



Chemistry and Physics of Materials Unit

2019-20

Jawaharlal Nehru Centre for Advanced Scientific Research





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Welcome Note from the Chairman

Welcome to the Chemistry and Physics of Materials Unit. It gives me pleasure to present the CPMU brochure for the year 2019-2020. 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 1994, the Unit has expanded its research activities on materials science and grown vertically over the years. This year, the Unit has touched a milestone of Silver Jubilee, which is a momentous occasion for us. The Silver Jubilee celebrations begin from the Unit day on 7th September 2019 and will continue with various academic events for a year.

The Unit fosters interdisciplinary research on cutting edge materials by involving highly skilled 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 area 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 Ph.D program, the Unit offers an Integrated Ph.D program in materials jointly with the Theoretical Sciences Unit (TSU). Recently, CPMU has played a leading role in establishing a virtual center of School of Advanced Materials (SAMat), which includes faculty members of TSU and New Chemistry Unit (NCU) of this Centre.

A Sundaresan
Chair, CPMU



Faculty Members

Founder Chair

CNR Rao, FRS

Chair

A Sundaresan

Professors

K S Narayan FNASc, FASc

S Balasubramanian, FASc

Chandrabas Narayana

G U Kulkarni FNASc, FASc on lien

S M Shivaprasad* on lien

M Eswaramoorthy



Tapas Kumar Maji

Ranjan Datta*

Rajesh Ganapathy*

Sridhar Rajaram*

Sarit S Agasti#

Bivas Saha*

* Jointly with ICMS

Jointly with NCU

**Associate Members from the
Theoretical Sciences Unit**

Shobhana Narasimhan FNASc

Swapan K Pati FNASc, FASc

Srikanth Sastry FNASc, FASc

Umesh V Waghmare FNASc, FASc

N S Vidhyadhiraja



C.N.R. Rao

Linus Pauling Research Professor
Honorary President of JNCASR

Phone: +91-80-2208-2761

Email: cnrrao@jncasr.ac.in

www.jncasr.ac.in/cnrrao

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 1650 research articles and over 50 books and has received honoris causa doctorate degrees from 79 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 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 Direction

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

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.

Publication:

1. A. Roy, A. Singh, S.A. Aravindh, S. Servottam, U.V. Waghmare, and C.N.R. Rao, Cadmium phosphohalides with novel features exhibiting HER activity, *Angew. Chem. Int. Ed.*, 58, 6926 (2019).
2. K. Manjunath, S. Prasad, S. Servottam, U.V. Waghmare, C.N.R. Rao, front Cover: Hg₂NF Analogue of HgO (*Eur. J. Inorg. Chem.* 19/2019, , *European Journal of Inorganic Chemistry* (19), 2396-2396 (2019).



Balasubramanian Sundaram

Professor

Phone: +91-80-2208-2808 +91-948287708

Email: bala@jncasr.ac.in

www.jncasr.ac.in/bala



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 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 are employed to investigate microscopically, the emergent behaviour in these systems.

Publication:

1. NVS Avula, A. Mondal, S. Balasubramanian, Charge Environment and Hydrogen Bond Dynamics in Binary Ionic Liquid Mixtures: A Computational Study” J. Phys. Chem. Lett., 9, 3511-3516 (2018).

Research Direction

- ♦ High Performance Computing
- ♦ Self-Assembly, Supramolecular Interactions
- ♦ Ionic Liquids for Energy Storage
- ♦ Gas Storage
- ♦ Enzyme modelling

Research Contribution:

The research group has had several breakthroughs, including the demonstration of fractional ionic charge in RTILs, the reversal of handedness upon reversal of electric field direction on a supramolecular polymer film -- a discovery which can be employed in chiral amplification, the enhancement of interfacial affinity of lipases by suitable mutations, etc.

2. DB Korlepara, WR Henderson, RK Castellano, S Balasubramanian, “Differentiating the mechanism of self-assembly in supramolecular polymers through computation” ChemComm, 55, 3773-3776 (2019).





Bivas Saha

Assistant Professor

Phone: +91-80-2208-2619; +91-6360126595

Email: bsaha@jncasr.ac.in ; bivas.mat@gmail.com

Web : www.jncasr.ac.in/bsaha

Biosketch:

Dr. Saha graduated with Ph.D. degree from Purdue University's Birck Nanotechnology Center and School of Materials Engineering in 2014, M.S. degree from JNCASR in 2010 and B.Sc. degree from Jadavpur University in 2007. Prior to joining JNCASR as a faculty member, he was a Postdoctoral Scholar in Department of Materials Science and Engineering and Center of Energy Efficient Electronic Sciences in University of California Berkeley.

Research Description:

Heterogeneous Integration Research Group directed by Dr. Saha specializes in the development of novel functional and artificially structured materials, understand and engineer their energy transport and conversion mechanism, and develop devices for applications in energy harvest and energy efficient electronic systems such as in thermoelectrics, plasmonics and energy efficient computing. The group envisions to drastically reduce energy consumption in electronics and optoelectronics, as well as develop highly efficient energy conversion devices, which will help our nation achieve energy security as well as address climate change.

Research Direction

- ♦ Heterostructure and Metamaterials.
- ♦ Nano-photonics
- ♦ Thermal and Thermoelectric Energy Conversion.

Research Contribution:

Dr. Saha developed the first epitaxial single crystalline metal / semiconductor superlattices, which has emerged as a novel kind of "man-made" crystal for applications in solid state energy conversion devices. His research has also demonstrated sub- 50 mV mechanical relay switch devices for mechanical computing devices.

Publication:

1. S. Nayak, M. Baral, M. Gupta, J. Singh, M. Garbrecht, T. Ganguli, S.M. Shivaprasad and B. Saha, "Rigid-Band Electronic Structure of Scandium Nitride (ScN) across the n to p- type Carrier Transition Regime " Phys. Rev. B Rapid Communication, 99, 161117(R), (2019).
2. B. Biswas, B. Saha, "Development of Semiconducting ScN" Phys. Rev. Materials, 3, 020301 (2019).



Chandrabhas Narayana

Professor

Phone: +91-80-2208-2810 +91-9448682721

Email: cbhas@jncasr.ac.in; cbhasi@gmail.com

www.jncasr.ac.in/cbhas



Biosketch:

Prof. Chandrabhas Narayana graduated with PhD degree from Indian Institute of Science, Bangalore's Department of Physics in 1995, MScEd degree from RCEM, Mysore University in 1988 and BScEd degree from RCEM, Mysore University in 1986. Prior to joining JNCASR as a faculty member, he was a Postdoctoral Associate in Department of Materials Science and Engineering, Cornell University, NY. He is currently the Dean, Research and Development at JNCASR.

Research Description:

Prof. Chandrabhas Narayana's group uses Raman, Brillouin and Synchrotron as a probe to under the physical properties of materials. The main emphasis of the lab is to provide the insight into why a particular property, like Topological transitions, multi-ferroic behavior, skyrmions, occur in the material and how this can be achieved or predicted in new materials. In order to perturb the system two thermodynamic variables are used, namely temperature and pressure. The group is one of the pioneers in the area of high pressure research in materials. The group also looks at synthesizing MOFs and its composites and nano-materials to elucidate the interesting properties they exhibit from a molecular perspectives. The group also specializes in developing bio-diagnostics and study of biologically important molecules like protein, nucleic acids with a aim to tailor its properties.

Research Direction

- ♦ Optical spectroscopy (Raman and Brillouin spectroscopy) for nanomaterials, strongly correlated systems, bio-systems.
- High Pressure research
- Bio-diagnostics and nano-biotechnology.

Research Contribution:

The group is pioneers in developing research tools like Raman spectrometers. The group has been one of the early groups to use Raman spectroscopy to study protein structure function and drug protein interactions. The group specializes in developing and use of High Pressure research in material science. The group have been recently able to use High Pressure Raman to elucidate new topological phases

Publication:

1. V. Rajaji, Raagya Arora, Saurav Ch. Sarma, B. Joseph, Sebastian C. Peter, Umesh V. Waghmare and Chandrabhas Narayana, Phonon signatures of multiple topological quantum phase transitions in compressed TlBiS₂: A combined experimental and theoretical study, Phys. Rev. B 99, 184109 (2019).
2. Amit Pawbake, Christophe Bellin, Lorenzo Paulatto, Keevin Beneut, Johan Biscaras, Chandrabhas Narayana, Dattatray J. Late and Abhay Shukla, Pressure-Induced Phase Transitions in Germanium Telluride: Raman Signatures of Anharmonicity and Oxidation, Phys. Rev. Let. 22, 145701 (2019).





M. Eswaramoorthy

Professor

Phone: +91-80-2208-2870 +91-9448829121

Email: eswar@jncasr.ac.in; ameswar@gmail.com

www.jncasr.ac.in/eswar

Biosketch:

Prof. Eswaramoorthy received his Ph.D degree from Anna University in 1996, Chennai. He did his postdoctoral research at JNCASR(1996-1999), AIST, Tsukuba/Sendai, Japan(1999-2001 and 2003-2004) and at Bristol University, UK(2001 to 2003). He joined JNCASR in 2004 as a faculty and is currently a Professor in Chemistry and Physics of Materials Unit.

Research Description:

Research work in our laboratory mainly focuses on synthesis and modification of nanomaterials possessing desired properties towards various applications in the fields of energy, environment and health. Synthesis of high surface area metal nanostructures for catalysis, nanoporous materials for adsorption and energy storage, development of 2D membranes for gas separation, application of carbon spheres for the delivery of drug molecules to the brain cells are some of the specific areas we are interested in.

Research Direction

- ♦ Nanomaterials for Catalysis
- ♦ Gas separation by membrane
- ♦ Electrocatalysis
- ♦ Energy storage
- ♦ Drug delivery

Research Contribution:

Fabricated sub-micrometer thick MoS₂ membranes showing highly efficient H₂/CO₂ separation along with very high H₂ Permeability. Demonstrated the use of glucose derived carbon spheres for the efficient delivery drug molecules into the brain. A strikingly simple method to synthesise high surface area noble metal nanostructure which find applications in catalysis has been established.

Publication:

1. Sonu K P, Sushmitha Vinikumar, Shikha Dhiman, George S J and Eswaramoorthy M, "Bio-inspired temporal regulation of ion-transport in nanochannels", *Nanoscale Advances*, 1, 1847 - 1852 (2019).
2. Gond R, Dheeraj K S, Eswaramoorthy M and Barpanda P, "Sodium Cobalt Metaphosphate as an Efficient Oxygen Evolution Reaction Catalyst in Alkaline Solution", *Angew. Chem. Int. Ed.*, 58, 1 - 6 (2019).



Giridhar U. Kulkarni

Professor

Phone: +91-80-2208-2814 ; +91-9448825386
Email: kulkarni@jncasr.ac.in ; gukulk@gmail.com
www.jncasr.ac.in/kulkarni



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. He is a Professor (on lien) since taking charge as Director, Centre for Nano and Soft Matter Sciences (CeNS) in April 2015.

Research Description:

The Kulkarni Group excels in developing new strategies for synthesis of nanomaterials directly suited to nanopatterning and device 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 – all aimed at possibility of translation towards potential technology.

Research Direction

- ♦ Metal network based devices
- ♦ Twisted Graphene stacks
- ♦ Supramolecular energy storage devices
- ♦ Morphology controlled Metal crystallites

Research Contribution:

The highlights include producing metal nanomesh based transparent conductors and a number of transparent devices made from the invention such as flexible touch screens, defrost and defogging panels, EMI shields and smart windows. In addition, molecular energy devices, circuit elements, memory devices and sensors as well as new family of twisted graphene have been fabricated. Further, gold microcrystallites have been grown bearing unconventional lattices as also properties-nobler in many ways than the conventional gold.

Publication:

1. S. Kundu and U. Mogera and S. J. George and G. U. Kulkarni, A planar supercapacitor made of supramolecular nanofibre based solid electrolyte exhibiting 8 V window, Nano Ener., 61: 259, 2019.
2. B. Bannur, K.D.M. Rao, K. N. Harish & G. U. Kulkarni, A Solution-Based Fast Fabrication of a High-Performance Unlimited Area Au Nanostructure/Si Heterojunction Photodetector, ACS Appl. Elec. Mater., 1: 577, 2019.





K.S. Narayan

Professor

Phone: +91-80-2208-2822

Email: narayan@jncasr.ac.in

www.jncasr.ac.in/narayan

Biosketch:

Msc from IIT Bombay, PhD from The Ohio State Univ, 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–India and Fellow of Indian Academy of Sciences.

Research Description:

Developing microscopic and spectroscopic techniques specifically to understand the various optical and electrical phenomena in low-dimensional materials is actively pursued. Transient electrical and optical measurements are carried out to probe and understand 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 is utilized.

Research Direction

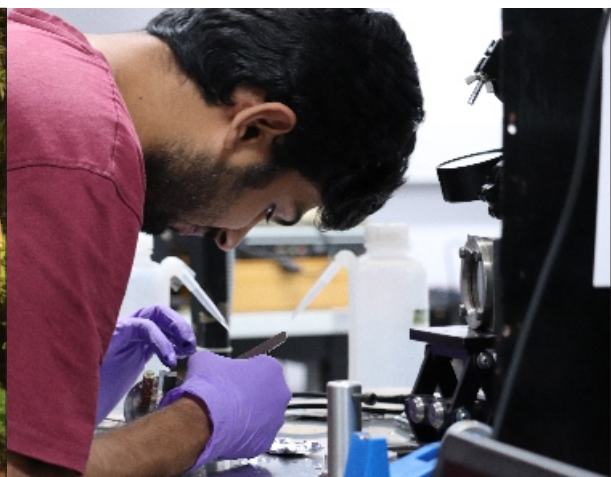
- ♦ Studies of optical, optoelectronic and electronic phenomena in organic/molecular systems
- ♦ Understanding and probing retinal system using soft interfaces and long-term neuronal recordings
- ♦ Translate devices and techniques to the commercial space.

Research Contribution:

His laboratory has contributed to several pioneering aspects of plastic optical-field effect transistors, organic solar cells and light emitting diodes. He has also contributed to research area of these soft-electronic polymers in biomedical arena where these materials have exhibited utility in tissue engineering and for vision prosthetic elements.

Publication:

1. P. Kumar, N. Ganesh and K. S. Narayan *Electrospun Fibers Containing Emissive Hybrid Perovskite Quantum Dots*, *ACS Appl. Mater. Interfaces*, DOI: 10.1021/acsami.9b08409 (2019).
2. S. Das and K. S. Narayan *Significant Increase in Electrical Transport of Conducting Polymers Confined in Alumina Nanopores* DOI:10.1021/acs.jpcc.9b01563, *The Journal of Physical Chemistry C* (2019).



Rajesh Ganapathy

Professor

Phone: +91-80-2208-2572 ; +91-9880671639

Email: rajeshg@jncasr.ac.in ;
rajesh.ganapathy@gmail.com

www.jncasr.ac.in/sml/



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 as a Faculty Fellow. He is currently an Associate Professor (since 2015) at ICMS, JNCASR.

Research Description:

Research in our group strives to unravel the physics of soft matter. From particle laden suspensions to biological cells and liquid crystal displays, soft materials are ubiquitous in our daily lives. A key unifying attribute of soft materials is that they comprise of mesoscopic structures held together by weak entropic forces. External perturbations therefore couple strongly to soft matter microstructure which, in turn determines their macroscopic response. Understanding this structure-response relationship is central to identifying properties exclusive to this class of condensed matter.

Research Direction

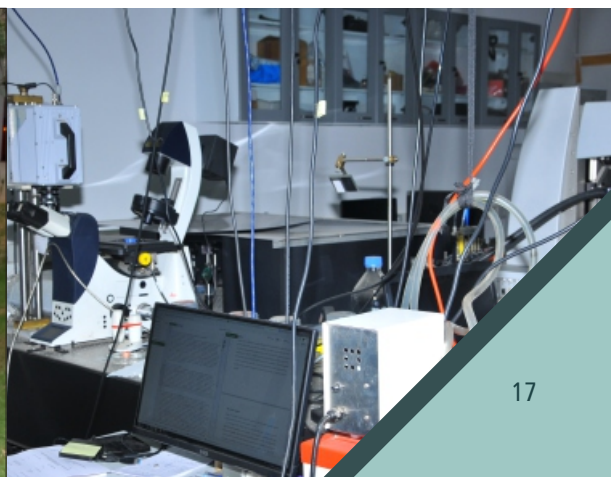
- ♦ Amorphous and crystalline solids: memory, glass transition
- ♦ Active matter
- ♦ Flow of suspensions: shear-thickening, tunable-rheology

Research Contribution:

Our key research contributions recently have been (1) Exploring the formation of mechanical memories in amorphous solids. (2) Exploiting atomic heteroepitaxy concepts to steer colloidal self-assembly (3) Unravelling the mechanisms by which dense suspensions of anisotropic particles shear-thicken.

Publication:

1. Srimayee Mukherji, Neelima Kandula, A K Sood and Rajesh Ganapathy, "Strength of mechanical memories is maximal at the yield point of a soft glass" *Phys. Rev. Lett.*, **122**, 158001, (2019).
2. Vikram Rathee, Srishti Arora, Daniel Blair, Jeff Urbach, A K Sood and Rajesh Ganapathy "Unravelling the role of frictional contacts and particle orientational order during shear-thickening in suspensions of colloidal rods" (*manuscript at revision 2019*).





Ranjan Datta

Professor

Phone: +91-80-2208-2571; +91-9513471098

Email: ranjan@jncasr.ac.in

www.jncasr.ac.in/ranjan

Biosketch:

Professor Ranjan Datta obtained his PhD in 2006 in Materials Science and Metallurgy, University of Cambridge, UK. After that he did his postdoctoral research from School of Materials from 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.

Research Description:

Prof. Ranjan Datta's group was involved in developing atomic and sub-atomic length scale HREELS and 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 Direction

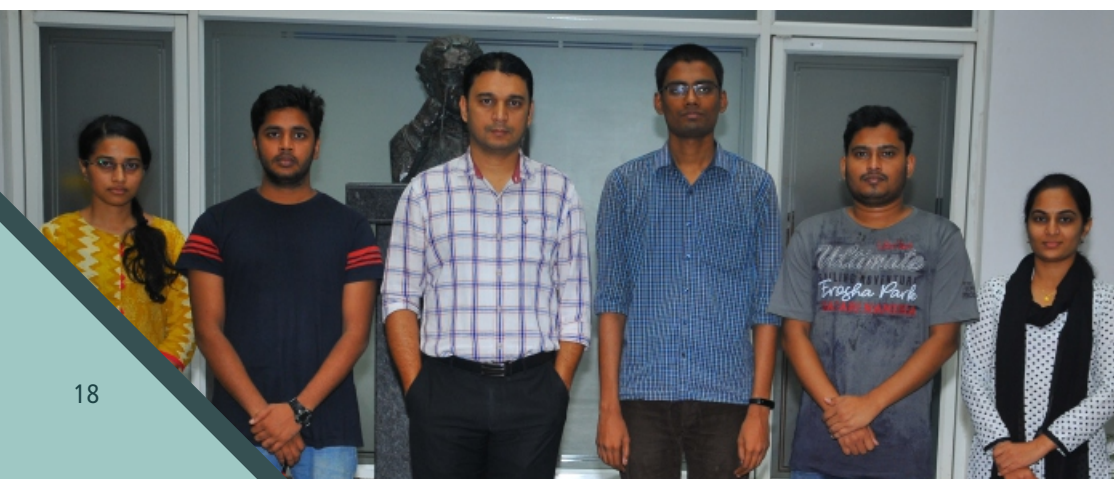
- ♦ Quantitative Imaging and spectroscopy at atomic length scale in an aberration corrected transmission electron microscope.
- ♦ HREELS for probing low dimensional magnetism and various electronic states of mater.
- ♦ Thin film growth and structure property investigation of layered 2D materials and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

Research Contribution:

Development of quantitative electron magnetic circular dichroism techniques (EMCD) at nano scale, quantitative magnetic order and spin canting measurement at atomic plane resolution and band gap measurement by HREELS.

Publication:

1. D.S. Negi, H Sharona, U Bhat, S Palchoudhury, A Gupta, **Ranjan Datta**, Surface spin canting in Fe₃O₄ and CoFe₂O₄ nanoparticles probed by high resolution electron energy loss spectroscopy, **Phys. Rev. B**, 95, 174444 (2017).
2. R Sahu, U Bhat, Nitin M Batra, H Sharona, B Vishal, S Sarkar, S Assa Aravindh, SC Peter, Iman S Roqan, PMFJ Costa, **Ranjan Datta**, Nature of low dimensional structural modulations and relative phase stability in Re_xMo(W)_{1-x}S₂ transition metal dichalcogenide alloys, **Journal of Applied Physics**, 121, 105101 (2017).



Sarit S. Agasti

Assistant Professor

Phone: +91-80-2208-2628 +91-7022256285

Email: sagasti@jncasr.ac.in ; saritagasti@gmail.com

www.jncasr.ac.in/sagasti



Biosketch:

Dr. Sarit S. Agasti received his BSc degree from the Ramakrishna Mission Vidyamandira, Belur Math in the year 2003 and completed his Master's degree from IIT, Kanpur in 2005. He pursued his doctoral research at the University of Massachusetts, Amherst (advisor: Prof. Vincent M. Rotello) and graduated in the year 2010. He then proceeded to take up postdoctoral position at the Harvard University from 2011–2015 with Prof. Ralph Weissleder and Prof. Peng Yin respectively. From 2015 onwards, he has been a faculty member at JNCASR.

Research Description:

Dr. Sarit Agasti leads the programmable molecular design lab which is interested in employing molecular systems for targeted imaging, critical for labeling and tracking specific molecules or cellular events in vivo. The group aims to utilize supramolecular interactions for achieving precise control and tunability in spatiotemporal labelling of cellular organelles. The lab expertise also includes use of DNA as a programmable nanomaterials for biological applications. The DNA based materials, viewed as “molecular breadboard”, provides precise addressability and enormous scope for a wide variety of applications ranging from sensing, imaging, and targeted drug delivery.

Research Direction

- ♦ Small molecule based systems for targeted bioimaging
- ♦ Programmable molecular materials and DNA origami
- ♦ Super-resolution optical microscopy
- ♦ Diagnostic sensing and therapeutics

Research Contribution:

Dr. Sarit Agasti has significantly contributed to the super resolution imaging method “DNA PAINT” which utilizes the programmable autonomous blinking of DNA probes. He has developed this method as a multiplexed super resolution-imaging platform for application in cellular systems. He is currently developing programmable molecular assemblies in the living system based on a synthetic host-guest system. These assemblies are employed for imaging in living systems.

Publication:

1. R. Sasmal, N. Das Saha, M. Pahwa, Sushma Rao, D. Joshi, M. S. Inamdar, V. Sheeba, and Sarit S. Agasti. "Synthetic Host–Guest Assembly in Cells and Tissues: Fast, Stable, and Selective Bioorthogonal Imaging via Molecular Recognition." *Analytical chemistry* 90, no. 19 (2018): 11305–11314.
2. S. Sinha, N. Das Saha, R. Sasmal, D. Joshi, Soumya C., Monica S. Bosco, and Sarit S. Agasti. "Reversible encapsulations and stimuli-responsive biological delivery from a dynamically assembled cucurbit [7] uril host and nanoparticle guest scaffold." *Journal of Materials Chemistry B* 6, no. 44 (2018): 7329–7334.





Shivaprasad S M

Professor

Phone: +91-80-2208-2947 ; +91-9900382352

Email: smsprasad@jncasr.ac.in

smsprasad8@gmail.com

www.jncasr.ac.in/smsprasad

Biosketch:

Shivaprasad did post-doctoral research at Univ of Sussex and IIT, Delhi after obtaining Ph D from Karnatak University. He established and headed (1985-2007) Surface Physics and Nanostructure Group at National Physical Laboratory, New Delhi and Professor at JNCASR since 2007. He was Visiting Scientist at NIST, Rutgers Univ, Tohoku Univ and Univ of Ulm. He is recipient of Young Scientist and Outstanding Scientist Awards from CSIR; Medal, Superconductivity & Materials Science and Distinguished Lecturership awards from MRSI; CNR Rao Oration and Rajaramanna Awards and Honorary D. Sc from VSK University, Bellary.

Research Description:

With expertise in epitaxial growth of ultra-thin films, Shivaprasad has elucidated on several metal-metal-semiconductor systems by mapping novel phase diagrams. He has established a sophisticated Epitaxy lab with Molecular Beam Epitaxy and E-beam Evaporation with several state-of-the-art characterization facilities. He is of late working on the heteroepitaxial growth of Gp-III Nitride wide-band-gap semiconductors, probing their structure, alloying and morphology relations with optical, electrical and magnetic properties. The studies of morphology dependence of properties show very exciting novel properties, making materials multi-functional.

Research Direction

- ♦ Heterostructures and Nanomaterials
- ♦ Surface Physics of Epitaxial Growth
- ♦ Wide band-gap Semiconductors

Research Contribution:

Shivaprasad has mapped novel 2D phase diagrams of several metal-semiconductor interfaces. His work of nanostructured GaN has resulted in exciting new results. He has demonstrated huge light emission from the nanowalls network of GaN. The manifestation has shown strong ferromagnetism, 2D gas formation and superconductivity in this system. Ag nanoparticle adsorption on this system makes this a very good substrate for SERS detection of biomolecules.

Publication:

1. S Nayak, M Gupta, U V Waghmare, S M Shivaprasad, Origin of Blue Luminescence in Mg-Doped GaN, Physical Review Applied 11 (1), 014027, 2019
2. P Kumar, P Devi, R Jain, S M Shivaprasad, RK Sinha, G Zhou, R Nötzel, Quantum dot activated indium gallium nitride on silicon as photoanode, Nature Communications: Chemistry 2 (1), 4, 2019



Sridhar Rajaram

Associate Professor

Phone: +91-80-2208-2560

Email: rajaram@jncasr.ac.in

www.jncasr.ac.in/XXX



Biosketch:

Dr. Sridhar Rajaram obtained his Ph.D. from the Department of Chemistry at the University of Utah. After a post-doctoral stint at the University of California, Berkeley, Dr. Rajaram joined JNCASR as a Faculty Fellow. Currently, he is an Associate Professor in JNCASR

Research Description:

Dr. Rajaram's group is working on synthesizing bio-degradable polymers through an organocatalytic Ring Opening Polymerization (ROP). The regio and stereo-regularity of bio-degradable polymers have a direct impact on their mechanical properties. Dr. Rajaram's group is developing organo-catalysts that can give polymers with a high degree of regio and stereo-regularity. Apart from this, Dr. Rajaram's group is also involved in the development strong organic bases for enantioselective synthesis of small molecules

Research Direction

- ♦ Synthesis of Novel Bio-degradable Polymers
- ♦ Effect of Polymer Microstructure on Bulk Properties
- ♦ Enantioselective Synthesis of Small Molecules

Research Contribution:

Dr. Rajaram's group has developed non-planar perylene diimides as electron transporters for organic solar cells. They have also novel hydrogen-bond donors for the enantioselective synthesis of small molecules.

Publication:

1. Shivanna, R.; Rajaram, S.; Narayan, K. S. Role of Charge-Transfer State in Perylene-Based Organic Solar Cells, *ChemistrySelect* **2018**, 3, 9204-9210.
2. Jain, P; Patra, R. S.; Rajaram, S.; Narayana, C. Designing Dendronic-Raman Markers for Sensitive Detection Using SERS. Manuscript Submitted.





A. Sundaresan

Professor

Phone: +91-80-2208-2824 +91-9880002184

Email: sundaresan@jncasr.ac.in ;

sundajnc@gmail.com

www.jncasr.ac.in/sundaresan

Biosketch:

He obtained his PhD (1994) in Chemistry from IIT Bombay. He was a post-doctoral fellow at Laboratoire Crystallography, Caen, Invited Researcher, LEPEs, CNRS, Grenoble, France and Researcher, JST-CREST, AIST Tsukuba, Japan before joining JNCASR in 2004.

Research Description:

The main focus of the research is to study structure-property relationship in transition metal oxides. Apart from conventional synthesis of oxides, high pressure and high temperature methods have been applied to make metal stable materials. Synchrotron and neutron diffraction studies are used to determine crystal and magnetic structures. Electrical and magnetic properties have been investigated down to 2 K. A special attention is given to exploring new magnetoelectric and multiferroic materials, magnetic materials showing temperature induced magnetization reversal and superconductivity.

Research Direction

- ♦ Structure-property relationship in transition metal oxides
- ♦ Magnetism, Ferroelectricity and Multiferroicity
- ♦ Superconductivity

Research Contribution:

Universal surface ferromagnetism was discovered in nanoparticles of otherwise nonmagnetic inorganic materials. An unusual temperature induced magnetization reversal phenomenon has been investigated in several transition metal oxides. A successful method to identify intrinsic ferroelectricity in type-II multiferroics has been demonstrated. Several new magnetism induced multiferroic material have been discovered.

Publication:

1. Chandan De, R. Bag, S. Singh, F. Orlandi, P. Manuel, S. Langridge, M. K Sanyal, C. N. R. Rao, Maxim Mostovoy and A. Sundaresan, Highly tunable magnetic spirals and electric polarization in $\text{Gd}_{0.5}\text{Dy}_{0.5}\text{O}_3$, Phys. Rev. Mat., 03, 044401 (2019).
2. A. Sen, D. Swain, T. N. Guru Row and A. Sundaresan, Unprecedented 30 K Hysteresis across Switchable Dielectric and Magnetic Properties in a Bright Luminescent Organic-Inorganic Halide $(\text{CH}_6\text{N}_3)_2\text{MnCl}_4$, J. Mater. Chem. C, 4838 (2019).



Tapas Kumar Maji

Professor

Phone: +91-80-2208-2826

Email: tmaji@jncasr.ac.in, tmaji74@gmail.com
www.jncasr.ac.in/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:

Prof. Maji's group has been working on inorganic-organic hybrid materials (known as metal-organic frameworks (MOFs) in bulk and nanoscopic forms and porous organic polymers (POPs) towards renewable energy and environmental applications. Armed with an expansive synthetic tool-kit, Maji's group has made significant contributions on porous materials and has explored them for selective capture and separation of carbon dioxide, adsorptive based separation of hydrocarbons, and his research work has direct impact on industry. Recently, his group has been working on coordination polymer gel for optoelectronic applications and also studied for photocatalytic water splitting and CO₂ reduction, Organic porous polymers developed by his group have found to be active for metal free for photo/electrocatalysis for energy generation and conversion.

Research Direction

- ♦ Porous Materials (MOFs and Organic Porous Polymers)
- ♦ Nanoscale MOFs & Composites for Water Storage and Harvesting.
- ♦ Functional Processable 'soft' Organic/hybrid Gel Materials

Research Contribution:

Prof. Maji research work has a direct impact in the chemical industry as in the cost-effective separation of chemical feedstock, geometrical isomers and removal of toxic heavy metal ions from aqueous solution. In a pioneering work from India, using a novel breakthrough measurement setup, he has demonstrated the separation of CO₂ from CO₂/N₂ or CO₂/CH₄ mixture and of olefin from paraffin at ambient conditions.

Publication:

1. D. Samanta, S. Roy, R. Sasmal, N. Das Saha, R. Viswanatha, S. S. Agasti, T. K. Maji, Solvent Adaptive Dynamic Metal-Organic Soft Hybrid for Imaging and Biological Delivery, *Angew. Chem. Int. Ed.*, 58, 5008-5012 (2019)
2. P. Sutar, V. M. Suresh, K. Jayaramulu, A. Hazra, T. K. Maji, Binder driven self-assembly of metal-organic cubes towards functional hydrogels, *Nat. Commun.*, 9, 3587 (2018)



Faculty Awards and Student Awards



A. Sundaresan

MRSI-ICSC & Materials Science Annual Prize (2019)
National Prize for Research on Solid State and Materials Chemistry (2018)

Prof. Kulkarni's

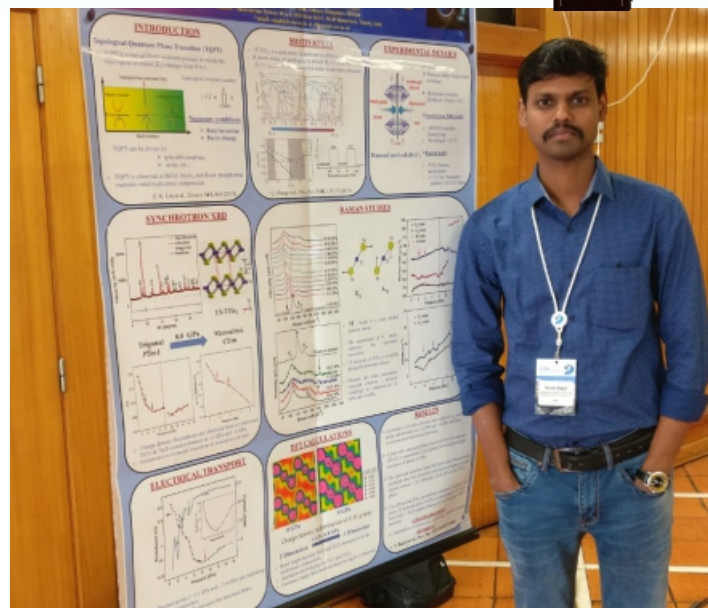
SASTRA-CNR Rao Award for Excellence in Chemistry & Materials Sciences (2019 - 20) MRSI-Distinguished Lectureship Award (2019-20)

Prof. Sarit S Agasti

Journal of Materials Chemistry B 2018 Emerging Investigator

Prof. Eswaramoorthy

CNR Rao National Prize for Chemical Research 2018



Mr. Yanda Premakumar

Best poster award in "Magnetic Crystallography; The 53rd Course of the International School of Crystallography" in Erice, Italy from 31 May - 9 June, 2019

Mr. PN Ravishankar

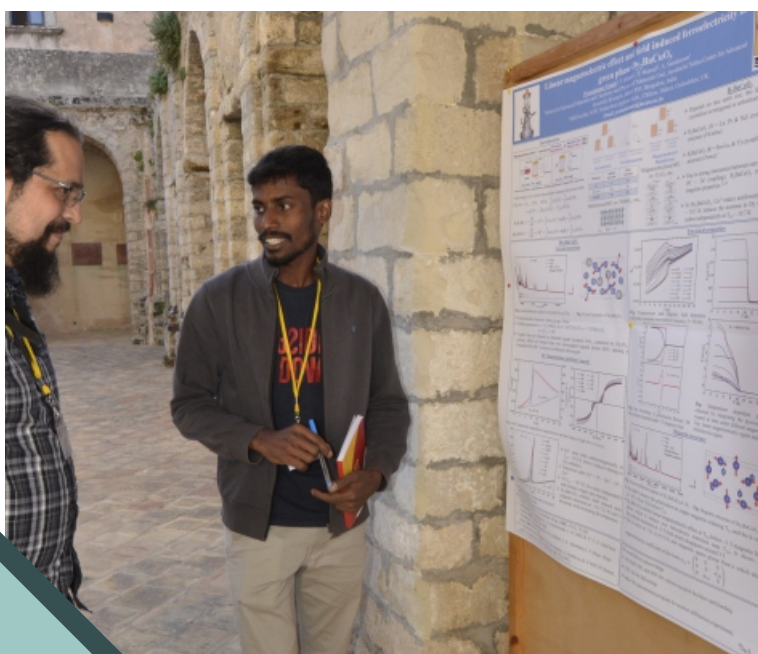
Best poster award in "MRSI AGM 2019", IISc., Bangalore from February 12-15, 2019.

Chaitali Sow

Best poster award Poster title: Ar⁺ Ion Induced Generation of a Series of BCT Phases During Phase Transformation of Non-Cubic Au Microcrystallites to Cubic Lattice Contributors: Chaitali Sow and G. U. Kulkarni Conference: 10th International Conference on Materials for Advanced Technologies (ICMAT), 23-28 June 2019 | Marina Bay Sands, Singapore

Mr. Rajaji Vincent

Ph.D student of Prof. Chandrabhas Narayana, CPMU has been awarded the best poster presentation award at the 56th European High Pressure Research Group (EHPRG) meeting, held in Aveiro, Portugal, from 2nd to 7th September, 2018.





Courses Offered

August - December Session

JC 304	Chemistry of Materials	3:0
JC 307	Physics of Materials	3:0
JC 206	Physical Chemistry	3:0
JC 213	Inorganic Chemistry	3:0
JT 205	Quantum Mechanics	3:0
JT 204	Statistical Mechanics	3:0
JC 214	Laboratory-I	0:4
JT 208	Computational Methods for Condensed Matter	2:0
JC 218	Materials Laboratory	0:4
JC 221	Summer Project	0:3
JC 223	Mathematics	3:0
JNC 202	Organic Chemistry	3:0
JNC208	Characterization of Materials	3:0

January - April Session

JC 210	Group theory and Vibrational Spectroscopy	3:0
JC 205	Seminar Course	1:0
JC 209	Basics of Nanoscience	2:0
JC 215	Electromagnetism	3:0
JJ 301	Matter	1:0
JC 216	Laboratory-II	0:4
JNC307	Quantum Chemistry and Chemical Bonding	3:0
JC 224	Computer Programming in Fortran	1:2
JC 220	Topics in Physical Metallurgy	1:0
JN 203	Scientific Communication –II	0:1
JT 201	Solid State Physics	3:0
JJ 302	Transmission Electron Microscopy and Spectroscopy	2:0
JC226	Solid State Electronics	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:
<http://www.jncasr.ac.in/fe>

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:
<http://www.jncasr.ac.in/fe>



Academic Programmes

Ph. D. in CPMU Unit

Candidates are selected based on their performance in a National level entrance examination such as GATE/JEST/CSIR-UGC-NET and an on-site interview. Eligibility for this programme is M.Sc. in Chemistry /Physics or M.E./M.Tech. in relevant disciplines such as Chemical Engineering / Electrical Engineering etc. with a minimum of 55% marks. Students are admitted in August and January of every year.

Selected candidates have to 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 from the date of registration.

For more details, visit : <http://www.jncasr.ac.in/admit>

M.S. (Engg.) in Materials Science

Candidates are selected based on their performance in a National level entrance examination such as GATE, CSIR-UGC-NET etc., and an on-site interview. Eligibility for this program is M.Sc. in Chemistry/Physics or B.E./B.Tech. in relevant disciplines such as Chemical Engineering / Electrical Engineering etc. with first class or equivalent. The duration of the course is two years.



Selected candidates have to 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 has to submit a thesis and defend it in front of an expert committee.

Based on the performance of the candidate in the M.S. programme, the department can recommend him/her 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:

<http://www.jncasr.ac.in/admit>

Integrated Ph. D. in Materials Science

Integrated Ph.D. in Materials Science is a one of its kind program in the country and is jointly conducted with the Theoretical Sciences Unit since August 2014. Students


with Bachelor's degree in any branch of Science can apply. Those with Bachelor's degree in Engineering with an aptitude towards 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 through a written test conducted in JNCASR or JAM examination 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 towards a M.S. degree in Materials Science, and (iii) doctoral research leading towards a Ph.D. degree to be pursued in the succeeding two to four years.

For more details, visit: <http://www.jncasr.ac.in/admit>

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 Spectrometer*
- 8) *Micro- and indigenously built Raman Spectrometers*
- 9) *Photoluminescence emission and excitation spectroscopy*
- 10) *Zetasizer Nano ZS particle size analyzer*
- 11) *Precision Workstation for dielectric measurements*
- 12) *SQUID magnetometer*
- 13) *Super Computer facility*
- 14) *Molecular Beam Epitaxy*
- 15) *High Pressure High Temperature Synthesis facility*
- 16) *TEM*
- 17) *TRC-Nanoscriber highest resolution 3D Printer*



Unit Statistics

Total Publications

1,733

h-index

120

Average citations per item **41.92**

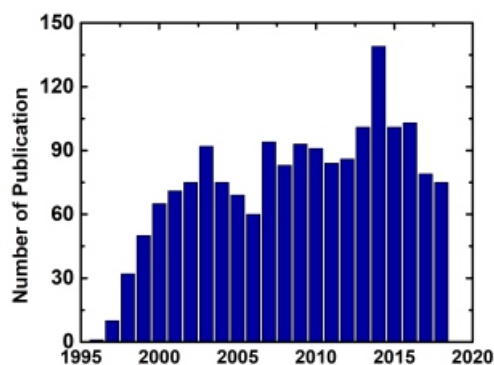
Sum of Times Cited

72,651

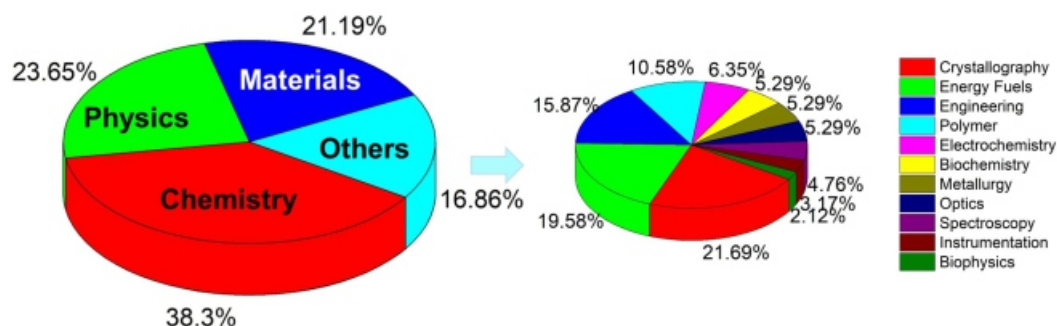
Citing articles

53,627

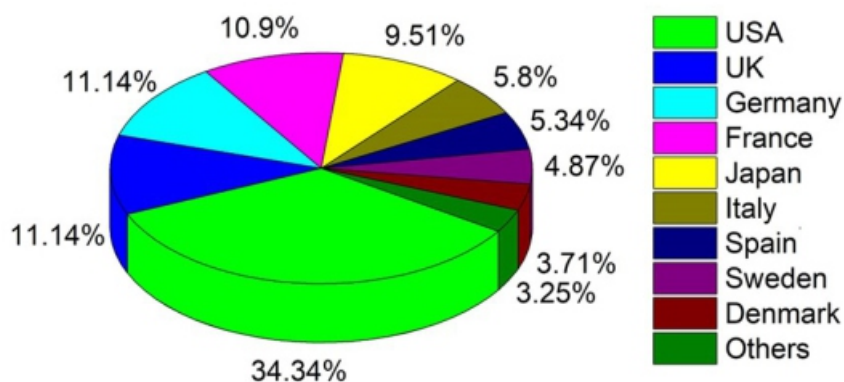
Publications from CPMU



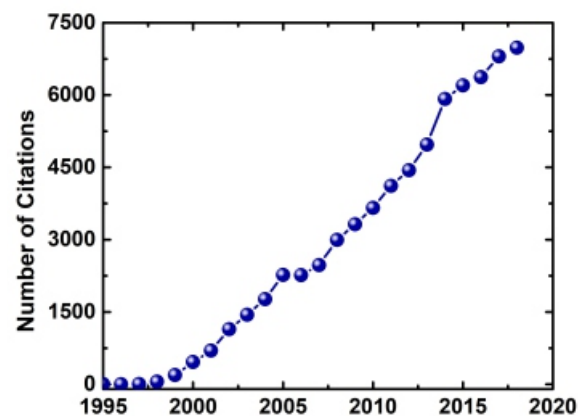
Diversity of Research in CPMU



Global CPMU: Collaborative Publications



Citations of CPMU Publications





Technical & Administrative Staff

Senior Technical Officers

V Sreenath

S Srinivas

Senior Laboratory Assistants

J Anil Kumar

A Srinivasa Rao

Consultant

Usha Tumkurkar

Lab Assistant (Grade – I)

B S Vasudeva

Office

Radha V

Workshop

Rajakumar D

Helper (on contract)

Balraj

Sunil





"School of Advanced Materials (SAMat) is a virtual research centre 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."



➔ **School of Advanced Materials (SAMat)**



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 Saqr Laboratory Located in the premises of the International Centre for Materials Science, is the state-of-the-art centre devoted to high impact, interdisciplinary scientific research in the area of materials chemistry and chemical biology.



*I too have worshipped
at the shrine of science*

- Jawaharlal Nehru



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)
Jakkur P.O., Bangalore 560 064, INDIA

Tel : +91 80 2208 2750 / 2208 2875 ; Fax : +91 80 2208 2766

Email : cpmuchair@jncasr.ac.in ; Web : <http://www.jncasr.ac.in/cpmu>

