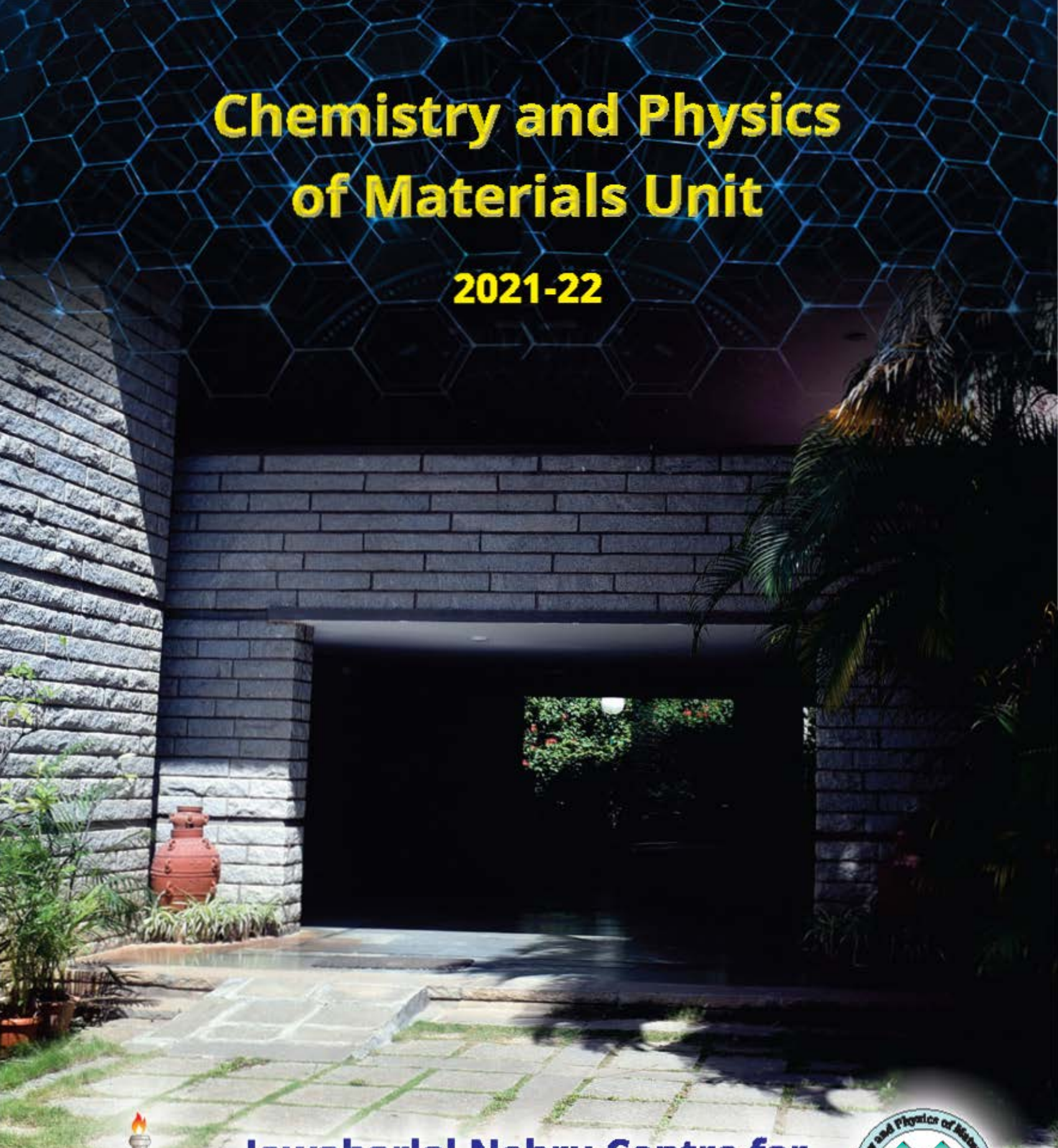
Chemistry and Physics of Materials Unit

2021-22



JNCASR

Jawaharlal Nehru Centre for Advanced Scientific Research

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A Note from the Founder Chairman

I can never forget the day, the CPMU was created. This is the first department in JNC. I congratulate the people who have contributed immensely. Let us wish CPMU lots of luck !

Prof. C. N. R. Rao, F.R.S.
Linus Pauling Research Professor

Welcome Message from the Chair

Welcome to the Chemistry and Physics of Materials Unit. It gives me pleasure to present the CPMU brochure for the year 2021-2022. The CPMU was the first Unit to be established in this Centre under the stewardship of Bharat Ratna, Professor C.N.R. Rao. Since its inception in 1994, the Unit has expanded its research activities on materials science and grown vertically over the years. In 2019, we celebrated the Silver Jubilee of our Unit with various academic activities, notably bringing out a special issue on Functional Materials in Materials Research Bulletin and instituting CPMU Alumni Materials Lecture, a yearly event.

The Unit fosters interdisciplinary research on cutting edge materials by involving highly motivated and creative faculty, students, post-docs in chemistry, Physics and Engineering disciplines in a highly collaborative research environment. The Unit faculty members are leaders in their own areas of research and have contributed substantially to the advancement of the respective research fields. The Unit has constantly been at the forefront in terms of publications, patents, awards, and fellowships, attracting collaborations with other institutions in India and abroad.

The Unit has been playing pioneering role in various academic activities of this Centre. In addition to the regular PhD program, the Unit offers an Integrated PhD program in Physical Sciences (specialization in materials) jointly with the Theoretical Sciences Unit (TSU). Recently, to bring all the materials researchers in JNCASR under one umbrella, the CPMU played a significant role to establish School of Advanced Materials (SAMat).

Prof. A. Sundaresan

Faculty Members

Founder Chair

C. N. R. Rao, FRS

Chair

A. Sundaresan

Faculty

K. S. Narayan

S. Balasubramanian

Chandrabas Narayana (On lien)

G. U. Kulkarni

M. Eswaramoorthy

Tapas Kumar Maji

Sarit S. Agasti (Jointly with NCU)

Bivas Saha (Jointly with ICMS)

S. M. Shivaprasad (superannuated on 30th June 2022)

Associate Members from the International Centre for Material Science (ICMS)

Ranjan Datta

Rajesh Ganapathy

Sridhar Rajaram

Associate Members from the Theoretical Sciences Unit

Shobhana Narasimhan

Swapan K. Pati

Srikanth Sastry

Umesh V. Waghmare

N. S. Vidhyadhiraja

C. N. R. Rao

Linus Pauling Research Professor
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Biosketch

Prof. C.N.R. Rao is the Honorary President and Linus Pauling Research Professor at the Jawaharlal Nehru Centre for Advanced Scientific Research and is also an Honorary Professor at the Indian Institute of Science, Bangalore, India. He has received M.Sc. from Banaras Hindu University and Ph.D. from Purdue University in USA. Prior to serving as the Founding President of JNCASR, Prof. Rao have held academic positions in University of California Berkeley, IIT Kanpur and IISc. Bangalore. He has published over 1750 research articles and over 54 books and has received honoris causa doctorate degrees from 83 universities. Prof. Rao is a member of several academic societies around the world and is the recipient of the highest civilian award of the Republic of India, the Bharat Ratna.

Research Direction

- Photochemical Water Splitting for Energy Applications
- Synthesis and Properties of Layered Materials
- Oxide and Carbon-based Nanomaterials

Research Description

Prof. Rao's research group specializes in the synthesis, characterization and measurement of various inorganic and organic nanomaterials including oxides, nitrides, sulfides, and layered materials such as graphene and beyond. Current research interests of his group include solar photochemical hydrogen generation by splitting water, semiconducting metal chalcogenides and their physical properties, layer materials beyond graphene etc.

Research Contribution

Prof. Rao has been working in the solid-state and materials chemistry research for over sixty years and has contributed much to the research and development of electron and vibrational spectroscopy, oxides, nitrides, high-temperature superconductivity, carbon nano-materials, photochemical and electrochemical energy storage and conversion, etc. Apart from his giant contribution on the chemistry of materials research, Prof. Rao has contributed significantly to the development of academic and higher education research institutes in India and have mentored generations of young scientists and engineers in India and around the world.

Publications

1. Layered Nanocomposites of Polymer-Functionalized Reduced Graphene Oxide and Borocarbonitride with MoS_2 and $MoSe_2$ and Their Hydrogen Evolution Reaction Activity, K Pramoda, S Servottam, M Kaur, CNR Rao, ACS Applied Nano Materials 3 (2), 1792-1799, 2020.
2. Effects of Ga doping on the phase transitions of V2O3, Pavitra N. Shanbhag, Anjana Joseph, Fabio Orlandi, Pascal Manuel, R. Mahendiran, Francois Fauth, Chandrabhas Narayana, A. Sundaresan, and C.N.R. Rao, Phys. Rev. B 105, 064103, 2022.

Balasubramanian Sundaram

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Biosketch

Prof. Balasubramanian received his Ph. D. from the Indian Institute of Science, Bengaluru in 1994. He later served as a Postdoctoral fellow at the University of Pennsylvania, prior to joining JNCASR as a faculty in 1998.

Research Directions

- High Performance Computing
- Self-Assembly, Supramolecular Interactions
- Ionic Liquids for Energy Storage
- Gas Storage
- Enzyme modelling
- Machine Learning Models, Potentials

Research Description

The Molecular Modelling Group is interested in studies of interesting phenomena, processes and properties exhibited by soft materials. These include: Ionic Salts which are liquids (RTIL) at ambient conditions, Supramolecular Polymers (mechanism of formation, pathway complexity, etc.), carbon dioxide storage in porous materials including metal organic framework solids, and modelling the structure, dynamics and function of enzymes. Advanced computational methods, including machine and deep learning methods are employed to investigate microscopically, the emergent behaviour in these systems.

Research Contribution

The research group has had several breakthroughs, including the demonstration of fractional ionic charge in RTILs, hopping motion of lithium ions in high salt concentration battery electrolytes, unravelling the microscopic reasons behind the anomalous temperature dependence of gas uptake by some porous solids, etc.

Publications

1. A. Gaur and S. Balasubramanian, Conformer Selection upon Dilution with Water: The Fascinating Case of Liquid Ethylene Glycol studied via Molecular Dynamics Simulations, Chemistry Open, e202200132, 2022.
2. S. Behera, and S. Balasubramanian, Molecular simulations explain the Exceptional Thermal Stability, Solvent Tolerance and Solubility of Protein-Polymer Surfactant Bioconjugates in Ionic Liquids, Phys. Chem. Chem. Phys., 24, 21904, 2022.
3. A. Sharma, N. Dwarkanath and S. Balasubramanian, Thermally Activated Dynamic Gating Underlies Higher Gas Adsorption at Higher Temperatures in Metal-Organic Frameworks, J. Mater. Chem. A, 9, 27398, 2021.

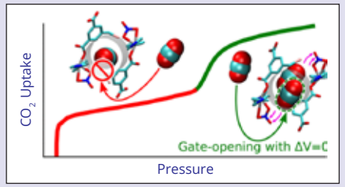

Illustration 1: Cooperative CO_2-CO_2 interactions enabled by flexibility of nitrate groups underpins the step in gas adsorption isotherm (see Dwarkanath and Balasubramanian, Inorg. Chem. 61, 10810 (2022).

Bivas Saha

Faculty Fellow

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Biosketch

Dr. Bivas Saha is an Assistant Professor at the International Center for Materials Science in the Jawaharlal Nehru Center for Advanced Scientific Research (JNCASR), India. He graduated with a Ph.D. from Purdue University in 2014, an M.S. from JNCASR in 2010, and a B.Sc. from Jadavpur University in 2007. Before joining JNCASR, he was a Postdoctoral Scholar at the University of California, Berkeley. Dr. Bivas Saha is an internationally recognized leader in thin film and heterostructure, III-V semiconductors, thermal and optical metamaterials research. He has published 56 research papers in international journals and three book chapters and holds a U.S. patent.

Research Direction

- Nanophotonic Materials and Devices
- Phase-change Materials
- Artificial Synaptic Devices
- First-principles Modeling of Materials

Research Description

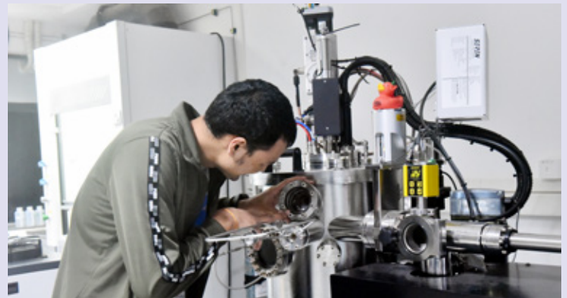
Dr. Bivas Saha's group specializes on thin film and heterostructure nanomaterials for nanophotonic, phase-change materials and artificial synaptic device applications. His group deposit high-quality epitaxial materials and metamaterials, study the fundamental energy transport and conversion mechanism and fabricate devices to improve the efficiencies. Dr. Saha's group also conduct cutting-edge modeling and simulation of materials to understand material and device properties.

Research Contribution

Dr. Saha is an internationally recognized leader in thin film and heterostructure nanomaterials for plasmonic and nanophotonic applications. Over the last four years, Dr. Saha's group has made fundamental contributions to the alternative plasmonic and polaritonic materials research. His group is also a leader in nitride-based phase change material and artificial synaptic devices.

Publications

1. K. C. Maurya, A. Chatterjee, S. M. Shivaprasad and B. Saha, *Nano Letters, 22, 23, 9606–9613 (2022).*
2. D. Rao, A. I. K. Pillai, M. Garbrecht and B. Saha, *Adv. Electron. Mater, 2200975 (2022).*
3. K. C. Maurya, D. Rao, S. Acharya, P. Rao, A. I. K. Pillai, S. K. Selvaraja, M. Garbrecht and B. Saha, *Nano Letters, 22, 13, 5182-5190 (2022).*
4. B. Biswas, S. Chakraborty, A. Joseph, S. Acharya, A. I. K. Pillai, C. Narayana, V. Bhatia, M. Garbrecht and B. Saha, *Acta Materialia 227, 117737 (2022).*



Chandrabhas Narayana

Professor

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Biosketch

Professor Chandrabhas obtained his PhD from the Indian Institute of Science, Bangalore in 1995 and carried out postdoctoral research in the Material Science and Engineering Department of Cornell University, New York from 1995 till 1998. He joined JNCASR as an assistant professor in 1998. Currently he is the Director of Rajiv Gandhi Centre for Biotechnology (RGCB), Thiruvananthapuram, Kerala.

Research Direction

- High Pressure Raman Spectroscopy
- Temperature and pressure dependent Raman studies to identify electronic and structural phase transitions
- Magneto-Raman studies
- Surface Enhanced Raman Spectroscopy studies on biomolecules
- Brillouin Scattering studies
- Development of miniature Raman spectrometers

Research Description

The group is involved in identifying and understanding electronic, structural, magnetic and topological phase transitions through temperature and pressure dependent Raman Spectroscopy, Magneto-Raman studies, X-ray diffraction studies, Brillouin Spectroscopy, Surface Enhanced Raman Spectroscopy of biomolecules for various applications in disease diagnosis.

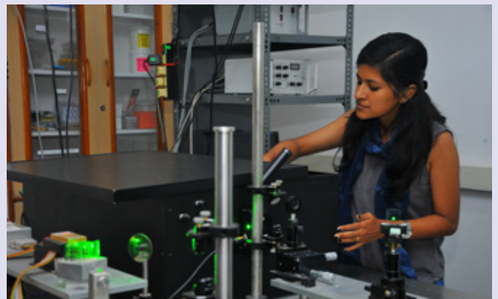
Research Contribution

Demonstration of large enhancement in Surface Enhanced Raman studies of various molecules using the Ag core Ag shell nanoparticles with hotspots which is better than silver nanoparticles.

Study of spin-phonon coupling in multiferroic $RCrO_3$ (R=Y, Lu, Gd, Eu and Sm) through Raman Spectroscopy showing the difference in phonon behavior of compounds with magnetic ions and nonmagnetic ions. Designing dendronic Raman markers for sensitive detection of biomolecules using Surface Enhance Raman Spectroscopy. The group has combined Raman Spectroscopy and Molecular Dynamics simulations to study protein aggregation mechanisms that play a role in neurogenerative diseases.

Publications

1. Priyanka Jain et.al, Polaronic Signatures in Doped and Undoped Cesium Lead Halide Perovskite Nanocrystals through a Photoinduced Raman Mode, ACS Applied Materials and Interfaces, 14, 5567, 2022.
2. Divya Chalapathi et al., Insights on Aggregation of Hen Egg-White Lysozyme from Raman Spectroscopy and MD Simulations, molecules, 27, 7122, 2022.



Eswaramoorthy M.

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Biosketch

Prof. Eswaramoorthy obtained his Ph.D. from Anna University, Chennai in 1996.

He did his postdoctoral research at JNCASR, AIST Japan and Bristol University. He joined JNCASR, Bangalore as a faculty fellow in 2004 and is a professor since 2016.

Research Direction

- Development of nanomaterials for applications in electrocatalysis, electrochemical energy storage and thermocatalysis.
- Designing porous materials for controlled release of various biomolecules
- Fabrication of membranes for gas separation and waste water treatment.

Research Description

Nanomaterials and Catalysis Laboratory, is currently focusing on developing different nanomaterials, composites, and porous materials by adopting new synthetic methodologies for different applications. These materials are used as catalyst for thermocatalytic reactions which includes alkane dehydrogenation, CO_2 hydrogenation and green synthesis of H_2O_2. There is also an increasing interest in carbon-based materials for energy storage applications. Membrane-based techniques are being developed for wastewater treatment and separation of gas mixtures. The lab also has expertise in designing controlled-drug release materials.

Research Contribution

Designing an efficient protocol to re-evaluate the performance of well claimed electrocatalysts for electrochemical nitrogen reduction reaction. (ACS Omega,2022, 7, 1874−1882; Chem. Rec., 2022, e202200139)

Tailoring nanocomposites (Ni-Fe LDH/1-T MoS_2) and metal phosphides (CoP, FeP and NiCoP) for electrochemical oxygen evolution reaction. (J. Mater. Chem. A., 2022, **10**, 22354-22362; ACS Appl. Mater. Interfaces, 2022, 14,28, 31951-31961; Materials Research Bulletin,140, 2021, 111312)

Development of anode materials for alkali metal ion batteries. (Electrochem. Sci. Adv., 2021, e2100019)

Publications

1. Bhutani D.; Maity S.; Chaturvedi S.; Chalapathi D.; Waghmare U.V.; Narayan C.; Vinod C. P.; Eswaramoorthy M.; Heterostructure from heteromixture: unusual OER activity of FeP and CoP nanostructures on physical mixing, J. Mater. Chem. A., 10, 22354-22362, 2022.
2. Biswas S.S.; Chakraborty S.; Saha A.; Eswaramoorthy M.; Electrochemical Nitrogen Reduction to Ammonia under Ambient Conditions: Stakes and Challenges, Chem. Rec., e202200139, 2022.

Giridhar U. Kulkarni

Professor

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Biosketch

Dr. Kulkarni obtained his Ph. D (1992) in Solid State and Structural Chemistry from Indian Institute of Science. He was a postdoctoral fellow at Cardiff University, UK, before joining JNCASR in 1995 as Faculty Fellow and is a professor since 2008. Having been the Chair of Materials Unit till 2011, he held Dean Academic Affairs (11-13) as well as Dean-Faculty Affairs (13-15) positions before moving to Centre for Nano and Soft Matter Sciences (CeNS) as the Director. Prof. Kulkarni returned to JNCASR in Jan 2020 to take over as the President while continuing to hold Adjunct Professorship at CeNS.

Research Direction

- Nanomaterials
- Nanolithography & fabrication
- Neuromorphic devices
- Molecular systems & properties

Research Description

The present research interests are focused on new strategies in synthesis of nanomaterials, nanopatterning and nanodevice fabrication including of molecular systems. The recipes emphasize the importance of simple design, near ambient working conditions, solution-based processing as well as low-cost instrumentation. Prof. Kulkarni's group strives to translate nano research finding into affordable technology.

Research Contribution

The unique chemical recipes employed have paved way, for the first time, to direct patterning of functional nanomaterials. The resulting patterns, by design or by self-forming, have been exploited in fabricating a wide range of device prototypes, from gas sensors to neuromorphic systems. Often, tailor-made molecules are incorporated to realize the desired functionality.

Publications

1. Second-Order Conditioning Emulated in an Artificial Synaptic Network, Bharath B, Bhupesh Yadav, and G. U. Kulkarni, ACS Appl. Electron. Mater.,4, 4, 1552–1557,2022.
2. Fabrication of dual-functional electrochromic smart window based on low-cost hybrid transparent electrode coated with a solution-processable polymer, SC Karumuthil, KG Mukhesh, I Mondal, AK Singh and GU Kulkarni, J. Mater. Chem. A,10, 23265-23273, 2022.

K. S. Narayan

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Biosketch

MSc from IIT Bombay, PhD from The Ohio State University, Scientist at Wright Patterson Air Force Base, USA and presently Silver Jubilee Professor, JNCASR. He is Fellow of Indian National Science Academy, Fellow of National Academy of Sciences and Fellow of Indian Academy of Sciences, Professor and Sir J. C. Bose National Fellow at JNCASR

Research Direction

- Studies of optical, optoelectronic and electronic phenomena in organic/molecular systems, Development of microscopy and photophysical probes to study Light emitting diodes and photonic structures.
- Solar Cells Fabrication, Measurements and Modelling
- Probing retina of different model systems and understanding vision processes for development of prosthetics.
- Study of cell growth and network on active substrates and neuronal recordings
- Translate Energy devices, sensors and techniques to the commercial space.

Research Description

Our laboratory is geared for studies which help us in understanding the electronic and optoelectronic processes in solution processed semiconductors and extended macromolecular systems. Bioelectronics for biophysical problems and utilize it in tissue engineering and for vision prosthetic elements. Developing microscopic and spectroscopic techniques to address various optical and electrical phenomena in low-dimensional materials. Transient electrical and optical measurements for charge carrier dynamics in molecular systems. Fabrication, measurement and analysis of organic-devices, 3-D printing and soft lithography to pattern structures for scaling, micro-optics and photonics, tissue engineering applications. Noise measurement and scanning-imaging techniques to predict the full life cycle of photovoltaic cells and modules.

Research Contribution

Our laboratory invented the POFET (photoactive organic field-effect transistor or polymer-based optical transistor, 2001). Recent studies of noise in photocurrent from organic solar cells and hybrid perovskite PVs suggest a novel rigorous approach to understand defects and degradation mechanisms. Our lab circumvented the laborious control protocols by using an embryonic chick retina in the early stage of development where photoreceptors are not functional and interfacing it with a more efficient polymer bulk heterojunction layer.

Publications

1. Light Controlled Signaling Initiated by Subretinal Semiconducting-Polymer Layer in Developing-Blind-Retina Mimics the Response of the Neonatal Retina, J. Neural Eng_,19036019 ,2022.
2. Confinement highlights the different electrical transport mechanisms prevailing in conducting polymers, Phys.Rev. Materials 6, 025602, 2022.

Rajesh Ganapathy

Professor

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Biosketch

Rajesh Ganapathy obtained his PhD in Physics from the Indian Institute of Science, Bangalore in 2007. From 2007 –2009 he was a Postdoctoral Fellow in the Dept of Physics, Cornell University USA. He joined the International Centre for Material Science (ICMS), JNCASR in 2009 where he is currently a professor.

Research Direction

- Phase transitions in colloids in flat and curved space
- Granular active matter
- Surface growth
- Stochastic machines
- Shear-induced transitions

Research Description

Research in Prof. Ganapathy's group strives to understand the emergent physics of soft matter systems, both passive and active. While passive/dead systems like, particle laden suspensions, liquid crystals, surfactant, and polymers have traditionally fallen under the umbrella of soft matter, more recently, soft matter has branched out to encompass systems where the constituents are endowed with an internal energy source making them self-propelled/active. Examples include motile bacteria, vibrated granules, confluent cell sheets to name a few. We use real-space imaging techniques to directly interrogate the physics of these systems.

Research Contribution

Some of our recent contributions include investigating the melting transition of colloidal crystals draped on the surface of a sphere, probing the glass transition in active granular liquids, and also exploiting machine-learning approaches to shed light on how a glass transforms into a crystal, a process known as devitrification.

Publications

1. Singh, N; Sood, A. K.; Ganapathy, R. Observation of Two-step Melting on a Sphere. Proc. Natl. Acad. Sci. U.S.A.,119, e2206470119 , 2022.
2. Arora, P.; Sood, A. K.; Ganapathy, R. Motile Topological Defects Hinder Dynamical Arrest in Dense Liquids of Active Ellipsoids, Phys. Rev. Lett., 128, 178002, 2022.
3. Ganapathi, D.; Chakraborti, D.; Sood, A. K.; Ganapathy, R. Structure Determines Where Crystallization Occurs in a Soft Colloidal Glass, Nature Phys., 17, 114, 2021.

Ranjan Datta

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Biosketch

Professor Ranjan Datta obtained his PhD in 2006 in Materials Science and Metallurgy, from University of Cambridge, UK. After that he did his postdoctoral research from the School of Materials Arizona State University, USA (2006-2208) before joining ICMS, JNCASR as Faculty Fellow on Dec 2008. Professor Datta did his B.E. and M.E. from Jadavpur University, Kolkata and Indian Institute of Science, Bangalore, respectively.

Research Direction

- Quantitative Imaging at atomic length scale in an aberration corrected transmission electron microscope.
- HREELS including momentum resolved EELS for probing low dimensional magnetism and various electronic states of mater.
- Thin film growth and structure property investigation of layered 2D materials and their heterostructures.

Research Description

Prof. Ranjan Datta's group is involved in developing atomic and sub-atomic length scale HREELS and advanced imaging techniques to characterize materials properties in an aberration corrected electron microscope. This work involves both experimentation and theoretical simulation.

Moreover, Prof. Datta's research work also involves thin film growth of various layered 2D materials and their heterostructures.

Research Contribution

Development of quantitative electron magnetic circular dichroism techniques (EMCD) at nano scale in an aberration corrected transmission electron microscope. Development of quantitative magnetic order and spin canting measurement at atomic plane resolution by HREELS. Surface spin canting geometry has also been revealed by the same technique with better information compared to a recently developed spin polarized neutron technique. Nanoscale band gap measurement by HREELS. Quantitative imaging at atomic length scale by both inline and off axis holography. Image simulation and reconstruction in advanced transmission electron microscopy. In materials, there are several contributions in p-doping of ZnO, Te and S doping of ZnO, large area epitaxial growth of various 2D materials and their heterostructures.

Publications

1. U Bhat, R Datta, Direct methods applied to phase retrieval in high resolution transmission electron microscopy, Journal of Physics Communications 6, 4, 045007, 2022.
2. U Bhat, R Datta, Quantitative counting of Zn and O atoms by atomic resolution off-axis and in-line electron holography, Journal of Applied Physics 125 ,15, 154902,2019.

Sridhar Rajaram

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Biosketch

Professor Sridhar Rajaram obtained his Ph.D. from the University of Utah, USA. After a postdoctoral stint in University of California, Berkeley, he joined as Faculty Fellow in ICMS. Currently he is a Professor in ICMS

Research Direction

- Biodegradable aliphatic carbonates as benign alternatives to aromatic polycarbonates
- Small molecule modulators of autophagy for treating neurodegenerative and neurodevelopmental disorders
- Organic-strong bases for enantioselective reactions

Research Description

Prof. Sridhar Rajaram's group is working on the development of aliphatic polycarbonates as alternatives to BPA-based aromatic polycarbonates. Currently, his group is exploring the use of these polycarbonates in coatings and as solid phase electrolytes in batteries. His group is also developing small molecule modulators of autophagy in collaboration with Prof. Ravi Manjithaya's group and Prof. James Chelliah's group. Apart from this, Prof. Rajaram's group has strong interest in developing organo-catalysts for polymerizations

Research Contribution

Aromatic polycarbonates are robust plastics with a variety of applications in daily life. A key problem with these plastics is that they release bis-phenol A upon biodegradation and due to this feature, they are banned from use in medical devices. We have developed aliphatic polycarbonates as alternatives as safe alternatives to aromatic polycarbonates. The rapid detection of low viral loads is important for early therapeutic interventions. Towards this end, we have developed dendronic raman-markers for amplification free detection of viral RNA. Autophagy is an important biological process for clearing and recycling cellular debris. In collaboration with Prof. Manjithaya and Prof. Chelliah we have shown that small molecular modulators of autophagy can be used to alleviate behavioral deficits in autistic mice. We have developed non-planar perylene diimides as alternatives to fullerenes in organic solar cells.

Publications

1. Verma, V.; Vijay Kumar, M. J.; Sharma, K.; Rajaram, S.; Muddashetty, R.; Manjithaya, R; Behnisch, T.; Clement, J. P. Pharmacological intervention in young adolescents rescues synaptic physiology and behavioural deficits in Syngap1+/- mice Exp. Brain Res. 240, 289-309,2022.
2. Ramesh, M. S., Rajaram, S. Organocatalyzed Regio-regular Ring Opening Polymerization of α-Phenyl Trimethylene Carbonate, Polymer 227:123803,2021.

A. Sundaresan

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Biosketch

Professor Sundaresan obtained his Ph.D. (1994) in Chemistry from IIT Bombay. He was a post-doctoral fellow at Laboratoire Crystallography, CNRS, Caen, Invited Researcher at LEPES, CNRS, Grenoble, France, and a Researcher (JST-CREST) at AIST, Tsukuba, Japan, before joining JNCASR in 2004. He is currently the Chair of CPMU. He is a Fellow of the Indian Academy of Sciences (FASc).

Research Direction

- Structure-property relationship in transition metal oxides.
- Magnetism, Ferroelectricity, Superconductivity, and Multiferroicity.
- High-pressure synthesis.

Research Description

Prof. Sundaresan's group's primary focus is studying the structure-property relationship in transition metal oxides. Apart from the conventional synthesis of oxides, the high-pressure and high-temperature method has been applied to make meta-stable materials. Synchrotron and neutron diffraction studies are used to determine crystal and magnetic structures. Physical properties such as magnetization, electrical transport, and heat capacity are carried out down to 2 K. A special focus is given to exploring new magnetoelectric multiferroic materials, quantum spin liquids, and superconductivity.

Research Contribution

Surface ferromagnetism was discovered in nanoparticles of otherwise nonmagnetic inorganic materials. Several transition metal oxides have been investigated to show unusual temperature-induced magnetization reversal phenomena. A new method has been demonstrated to identify intrinsic ferroelectricity in type-II multiferroics, particularly with low electric polarization. Several new spin-induced multiferroic materials have been discovered.

Publications

1. R. Kumar, and A. Sundaresan, Antisite-disorder driven cluster glass state and colossal magnetoresistance in $MnSb_2Se_4$, Phys. Rev. B 106, 134423, 2022.
2. D. P. Panda, D. Swain, and A. Sundaresan, Zero-Dimensional $(Piperidinium)_2MnBr_4$: Ring Puckering-Induced Isostructural Transition and Strong Electron-Phonon Coupling-Mediated Self-Trapped Exciton Emission, Inorg. Chem., 61, 11377, 2022.

Sarit S. Agasti

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Biosketch

Dr. Sarit S. Agasti obtained a Ph.D. degree in Chemistry from the University of Massachusetts-Amherst, working under the guidance of Prof. Vincent M. Rotello. He subsequently joined Harvard University to pursue his postdoctoral research, where he worked with Prof. Ralph Weissleder and Prof. Peng Yin. Dr. Sarit S Agasti is currently an associate professor at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore.

Research Direction

- Synthetic supramolecular host-guest interactions and their application in chemical biology.
- Development of new strategy and chemical probes for fluorescence imaging and super-resolution microscopy.
- DNA-based imaging.
- Biosensing and drug delivery using programmable molecular materials.

Research Description

The central theme of our research is molecular recognition in the synthetic system via supramolecular interactions: fundamental studies and applications in biology and materials. Our primary design relies on two types of molecular systems, macrocyclic host-guest, and DNA. We employ the concepts of molecular recognition in these systems to engineer molecules and materials to address challenges in various areas of biology and materials science, including bioimaging, sensing, drug delivery, and programmable and adaptive materials.

Research Contribution

Supramolecular chemistry facilitates programmable engineering of molecular systems through incorporation of various non-covalent recognition motifs. In recent years, we have been working on combining synthetic host-guest systems with the biological interface to develop various novel technologies with relevance to both fundamental and medical research. Examples include biorthogonal imaging and sensing, methods for super-resolution imaging, and new approaches for the delivery and activation of therapeutic materials

In the area of programmable molecular materials, we are interested in synthetic DNA nanostructures called DNA origami. The other exciting application of this system is to employ the programmable nature of DNA hybridization to generate probes for super-resolution microscopy.

Publications

1. Kundu, K.; Acharyya, P.; Maji, K.; Sasmal, R.; Agasti, S. S.*; Biswas, K.* Synthesis and Localized Photoluminescence Blinking of Lead-free 2D Nanostructures of $Cs_3Bi_2I_6Cl_3$ Perovskite. Angew. Chem. Int. Ed., 59, 13093, 2020.

Tapas K. Maji

Professor

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Web : www.jncasr.ac.in/faculty/tmaji

Biosketch

Prof. Maji graduated with Ph.D. Degree from IACS (Kolkata) in the year of 2002, M.Sc. (in 1997) and BSc. (In 1995) degree from Burdwan University (W. B). prior to joining JNCASR as a faculty member. He was a Lecturer at Jadavpur Univ. Kolkata. He was a JSPS Post-doctoral Fellow Kyoto University, Japan.

Research Description

Developing functional metal-organic frameworks (MOFs) and porous organic polymers (POPs) is the main focus of this laboratory. By judicious functionalization of nano-spaces of MOF and POP materials, our group emphasises on the capture and cost-effective separation of different chemical feedstocks (CO_2/H_2, CO_2/N_2, and olefin/paraffin), geometrical isomers and toxic elements in the aqueous medium. By introducing suitable light-harvesting or redox active building units in MOFs and POPs, we are working on the development of cost-effective and efficient catalysts for photo and electrochemical energy storage and conversion processes such as hydrogen evolution from water and CO_2 reduction to different fuels. To further enhance the processability of metal-organic hybrid material, our group has been working on developing 'soft' gel materials by self-assembling low molecular weight gelators (LMWG) with different metal ions.

Research Directions

Metal-Organic Frameworks, Porous Organic Polymers, Metal-Organic Gels, Energy Storage, H_2 Generation and CO_2 Capture and Reduction.

Research contribution

Today's world is witnessing the struggle of more than 4.3 billion people (71% of the global population) in accessing clean, ample, and safe drinking water. Introducing atmospheric water harvesting (AWH), beyond the arid atmosphere, under comfortable indoor humidity and temperature regime has its urgency in terms of commercialization and addressing the worldwide freshwater crisis. We have developed of a series of binary (aminopropyl functionalized magnesium phyllosilicate or aminoclay, and CuBTC) and ternary (aminoclay, graphene oxide, and CuBTC) MOF nanocomposites and their water storage and harvesting properties from the indoor atmosphere. We have designed and fabricated a prototype water harvester where the ternary nanocomposite enables 0.431 gg−1 of water at 90% relative humidity with a maximum value of 0.445 gg−1 indoor water collections per day.

Publications

1. P. Verma, F. A. Rahimi, D. Samanta, A. Kundu, J. Dasgupta, T. K. Maji, Visible Light Driven Photocatalytic CO_2 Reduction to CO/CH_4 using Metal-Organic 'Soft' Coordination Polymer Gel, Angew. Chem. Int. Ed.,61, e202116094,2022.
2. S. Laha, T. K. Maji, Binary/Ternary MOF Nanocomposites for Multi-Environment Indoor Atmospheric Water Harvesting, Adv. Funct. Mater., 2203093,2022.

Faculty and Student Awards

Prof. G. U. Kulkarni

- Dr Raja Ramanna State Award 2019 -Karnataka State Council for Science and Technology (KSCTC)
- The Prof. C.N.R. Rao National Prize for Chemical Research-2020, by Chemical Research Society of India (CRSI)
- Kannada Rajyotsava Award – 2021
- Young Scientist Research Award, Board of Research in Nuclear Sciences (BRNS) of Department of Atomic Energy, India, 2020.
- CNR Rao Prize Lecture in Advanced Materials 2022 by Materials Research Society of India (MRSI)
- Hon. Fellowship of Karnataka S&T Academy (KSTA) 2020, Bengaluru
- Adjunct Professor of the Centre for Nano and Soft Matter Sciences
- Adjunct Faculty at Manipal Academy of Higher Education (MAHE)
- Fellow of the Indian National Science Academy
- Fellow of the Indian National Academy of Engineering

Prof. Bivas Saha

- Editor, Solid State Communications (08/2022- Cont.)
- Sheikh Saqr Career Award Fellowship, (2022-Cont.)
- Associate, Indian Academy of Sciences, (2020- Cont.) Young Scientist Research Award,
- Board of Research in Nuclear Sciences (BRNS) of Department of Atomic Energy, India, 2020.

Prof. Chandrabhas Narayana

- Platinum Jubilee lecture award of Indian science Congress (2020) Honorary Fellow of Indian Society of Analytical Scientists

Prof. Sarit Agasti

- Merck Young Scientist Award (2021)
- Editorial Advisory Board of ACS Journal Bioconjugate Chemistry (2022).
- Invited to organize a “Focused Cluster” on the topic of “Synthetic Host-Guest Chemistry in Biology” for the ACS journal Bioconjugate Chemistry (2022).
- INSA Medal for Young Scientist (2022)

Students

Tejaswini S Rao

- Best Student Talk at the ‘In-house symposium (IHS) 2021’, JNCASR

Rohit Attri

- Best Poster award at the following conferences:
- International Winter School on Frontiers in Materials Science - 2020
- Bengaluru India Nano – 2022

Sourav Rudra

- CSIR SHYAMA PRASAD MUKHERJEE FELLOWSHIP, 2021.

Rahul Kumar

- Winning the ICDD grant for the 2022-2023 cycle under the proposal title,"*Diffraction pattern of new low-dimensional materials.*"

Divya C

- Best Talk, ICOPVS, 2020

Anjana Joseph

- Best poster 2021, In-house symposium

Janaky Sunil

- Best Talk: 2020, In-house symposium

Simanta Kalita

- Best poster prize in International Conference on Chemistry and Applications of Soft Materials (CASM 2022), CSIR-NIIST

Dheemahi Rao

- Best Poster Award, 2021, In-house symposium, JNCASR.

Courses Offered

Aug-Dec session		
JT 205	Quantum Mechanics	3:0
JT 207	Mathematical Methods	3:0
JC 201	Basic Electronics	2:1
JC 213	Inorganic Chemistry	3:0
	Solid State Physics-II	3:0
JT 205	Quantum Mechanics	3:0
	Fundamentals of Optics	3:0
JC 214	Laboratory – I	0:4
JC 218	Laboratory-III (Materials Laboratory)	0:4
JC 307	Physics of Materials	3:0
JC 228	Classical Mechanics	3:0
JC 304	Chemistry of Materials	3:0
JNC 208	Characterization of Materials	3:0
JNC 311	Molecular Structure and Spectroscopy	3:0
JC 308	Fundamentals of Computational Statistical Mechanics	3:0
JNC 202	Organic Chemistry	3:0

Jan-Apr session		
JC 215	Electricity and Magnetism	3:0
JT204	Statistical Physics	3:0
JT 201	Solid State Physics	3:0
JC 309	Computational Methods	3:0
JC 216	Laboratory-II	0:4
JI 302	Transmission Electron Microscopy and Spectroscopy	3:0
JT208	Computational methods for condensed matter and materials science	2:0
JNC 306	Advanced Inorganic Chemistry	3:0
JNC 301	Reaction Mechanisms	3:0

Extension Programmes

- Summer Research Fellowships Programme (SRFP)
- CPMU hosts around twelve students every summer as part of JNC’s Summer Research Programme.
- For more details, visit: https://www.jncasr.ac.in/academic/fandeprogrammes

Visiting Fellowship Programme

- The Unit hosts around two to three visiting researchers holding permanent positions from various Universities and laboratories, every year.
- For more details, visit: https://www.jncasr.ac.in/academic/fandeprogrammes

Academic Programmes

Ph.D.

Candidates are selected based on their performance in national-level entrance examinations such as GATE/JEST/CSIR-JRF/UGC-JRF/DBT-JRF/ICMR-JRF/ INSPIRE-JRF and an on-site interview. Eligibility for this programme is (i) Master's Degree in Science or equivalent in Electronics, Chemical/Mathematical/ Physical/ Materials Science, (ii) Bachelor's Degree in Engineering/Technology/4-year, Bachelor of Science or equivalent in Electrical/Electronics/Metallurgy/ Polymer/ Engineering Physics/Nano Technology/ Chemical (iii) Master's Degree in Engineering/ Technology or equivalent in Electrical/Electronics/ Metallurgy/Polymer/Engineering Physics/Nano Technology/Chemical Engineering with a minimum of 55% marks. Students are admitted in August and January of every year. Selected candidates must earn 12-course credits in a span of two-to-three semesters and should maintain a Cumulative Grade Point Average (CGPA) of 5.5. In the subsequent years, the candidate will carry out original research work under the supervision of a faculty. The student should pass a comprehensive examination (viva voce) within two years of registration.

For more details, visit: https://www.jncasr.ac.in/admission/degree-programmes/phd

M.S. (Engg.) in Materials Science

Candidates are selected based on their performance in national-level entrance examinations such as GATE/JEST/CSIR-JRF/UGC-JRF/DBT-JRF/ICMR-JRF/ INSPIRE-JRF and an on-site interview. Eligibility for this program is the same as required for the Ph.D. programme or bachelor's degree in Engineering/ Technology/4-years Bachelor of Science or equivalent in Electrical/Electronics/Metallurgy/Polymer/ Engineering Physics/Nano Technology/Chemical Engineering with first class or equivalent. The duration of the course is two years.

Selected candidates must earn 12-course credits in a span of two-to-three semesters. The minimum CGPA required is 5.5. After the first semester, the candidate will carry out original research work. At the end of the second year, the candidate must submit a thesis and defend it in front of an expert committee.

Based on the candidate's performance in the M.S. programme, the department can recommend the candidate to join its Ph.D. program. The stipend and the fee structure are similar to those for the Ph.D. program. Students are admitted in August and January of every year.

For more details, visit: https://www.jncasr.ac.in/admission/degree-programmes/ms

Integrated Ph. D. in Physical Sciences (Materials)

For the academic year starting Aug 2022 onwards, CPMU Unit, JNCASR, has a new Integrated Ph.D. programme in Physical Sciences (specialization in Materials). The programme is jointly conducted with the Theoretical Sciences Unit; JNCASR aims to provide students with a strong foundation in physics and materials research. Students with Bachelor's degrees in physics and chemistry can apply. Those with Bachelor's degrees in Engineering with an aptitude for scientific research are also considered. Candidates should have a minimum of 55% marks at the Bachelor's (B.Sc./B.E./ B.Tech.) level. Students are chosen based on the national-level examination, and their marks in pre-university or equivalent, followed by an on-site interview.

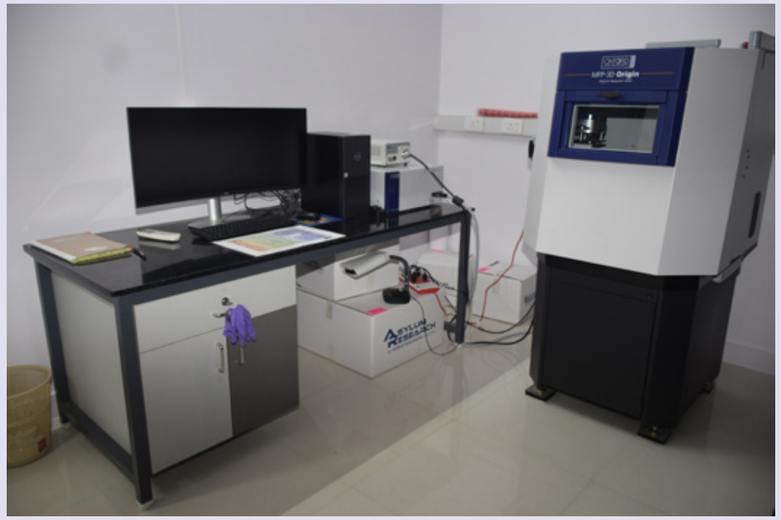
The program commences in August, every year. It consists of three parts (a) course work spanning three-four semesters, (ii) research over another two-three semesters culminating in a thesis toward an M.S. degree in Physical Science, and (iii) doctoral research leading toward a Ph.D. degree to be pursued in the succeeding two to four years.

For more details, visit: https://www.jncasr.ac.in/sites/default/files/users/user277/Int.%20PhD_Physical%20Sciences.pdf

On-campus hostel and medical facilities are available for all students.

Research Facilities

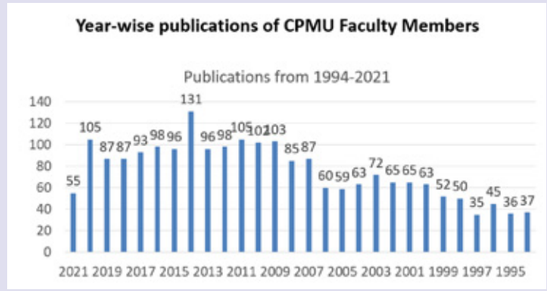
1. Single Crystal X-ray diffractometer with CCD facility
2. Catalyst characterization with Gas chromatograph
3. Powder X-ray diffractometers
4. Fourier Transform Infra-red Spectrometer
5. Thermal characterization (TGA, DSC)
6. UV-VIS Lambda 750 spectrometer
7. Brillouin and Raman Spectrometers
8. Photoluminescene emission and excitation spectroscopy
9. Zeta sizer Nano ZS particle size analyzer
10. Precision Workstation for dielectric measurements
11. PPMS and SQUID magnetometer
12. Super Computer facility
13. Molecular Beam Epitaxy
14. High Pressure High Temperature Synthesis facility
15. Transmission electron microscope (TEM) and FESEM
16. Atomic force microscope (AFM)
17. Nanoscriber highest resolution 3D Printer
18. Clean room facility
19. Ellipsometer

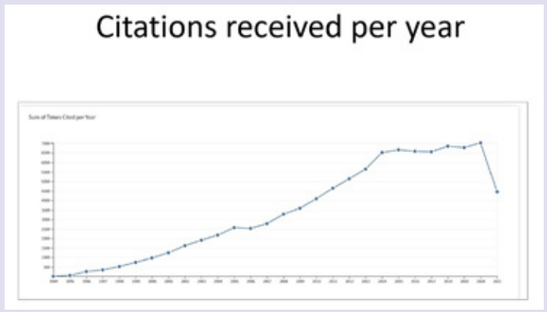


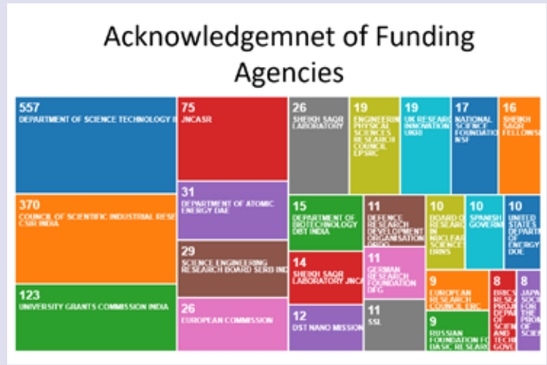
Unit Statistics

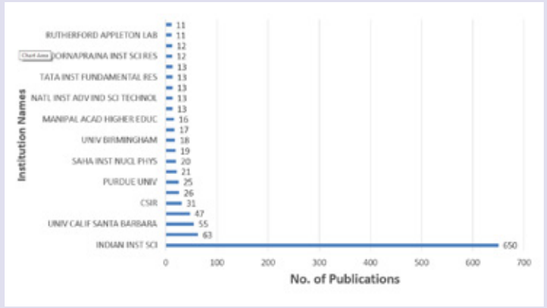
Overview

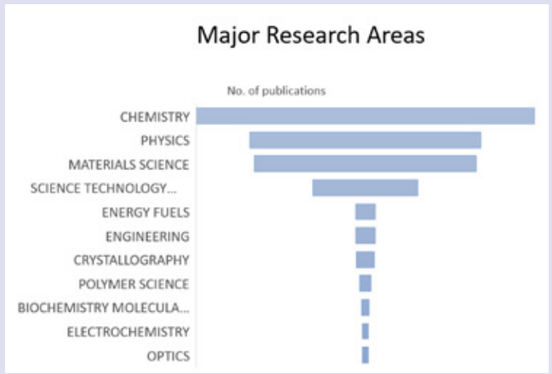
Total number of publications	2130
h-index	139
Average citations per item	44.87
Total citations	95,572
Total Citations (without self-citations)	88,128











Technical & Administrative Staff

Senior Technical Officers
V Sreenath
S Srinivas

Senior Laboratory Assistants
J Anil Kumar
A Srinivas Rao
B S Vasudeva

Technical Assistant
Arun Aravindakshan K V
Sreehari Mohan

Office
M Uma Usha

Workshop
Rajkumar D

Helper
Balraj

School of Advanced Materials (SAMat)

"School of Advanced Materials (SAMat) is comprising researchers from Chemistry and Physics of Materials Unit (CPMU), New Chemistry Unit (NCU) and Theoretical Sciences Unit (TSU) in JNCASR. SAMat is headed by CPMU and fosters collaborative research across different disciplines to address important and pressing scientific and engineering challenges."

ICMS & SSL

International Centre for Materials Science

International Centre for Materials Science (ICMS), established in 2007, is the first international centre of its kind in India, devoted to research, education in Materials Science, established in the confines of scientific cum educational institution. The centre was envisaged by the Department of Science and Technology (DST), Government of India. JNCASR has taken the lead and necessary step to establish it.

Sheikh Saqr Laboratory (SSL)

Sheikh Squr Laboratory Located in the premises of the Inter national Centre for Materials Science, is the stateof- the-art centre devoted to high impact, interdisciplinary scientific research in the area of materials chemistry and chemical biology.

CPMU Alumni Materials Lecture

2021

Prof. Chilla Malla Reddy

Professor, Department of Chemical Sciences
Indian Institute of Science Education and Research Kolkata

Crystal Engineering of adaptive smart materials: from mechanical bending to self-healing

On September 4, 2021

2022

Prof. Chandni U

Assistant Professor, Department of Instrumentation and Applied Physics
Indian Institute of Science Bangalore

Emergent Phases of Matter in Twisted Bilayer Graphene

October 01, 2022

Chemistry and Physics of Materials Unit

Jawaharlal Nehru Centre for Advanced Scientific Research

(A Deemed University)

(Supported by the Department of Science & Technology, Govt. of India)

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