable and hence it is not possible to prepare them by conventional synthesis methods. Of late, the focus of research has been shifted to multi-functional materials i.e., the materials which can possess two or more than two synergistic or antagonistic functionalities. Several materials with unusual coordination number and oxidation states will be discussed in this presentation. Rational concepts like tuning of radius ratio, degree of disorder, distortion, point defects engineering, unusual polyhedral sharing, unusual coordination numbers and counter-ion polarisability to prepare many new materials with desired functional properties. Some typical materials are La_{1-x}Ce_xCrO₃, Pr_{1-x}Ce_xScO₃ (materials with tunable band gap and magnetic properties), CeScO₃ (with unusual reversible conversion to fluorite lattice), $Gd_{1-x}Y_xInO_3$, $GdSc_{1-x}In_xO_3$, $YIn_{1-x}Fe_xO_3$ (tunable dielectrics) and several lead-free relaxor materials. Several interesting pyrochlore-based oxygen storage materials, viz. $Ce_2Zr_2O_{7+x}$ (x = 0.0 to 1.0), Gd₂- $_{x}Ce_{x}Zr_{2}O_{7}$ and $Gd_{2x}Ce_{x}Zr_{2-x}Al_{x}O_{7}$ (x = 0.0 to 2.0) have been prepared, which have shown interesting redox catalysis. The simple concepts like r_A/r_B ratio of A₂B₂O₇ pyrochlores could be used to tailor the properties like dielectric and catalytic behavior. Some recent results in the field of energy storage and photocatalysis will also be discussed. The major focus of this talk will be on the role of synthesis, novel properties exhibited by these functional materials, and their crystallographic correlation. Several examples for technologically important materials will also be discussed.



Dr. A. K. Tyagi, is presently Dean and Senior Professor, at Homi Bhabha National Institute (HBNI), Mumbai, and was immediate past Director, Chemistry Group, and Director, Bio-science Group, Bhabha Atomic Research Centre (BARC), Mumbai, and Distinguished Scientist, Department of Atomic Energy (DAE). He joined BARC through BARC training School (29th batch, 1985-86) and obtained PhD in chemistry from BARC/Mumbai University in the year 1992. His research interests are in the field of nanomaterials, functional materials, nuclear materials, metastable materials and Hybrid materials. He did postdoctoral research at Max-Planck Institute, Stuttgart, Germany (1995-96). He has published about 681 papers in international journals, more than 10 books and several review articles. *His four-decade journey in the field of solid-state chemistry and a detailed scientific profile is appended at the end of this booklet*.

In brief, he is a fellow of various premier national and international scientific academies and societies. He has been conferred with a number of prestigious national and international awards notable among which are DAE-Homi Bhabha Science and Technology Award, DAE-SRC Outstanding Researcher Award, MRSI Medal; MRSI-CNR Rao Prize in Advanced Materials; CRSI-CNR Rao National Prize in Chemical Sciences; CRSI-Silver Medal; Medal of Indian Nuclear Society; IANCAS-Dr. Tarun Datta Memorial Award; R. D. Desai Memorial Award of Indian Chemical Society; Rajib Goyal Prize in Chemical Sciences; ISCB Excellence Award

in Chemical Sciences; ISCA Platinum Jubilee Lecture Award in Materials
Science; Metallurgist of the Year award from Ministry of Steel, GoI;
JNCASR-National Prize in Solid State and Materials Chemistry; ISCA
Acharya PC Ray Memorial Award; NASI – Prof. N.R. Dhar Memorial
Award; JNCASR-Prof. AV Rama Rao Foundation Lecture Award.

IT-1 Magnetoelectric properties of chemical ordering-induced pyroelectric oxides

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Abstract: Combining ferroelectricity and magnetism in the same material remains a challenge because it involves complex crystal chemistry and stringent symmetry requirements. In conventional ferroelectrics, the polarization arises from the second-order Jahn–Teller effect associated with cations of d^0 or s^2 lone pair electronic configuration. Conversely, magnetism arises from cations with partially filled d or f electrons. Materials incorporating these two kinds of cations in different crystallographic sites exhibit multiferroic properties but weak coupling between magnetism and ferroelectricity. On the other hand, a strong cross-coupling occurs in some materials, where specific spin structures induce weak ferroelectricity below the magnetic ordering temperature. In this talk, we discuss a new class of multiferroics where the polar distortion results from chemical ordering. These polar oxides are mainly pyroelectric in the entire temperature range and exhibit magnetoelectric coupling below the magnetic ordering temperatures.



Dr. A. Sundaresan currently holds the position of Chair and Professor at the Chemistry and Physics of Materials Unit, JNCASR. His academic pursuits revolve around the intricate interplay between structure and property, specifically emphasizing the realms of magnetism, superconductivity, and multiferroics.

Targeting Functional Materials by Exploratory Solid State Chemistry Approach and by Rational Design

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Abstract: Synthesis and structural characterization of novel solids by exploration is the first and foremost significant step crucial for the fundamental understanding of structure property relation, and ultimately the pathway leading to a vast number of functional materials. The quest for materials ranges from electrodes, electrolytes for the various rechargeable batteries, for second harmonic generation, dielectric, ferroelectric, catalysts, and photocatalysts that are essential to provide a cleaner, greener energy, and environment. Our exploratory approach has been based on the systematic screening of the phase diagrams or careful modification of the cations and/or anions in the known structures or both, and possibly by rational design in few cases. Concurrent adaptation/development of appropriate synthetic methodologies has also been given simultaneous attention. Few selected examples will be discussed in this talk to emphasize the outcome of the mentioned aspects including those of the family of oxides possessing honeycomb ordered rocksalt superstructures.

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Prof. Sitharaman Uma joined the Department of Chemistry, University of Delhi, as a Reader in January, 2006 and became Professor in 2012. She obtained her Ph.D in Solid State Chemistry, from the Indian Institute of Science, Bangalore in the year 1995, with Professor J. Gopalakrishnan, FASC, FNA, FNASC. Her post-doctoral experience includes, Ames Laboratory, Iowa State University, Ames, Iowa, USA, followed by Department of Chemistry, Oregon State University, USA and at Kansas State University, USA. Her area of research interest is Solid State Material Chemistry, focusing on the synthesis of new materials, crystal structure evaluation, studying structure-property relationship, particularly interested in materials relevant for solid electrodes, electrolytes, ionic conductors, and optical materials and photocatalysts for environmental remediation and energy. She has received the K.P. Abraham Gold Medal and cash award for the Best Thesis in Materials Chemistry, IISc., Bangalore and also been awarded the Maya Devi Juneja Gold Medal in the ISCA-2015 for contribution in the area of Solid-State Chemistry and Allied Areas. She has member affiliations with ACS, MRS and SMC and the Editorial Board Member of the Journal of Chemical Sciences.

Molecular and Framework Metal Phosphates for Applications in Energy, Catalysis, and Magnetism

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Abstract: Reaction of phosphonic acids and phosphate monoesters with a divalent metal such as Zn^{2+} in a donor solvent (L) leads to the isolation of tetranuclear metal phosphates $[(R)PO_3Zn(L)]_4$ (R = alkyl/aryl or alkoxy/aryloxy), whose inorganic core resembles the zeolitic D4R secondary building units (SBUs).^{1,2} In recent times, we have unravelled that it is possible to isolate even larger SBUs through small variations in the reaction conditions.³ On the other hand, the reactions of phosphoric acid esters yield either 1-D or 2-D materials which thermally anneal below 300 °C to produce ceramic materials.⁴ Rationalization of building principles along with the use of this class of compounds in catalysis, energy, and molecular magnetism⁵ will be highlighted in this lecture.

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IT-3

Design and Synthesis of Alkali Metals (Na and K) Based CP and MOF: Rare to Novel Topology and Solid-State Structural Transformation

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Abstract: We report rare example of facile in-situ synthesis of Na-MOF1 that undergoes vacuum mediated SCSC transformations from rare parallel polycatenated kgd nets to new and novel 3-periodic 3,3,12-c net topology (named smm1). Further, SCSC transformation of Na-MOF1 to Na-MOF2 reveals activation of N-N-atoms in 1,2,3-triazole unit. Na-MOF1 and Na-MOF2 were authenticated by single crystal X-ray studies and the bulk was confirmed by PXRD studies.¹ Furthermore, We report a facile in-situ access to a new three dimensional network of coordination polymer { $[K_6(L)_2(\mu_3-H_2O)_3(H_2O)_4]$ · H_2O }, KCP constructed with a tritopic carboxylate linker containing triazole moities, synthesized in mild conditions at RT. The compound was structurally characterized by single crystal X-Ray diffraction analysis, PXRD and TGA. The topology features of the KCP gave a reasonable and complicated novel 4,5,6,6,6,6,6,6,0,11-c underlying deca-nodal net.



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Solid State Chemistry of Nuclear materials

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Abstract: Materials plays a significant role at various stages of nuclear fuel cycle from front end to the back end. The development of futuristic nuclear technologies such as accelerator-driven systems and breeder reactors as well as design of advance materials for waste immobilisation, mitigating accidental conditions, radiation stable materials are all central to the sustained growth of nuclear energy for peaceful applications. In this context, exhaustive work has been done on understanding the structure, thermophysical and thermodynamic properties of nuclear materials with structure belonging to fluorite, pyrochlore, garnets, silicates, metals, glasses etc. Development of indigenous database on solubility, phase stability, expansivity, phase transitions, thermal conductivity, heat capacity, which are all significant inputs for reactor design, have been generated on variety of systems based on CeO₂, UO₂, ThO₂, ZrO₂ and metals like U, Th and Zr. Radiation response investigation on CeO₂ and ZrO₂-based materials as the function of different parameters such as energy & fluence of radiation, material's powder properties, grain boundaries and interphase boundaries, nature of boding etc. have helped in establishing guidelines for designing superior radiation-stable materials. Indigenous compositions for sacrificial materials for core-catcher application have been optimised to develop fail-safe materials for nuclear safety. Various sorbents based on TiO₂, ZrO₂, γ-Al₂O₃, SnO₂ and CeO₂ have been developed for removal of radioactive species from waste stream as well as for radionuclide generators for ⁹⁹Mo-^{99m}Tc, ¹⁸⁸W-¹⁸⁸Re and ⁶⁸Ge-⁶⁸Ga. The talk shall strive to give a glimpse of the solid state research dedicated to nuclear fuel cycle.

Dr. (Mrs.) Vinita Grover Gupta is presently working as Scientific Office (H), Chemistry Division, Bhabha Atomic Research Centre and Professor Homi Bhabha National Institute, Mumbai. She has done her M.Sc. from III Delhi and PhD from Mumbai University. She works extensively in the frontline areas of materials for nuclear and energy applications. Her area o expertise is design of superior ferroelectrics, relaxors and radiation stable materials based on crystal structure-controlled properties and morphologica attributes. She has to her credit about 100 journal publications in addition to several book chapters and a technology transfer. She is the recipient of severa awards that include Young Scientist awards bestowed by Department of Atomic Energy, Indian Nuclear Society and Indian Society of Chemists and Biologists, DAE Scientific and Technical Excellence Award, IANCAS-Dr	
Atomic Energy, Indian Nuclear Society and Indian Society of Chemists and Biologists, DAE Scientific and Technical Excellence Award, IANCAS-Dr.	
Tarun Dutta Memorial Award and DAE-SSPS- Young Achiever Award. She is also the Fellow of Maharashtra Academy of Sciences, Associate Academician, Asia Pacific Academy of Materials and Member. National	
Academy of Sciences India. Recently, she has been recognised among 75 women in chemistry by office of PSA, GOI and Royal Society of chemistry.	

IT-6 A Chemist's Perspective on Nanomaterial Synthesis: How to Bridge the Gap Between Laboratory and Market?

Bhagavatula L. V. Prasad,^{a,b}

^aCentre for Nano and Soft Matter Sciences, Bengaluru ^bPhysical & Material Chemistry Division, CSIR-National Chemical Laboratory, Pune, India

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Abstract: As the applicative domain of nanomaterials is increasing is a great demand for their largescale production. Conventional batch processes of nanomaterial synthesis have several limitations as they involve several steps and/or reagents. To scale-up any synthesis we need to reduce the number of steps/reagents/solvents involved. We have taken up this task and embarked on a journey to develop methods to synthesize nanomaterials in three different routes. These are, (i) One step synthesis of metal nanoparticles using micro-reactors and microwave methods (ii) "All-in-one" precursors for the preparation of semiconducting metal, metal sulfide and bimetallic sulfide nanocrystals (iii) Sol gel synthesis of nanocrystalline MgO with high surface area. In each of these cases systematic studies were carried out to understand the batch processes thoroughly and later extended the same knowledge for scaled up synthesis. In this talk we will first briefly introduce the different approaches for the chemical synthesis of nanomaterials and then take up each of the above-mentioned cases one by one and delineate the challenges involved in achieving large scale synthesis. Our efforts in successfully circumventing these problems to yield reproducible and reliable large-scale synthetic processes will be described.



Prof. Bhagavatula L. V. Prasad (FASc, FNASc and FRSC) is currently working as the Director of Centre for Nano and Soft Matter Sciences, Bengaluru. He also holds the position of Chief Scientist in the Physical/Materials Chemistry Division of National Chemical Laboratory (CSIR-NCL), Pune, India. He obtained a Master of Science and PhD degrees in Chemistry from University of Hyderabad. After two post-doctoral stints; one at Tokyo Institute of Technology and second at Kansas State; he joined NCL in 2003. In 2021 he has assumed the office of Director, Centre for Nano and Soft Matter Sciences, Bengaluru. His group is actively working in the general area of material synthesis and in particular nanoparticles and nanoscale materials. He has published close to 140 papers in international peer reviewed journals and has 8 international patents to his credit. He was invited as visiting professor by different universities in many countries, including Japan, USA, UK, France and Germany. 18 students have completed PhD under his supervision and another 6 are pursuing their PhD currently.

Disrupting the Trends in Rechargeable Batteries: Re-Injectable Architectures for Aluminium Ion Full Cells

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Abstract: Aqueous aluminium ion batteries (AIBs) have recently emerged as a promising battery technology owing to their inherent advantages such as: abundant and low-cost resources, safety and high theoretical capacity. However, the full-cell design, with optimum performance, has been a challenge. In this work, an efficient intercalation mechanism for AI^{3+} is demonstrated in electrochemically desodiated NaMnPO₄ (NMP) as a cathode material with 1 M AlCl₃ as an aqueous electrolyte. While possessing intense redox peaks in the cyclic voltammetry curves, the chosen cathode exhibits a high discharge capacity of ~246 mAh g⁻¹, at a relatively high current density of 0.2 A g⁻¹ in a three-electrode configuration along with an excellent cycle life of ~97% after 1000 charge-discharge cycles.

The full cell fabrication was done using desodiated-NMP as the cathode material and readily available aluminium sheet as a cost-effective anode in a novel re-injectable pouch cell architecture using industrially available PET-EVA pouches by employing a thermoforming process. The issue of electrolyte depletion during charge-discharge process is mitigated by using a re-injectable architecture consisting of a one-way flow valve. These are amongst the 1st such designs that are being reported, to the best of our knowledge and literature survey. The full cell shows a specific capacity of ~62 mAh g⁻¹ at current density of 0.1 A g⁻¹.



IT-8 Graphitic Carbon Nitride: Strategies to enhance its photocatalytic activity

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Abstract: Graphitic carbon nitride $(g-C_3N_4)$, a metal free organic semiconducting polymeric material having tris-s-triazine repeating moieties, consisting of a large number of graphitic planes belongs to an important class of semiconductor materials. The uniqueness of $g-C_3N_4$ include high thermal and chemical stability, eco-benignity, and proper electronic band structure for required photo catalytic reactions. On the contrary, sluggish electron transfer, inadequate reaction active sites, lower solar radiation harvesting capacity, low specific surface area impedes its efficiency towards photocatalysis. In our group, we have rationally adopted many modification strategies such as morphology modification, exfoliation to form nanosheets, heterojunctions with oxides, perovskites, ferrites, layered double hydroxides, RGO, h-BN, thiospinels, metal alloys, intrinsic doping with non-metallic heteroatometc. The structure, morphologies optical, electrochemical characterisation of the as-synthesized photocatalysts was well-characterised. Thereafter, visible light absorption was identified by the UV-vis DRS spectroscopy and charge migration/separation efficiency was supported by PL, TRPL, and EIS analysis. All the synthesized photocatalysts were subjected towards eco-friendly solar to value-added chemical conversion reactions like H₂O₂ production, photocatalytic H₂ and O₂ evolution, reduction of Cr (VI), oxidation of phenolic compounds and antibiotics, which are regarded as promising and sustainable technologies. The optimised photocatalyst was investigated to show remarkable increment in photocatalytic activity. A detailed reaction mechanism study and an insight kinetic study with different affecting parameters were also carried out.



Prof. Kulamani Parida is a pioneer to explore the chemistry behind the core properties related to suppress the charge recombination process and enhancing the photocatalytic activities and quantum yield. He has a strong idea for designing new categorized materials based on oxides, borides, single crystal, nitrides, phosphides, perovskite, sulphides, quantum dots for nanoheterostructures, p-n heterojunctions, isotype and Z-scheme/ S-scheme oriented systems with outstanding activities for solar H₂ generation, O₂ reduction, N₂ reduction, H₂O₂ production, energy storage, and environmental remediation. He found a place in the global 2% scientist ranking in physical chemistry for the last three consecutive years (2020-2022). Prof. Parida also secured 1319th rank globally and 7th rank in India in the chemistry domain as per research.com survey. He has published 520 with an average impact factor of 6.7, granted 33 patents and supervised 56 PhD students. The important and current relevance of his work is amply reflected in a large number of citations ~ 32000 and h-index~98 in Google Scholar.

A four-decade journey of Prof. A. K. Tyagi in the field of solid-state chemistry

Dr. A. K. Tyagi, is presently Dean, Homi Bhabha National Institute and former Director, Chemistry Group, and Director, Bio-science Group, Bhabha Atomic Research Centre (BARC), Mumbai, and Distinguished Scientist, Department of Atomic Energy (DAE), Senior Professor, Homi Bhabha National Institute (HBNI), Mumbai embarked on his scientific journey at BARC, Mumbai in 1986, at young age of 22 years. Through an illustrious career spanning about four decades, he has gained tremendous expertise in the field of functional materials for applications in energy, environment and health sectors. He has established himself as an internationally acclaimed materials chemist. Dr. Tyagi has played a pivotal role in establishing state-of-the-art facilities to pursue world class research at BARC as well as to cater to scientific understanding and materials for diverse applications. His deep understanding in structure-property relationship along with sound knowledge in solid state chemistry, crystallography, defects engineering and thermodynamics has enabledhim to design and develop large number of innovative materials with superior properties. Dr. Tyagi has to his credit 377 entries in Inorganic Crystal Structure Database (ICSD), that clearly establishes him as a world leader in the field of structural inorganic chemistry. The innovative materials developed by him, have demonstrated superior functionalities in various fields, like photo-catalysis, magnetism, multiferroics, ionic conductors, materials for extreme conditions materials, highly selective inorganic ion exchangers, etc. His work is a remarkable blend of basic and applied sciences. Several materials and processes developed by him have transitioned from laboratory to field deployment for various departmental and societal benefits.

The research career of Dr. Tyagi is primarily focused on the art of designing materials through intricate structure-property relationships to synthesizehitherto unknown materials. He has developed variety of new non-equilibrium methods to synthesize materials with unusual composition, coordination number, oxidation states and lattice packing where the constraints due to thermodynamic, crystallographic and electronic reasons are surpassed. He has rationally used concepts like tuning of radius ratio, degree of disorder, distortion, point defects engineering, unusual polyhedral sharing, unusual coordination numbers and counter-ion polarizability to prepare many new materials with superior functional properties. Some of the notable examples and contribution of his studies are mentioned below.

Design of unusual materials with useful functionalities: Dr. Tyagi's research area covers a wide range of materials ranging from the oxide superconductors and their fluorination in the early research career to the designed multiferroics, catalysts and materials for nuclear fuel cycle in the present days. He has pursued research works in various internationally reputed laboratories as postdoc and later as visiting scientists. During his postdoctoral research at the Max-Planck Institute (MPI) in Stuttgart, Germany, from 1995 to 1996, Dr. Tyagi delved into the synthesis and properties of low-valent metal fluorides. Subsequently he has visited MPI, Stuttgart several times, and studied preparation and properties of unusual materials in oxides, fluoride and oxide-fluorides. One of the most notable contributions as preparation of hitherto unknown scheelite type $LiScF_4$ which is a unique optical hostcapable of accommodating both rare earth and transition metals ions. He has used an innovative high pressure-high temperature synthesis protocol to stabilize 8-fold coordination of Sc³⁺ ions, which is a pre-requisite of the scheelite structure. In addition, he has also prepared a number of several novel materials, like Li₃MF₆, $M = Ti^{3+}$, Ga^{3+} , Al^{3+} , $A_4B_3F_{17}$ and $A_7B_6F_{30}O$ type compounds with $A = Pb^{2+}$, Ba^{2+} and Sr^{2+} , B = trivalent rare-earth ions, and determined their structure by single crystal or powder X-ray diffraction methods. He has also studied crystal chemistry of wide variety of materials under extreme conditions, to understand their thermal expansion and compressibility behavior. The investigation on thermal expansion of avariety of framework materials, like cristobalite type AlPO₄, GaPO₄, BPO₄, framework type HfMo₂O₈, NbOPO₄, VP₂O₇, etc., deserves special mention. A close correlation between the inter-polyhedral angles, packing density, nature of coordination polyhedral and thermal expansion in such materials have been established in these systems. He has identified a number of metastable high-pressure phases and provided information on their structure and stabilities. Dr. Tyagi's research in unusual materials isreflected in the synthesis of RE_{1-x}Ce_xCrO₃ based tunable band-gap materials, excellent oxygen storage capacitors in Ce-Gd-Zr-O system, tunable-dielectrics in hexagonal-ABO₃ systems, new lead-free electro-active materialsand pyrochlore-based superior ionic conductors. An innovative-yet-simple two steps chemical synthesis protocol was developed to stabilize cerium in tri-valent oxidation state, which is otherwise unfavourable. Typical examples of such Ce³⁺ based oxides are CeCrO₃, La_{1-x}Ce_xCrO₃, CeScO₃, Ce₂Zr₂O₈etc. Multifunctional properties of CeCrO₃, such as antiferromagnetism, relaxor-like dielectric behavior, and an optical band gap in the visible region has been deciphered in these studies. The controlled oxidation of varietyof benzylic alcohols with 100% conversion and selectivity (80-100%) using CeCrO₃ as catalyst has been established. Tunable magnetic properties and optical band gap has been achieved by tuning the composition of La_{1-x}Ce_xCrO₃ ($0.0 \le x \le 1.0$). Nanocrystalline La_{0.2}Ce_{0.8}CrO₃was found to show extraordinary coexistence of sign reversal of both magnetization and exchange bias field in it. Mechanistic understanding on the oxygen storage properties of Ce_{0.5}Sc_{0.5}O_{1.75}having fluorite type structure and pyrochlore type Ce₂Zr₂O₈ has led to pioneering work on their applicationas redox catalyst.

Fundamental and applied research on functional materials: Dr. Tyagi has explored a variety offluorite, pyrochlore and perovskite-based materials to develop efficient moderate temperature ionic conductors. His investigations on these materials revealthat an optimum degree of disorder in the structure is desired to have sufficient number of mobile species as well as minimum activation energy. The careful optimization of activation energy and pre-exponential factor by subtletuning of nonstoichiometry in Nd₂Zr₂O₇ system could yield ionic conductivity higher than the well-known YSZ. Dr. Tyagi has also investigated wide varieties of materials for development of high dielectric and multiferroic materials. Invokingthe concepts of polyhedral distortion, he could demonstrate giant dielectric constant and relaxor-ferroelectric properties in FeTiTaO₆. Subsequently, compositional control to tweak local structure to introduce fascinating electrical properties has been demonstrated in several perovskites type systems, like GdSc1-xInxO3, YIn1-xFexO3 and Gd1-xYxInO3. These studies indicated thattwo cations at B-site having different polyhedral preference create subtle local distortion, and that render classical relaxor behavior in the otherwise dielectric materials. Under his supervision, extensive studies towards the enhancement of multiferroic properties of BiFeO₃ via nanostructuring and doping/co-doping with Ba²⁺/Mn²⁺, Ca²⁺/Cr³⁺, Sc³⁺/Ti⁴⁺ and Sm³⁺/Zr⁴⁺ ions have been carried out by his group. Synthesis of new multiferroic materials like BaMF₄:Mn, Fe₃O₄-PVDF, Ni-PVDF composites, etc. are also few notableexamples of his studies. Additionally, he has also made great strides in devising protocols to develop nano-ink formulations for depositing these materials in form of thin films.New nano-sorbents based on oxides of Ti, Zr, Al and Ce have been developed by him for the⁹⁹Mo-^{99m}Tc, ¹⁸⁸W-¹⁸⁸Re and ⁶⁸Ge-⁶⁸Ga generators for the applications in cancer diagnosis and treatment in collaboration with Radiopharmaceutical Division, BARC. Additionally, he has contributed to the development of nanocrystalline NiS-PMMA composites for separation of ¹⁰⁶Ru, an important radio-isotope used for treatment of ocular cancer, from a low-level nuclear waste (in collaboration with Nuclear Recycle Group, BARC). His studies also led to the development of Ag@R6G hybrid optical sensor for detection of Pb^{2+} in potable water down to 50 ppb. Recently, he demonstrated Cu-doped TiO₂ as an efficient photocatalyst for selective reduction of CO₂ and moisture to methane and oxygen under visible irradiation without using any sacrificial agent. Mechanistic investigations on the process revealed important roles of Cu⁺ and O-vacancies for reduction of CO₂ and H_2O . His studies also led to the development of V_2O_5 -WO₃ dispersed on CeO₂ support as thermal catalysts for mineralization of A1 carcinogens like dioxin and furans at temperature as low as 120°C. This finding has paved away for its possible use in any incineration process.

Materials for nuclear applications: Dr. Tyagi has steered several projects of national importance, such as development of materials and processes for Advanced Heavy Water Reactor (AHWR), Molten salt Breeder Reactors (MSBR), Inert Matrix Fuels (IMF) for the plutonium utilization or minor actinide transmutation, and so on. His contributions on the generation of thermodynamics and thermophysical data on thorium-based fuels have been invaluable for designing the fuel pins of AHWR. As part of this activity, Dr. Tyagi and his group has investigated phase relations and thermal expansion behavior of large number of thoria based systems. The data on plutonium bearing thoria

fuel were simulated using ceria (CeO_2) as a surrogate material for plutonia (PuO_2) on account of their similar physico-chemical properties. In his recent activities, he has been involved in generation of high temperature properties of molten fluoride salts relevant for Indian design of MSBR. Exploratory studies have been carried out to unravel eutectic salts compositions for fuel, coolant and blanket liquids. With the aim to develop new Inert Matrix Fuels, extensive studies on phase relations in ternary systems containing CeO_2 , ThO_2 , ZrO_2 and Ln_2O_3 , Ln = Lanthanides, have been carried out.A large number of compositions have been extensively studied to construct ternary phase equilibria in these systems. Dr. Tyagi has carried out substantial studies on structure and radiation stability on pyrochlores and related oxides. Towards the nuclear waste management, he has been involved in development of glass, ceramics and glass ceramic matrices for immobilization of radioactive elements as well as ion exchangers, nano-sorbent for separation of radioactive elements for alternate applications (in association with Nuclear Recycle Group, BARC and Radiochemistry and Isotope Group, BARC. A large number of zircon and monazite type phosphate, hollandite type ferrotitantes, pyrochlore and zirconolite type titanates have been investigated to understand their prospects for immobilization of radionuclides. He has carried out extensive studies on new glasses like Barium borosilicate glasstowards their stability and dissolution capability for Th, U, F etc. By Raman and MAS-NMR (²⁹Si and ¹¹B) characterization of SiO_n and BO₃ and BO₄groups in glass, he had provided crucial information for the design and development of such glasses. During last few years, Dr. Tyagi has initiated research on development of materials for Li and Na ion batteries also. A novel synthesis protocol for carbon coated LiFePO₄ has been established to be used as cathode material for Lithiumion battery. His group has also developed several materials for sodium ion batteries. His hallmark is perfect balance between fundamental and applied aspects of chemistry.

Academic Achievements of Dr. A. K. Tyagi

Records of Publications and Invited Talks :				
1.	International Journals	:	681	
2.	Review Articles and Book Chapters	:	26	
3.	Articles in Bulletins and News Letters	:	16	
4.	Invited Talks and Keynote Lectures	:	415 [India : 376 ; Abroad : 39]	
5.	Books	:	13	
6.	Technology transfers to companies	:	12	

1.	PhD students	45 (Awarded: 35; Submitted :02; Currently working: 08)		
2.	MSc students	05 (Awarded : 0	5)	
Goog	le Scholar (Citations: 20303 ;	h-index: 69;	i_{10} index : 443)	
Scopus (Citations: 17469;		h-index: 63;	i_{10} index : 384)	
As on	31-03-2024			

Dr. Tyagi is a recipient of the following awards / Recognitions / Fellowships

S. No.	Government awards	Year	
1	J C Bose National Fellowship from Science and Engineering Research Board	2024	
2	Acharya PC Ray Memorial Award from Indian Science Congress Association	2020	
	(Conferred by Shri M. Venkaiha Naidu, Vice-president of India)		
3	Metallurgist of the Year Award, Ministry of Steel, GoI	2017	
4	Platinum Jubilee Lecture Award in Materials Science from Indian Science	2015	
	Congress Association		
5	DAE-SRC Outstanding Research Investigator Award	2010	
6	DAE- Homi Bhabha Science and Technology Award (2008)	2006	
	(Conferred by Dr. APJ Abdul Kalam, former President of India)		
	From NASI		
7	NASI – Prof. N. R. Dhar Memorial Lecture Award	2022	
	From Chemical Research Society of India (CRSI)		
8	CRSI Silver Medal	2018	
9	CRSI - Prof. CNR Rao National Prize in Chemical Sciences	2012	
10	CRSI Bronze Medal	2006	
	From Materials Research Society of India (MRSI)		
11	MRSI- Distinguished Materials Scientist of the year award	2023	
12	MRSI-Prof. CNR Rao Prize in Advanced Materials	2018	
13	MRSI-ICSC Materials Science Senior Award	2014	
14	MRSI Medal	2005	
From JNCASR, Bengaluru			
15	Honorary Professorship (2022 – 2025)	2022	
16	A V Rama Rao Prize Lecture	2022	
17	National Prize in Solid State and Materials Chemistry	2018	
International Fellowships			
18	UNESCO–University of South Africa (UNISA) Fellowship	2017	
19	Max-Planck Fellowship, Germany	1995-1996	

From other Scientific and Academic Bodies				
20	Gold Medal of Chirantan Rasayan Sanstha	2024		
21	Prof.SR Mohanty Memorial Lecture Award from Orissa Chemical Society	2024		
22	D N Agarwal Memorial Award from Indian Ceramic Society	2023		
23	Annual Special Oration in Inorganic Chemistry at Delhi University	2023		
24	NETZSCH - ITAS Award from Indian Thermal Analysis Society	2022		
25	Coastal Chemical Research Society's Award for Excellence in Chemical Sciences	2014		
26	Award for Excellence in Chemical Sciences (from Indian Society for Chemists	2013		
	and Biologists)			
27	Rajib Goyal Prize in Chemical Sciences (from Kurukshetra University)	2010		
28	RD Desai Memorial Award (from Indian Chemical Society)	2009		
29	Dr.Tarun Datta Memorial Award	2007		
	(from Indian Association of Nuclear Chemistry and Allied Scientists)			
30	Gold Medal of Indian Nuclear Society	2003		
	(Conferred by Director General, International Atomic Energy Agency, Vienna)			
31	Rheometric Scientific-ITAS award by Indian Thermal Analysis Society	2002		
32	Dr. Lakhsmi Award by Indian Association of Solid State Chemists	2001		
	DAE-Group Achievement Awards			
33	DAE Group Achievement Award	2018		
	(Contribution towards supply of rare-earth based liquid neutron poison for			
	Nuclear Reactor applications)			
34	DAE Group Achievement Award	2018		
	(Contribution to BARC Integrated Centre for Crisis Management)			
35	DAE Group Achievement Award	2018		
	(Contribution to project on development of thermo-dilatometer)			
36	DAE Group Achievement Award	2012		
	(Contribution to hex gas dry-reduction process)			
Fellow of the National Science Academies				
37	Fellow, Indian National Science Academy (FNA)	2024		
38	Fellow, Indian National Academy of Engineering (FNAE)	2022		
39	Fellow, Indian Academy of Sciences (FASc)	2013		
40	Fellow, National Academy of Sciences, India (FNASc)	2004		
41	Fellow, Maharashtra Academy of Sciences (FMASc)	2003		
Fellow / Academician of the International Science Academies				
42	Fellow, World Academy of Sciences (FTWAS)	2024		
43	Academician, World Academy of Ceramics (Italy)	2021		
44	Honorary Fellow, African Academy of Sciences	2021		
45	Academician, Asia Pacific Academy of Materials	2013		
46	Fellow, Royal Society of Chemistry (UK)	2011		

Books published by Dr. A. K. Tyagi

- "Advanced Techniques for Materials Characterization" Eds. A. K. Tyagi, M. Roy, S. K. Kulshreshta, S. Banerjee Trans Tech Publications Ltd, Switzerland (2009) ISBN-13 978-0-87849-379-1 (Number of pages: 513)
- "Nanotechnology Research in India" Eds. A. Vinu and A. K. Tyagi Special volume of International Journal of Nanotechnology Inderscience Publishers, Vol. 7 (2010) (Number of pages: 406)
- "Functional Materials: Preparation, Processing and Applications" Eds. S. Banerjee and A. K. Tyagi Elsevier Publishers 2011 (ISBN: 978-0-12-385142-0) (Number of pages: 706)
- "Materials under Extreme Conditions: Recent trends and future prospects" Eds. A. K. Tyagi and S. Banerjee Elsevier Publishers 2017 (ISBN: 978-0-12-801300-7) (Number of pages: 870)
- "International Year of Periodic Table: 150 Glorious years" Eds. A. K. Tyagi, S. Nath, V. Grover and R. Chakravarty Published by Board of Research in Nuclear Sciences, 2019 (Number of pages: 220)
- 6. "Synthesis strategies for advanced materials" Volume-I: Techniques and fundamentals Eds: A. K. Tyagi and R. S. Ningthoujam Springer Nature (2021) (ISBN: 978-981-16-1806-2) (Number of pages: 691)
- 7. "Synthesis strategies for advanced materials" Volume-II: Processing and functionalization of materials Eds: A. K. Tyagi and R. S. Ningthoujam Springer Nature (2022) (ISBN: 978-981-16-1802-4) (Number of pages: 856)
- "Synthesis strategies for advanced materials" Volume-III: Materials specific synthesis strategies Eds: A. K. Tyagi and R. S. Ningthoujam Springer Nature (2022) (ISBN: 978-981-16-1891-8) (Number of pages: 921)
- 9. *"Non-power applications of nuclear technologies"* Eds: A. K. Tyagi and A. K. Mohanty BARC Publication (2021) (ISBN: 978-81-954733-2-8) (Number of pages: 220)

- 10. "Atomic Energy in India: Achievements since Independence" Eds. A. K. Tyagi and P. R. Vasudeva Rao HBNI Publication (2022) (ISBN: 978-93-5659-052-6) (Number of pages: 278)
- "Engineered Biomaterials: Progress and Prospects" Eds. P. A. Hassan, Biji Balakrishnan and A. K. Tyagi World Scientific (2023) (ISBN: 978-981-16-1891-8) (Number of pages: 921)
- 12. "Handbook of Materials Science" Volume
 1: Optical Materials
 Eds: R. S. Ningthoujam and A. K. Tyagi and
 Springer Nature (2024)
 ISBN- 978-981-99-7144-2)
 (Number of pages: 751)
- **"75 Years of Chemistry in Indian Atomic Energy Programme: Rich Legacy and Way forward"**Eds: A.K. Tyagi and P. A. Hassan
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