

List of Speakers

Ganesh Bagler, Institute of Himalayan Bioresource Technology, Palampur
Suman Chakraborty, Department of Mechanical Engineering, IIT Kharagpur
Pratim Chattaraj, Department of Chemistry, IIT Kharagpur

Indra Dasgupta, Department of Solid State Physics & Center for Advanced Materials, Indian Association for the Cultivation of Science, Jadavpur, Kolkata

Yuan Ping Feng, Department of Physics, National University of Singapore

Dinesh Gupta, Structural and Computational Biology Group, ICGEB, New Delhi

Yuhui He, Institute of Scientific and Industrial Research, Osaka University

V.K.Jayaraman, Shiv Nadar University

Dilip G. Kanhere, Department of Physics, Central University of Rajasthan

Preston Macdougall, Department of Chemistry, Middle Tennessee State University, Murfreesboro, TN

G. Mugesh, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore

Soumyo Mukherji, Department of Biosciences & Bioengineering, IIT Bombay

Saroj Nayak, IIT Bhubaneswar & Rensselaer Polytechnic Institute, Troy, NY

Sourav Pal, National Chemical Laboratory, Pune

Biswarup Pathak, Department of Chemistry, IIT Indore

Dhwani Raghav, School of Biotechnology, Gautam Budh University, Greater NOIDA

Rampi Ramprasad, Chemical, Materials & Biomolecular Engineering/Institute of Materials Science, University of Connecticut, Storrs, CT

S.B. Rao, C R Rao Advanced Institute of Mathematics, Statistics & Computer Science, University of Hyderabad

P.Ravindran, Department of Physics, Central University of Tamil Nadu, Thiruvavur

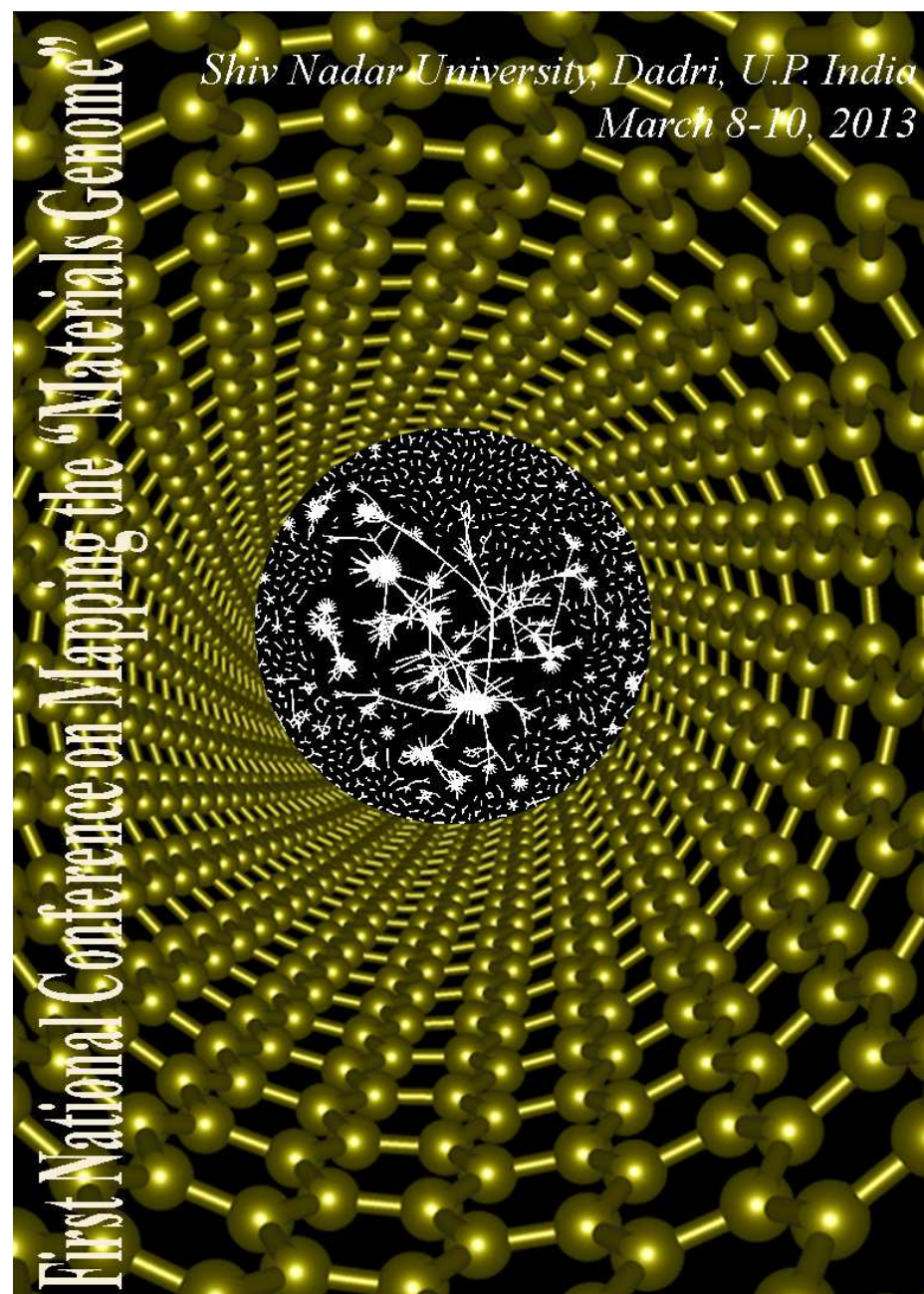
Vidya Ravindran, Center for Material Science & Nanotechnology, University of Oslo, Norway

G.Narahari Sastry, Molecular Modeling Group, Indian Institute of Chemical Technology, Hyderabad

Abhishek Kumar Singh, Materials Research Center, Indian Institute of Science, Bangalore

Somdatta Sinha, Department of Biological Sciences, IISER Mohali

C. Suguna, Centre for Cellular & Molecular Biology, Hyderabad



First National Conference on Mapping the “Materials Genome”

Hosted by the Center for Informatics and the School of Natural Sciences
Shiv Nadar University, Village Chithera, Tehsil Dadri, U.P., India

Dates: March 8-10, 2013 — The conference will start at 9:30 AM on Fri. March 8th and conclude at 4 PM on Sun. March 10th.

Aim & Scope:

Discerning and exploiting patterns in chemical and biological data lies at the heart of any systematic program for drug or materials design. Rapid advances in computational power during the last couple of decades have enabled theoretical characterization of many bio- and nano-materials using first principles computations, but the computational effort required is still formidable enough to preclude routine use of such methods in a high-throughput setting. Many problems in chemistry, biology and materials science are so complex and inter-connected that novel approaches based on the sciences of informatics, complex systems and network theory are required for their solution. Predictive informatics methods employing statistical techniques to process and analyze the huge volumes of data generated by robotic high-throughput assays in the wake of the Human Genome Project have led to rapid advances in bioinformatics. In the search for materials with specific properties, a similar combination of first principles computational studies with experimental work and heuristic statistical methods has the potential to leverage the power of each, thereby bringing high-throughput capability to the quest for predicting the characteristics of materials at the nanoscale. This approach has been termed the Materials Genome Initiative.

The scope of this conference will encompass various aspects of molecular and materials informatics, including data management and representation, multi-scale modeling, machine learning and *in silico* materials design associated with the discovery of molecules, polymers, drugs, gene products, bio- and nanomaterials. The conference will emphasize links between combinatorial experiments, high-throughput measurements, first-principles computations, statistical modeling and data analysis.

Outline of the Conference Topics and Call for Papers:

- First principles based Materials Modeling
- Multi-scale modeling: bridging the length scales
- Experimental characterization for Materials Design
- Bio-Materials, Nanoinformatics and the Nano-Bio Interface
- Systems and Network approaches to Materials Informatics
- Data Management, Data Visualization and Data Mining for Materials Informatics
- Informatics approaches to *In-silico* Materials Design

Contributed papers are invited in all of the above topic areas; of these, some will be selected for oral presentations and the rest as posters. Submit a 250 word abstract in MS Word or PDF format, with the title of the paper in bold face and the name of the presenting author underlined, to: gouriprasanna.roy@snu.edu.in

DEADLINES: Abstract submission deadline is Feb.15th. Accepted presenters will be notified by Feb.20th.

CONFERENCE FEES: There are NO registration fees.

Accommodations:

Accommodations will be provided for all accepted speakers and poster presenters.

Local Organizing Committee

Co-chairs:

[N. Sukumar \(n.sukumar@snu.edu.in\)](mailto:n.sukumar@snu.edu.in) Department of Chemistry & Center for Informatics, SNU
[Vijay Kumar \(vijay.kumar@snu.edu.in\)](mailto:vijay.kumar@snu.edu.in) Dr. Vijay Kumar Foundation & Center for Informatics, SNU

Members:

Sudepto Bhattacharya	Bimlesh Lochab	Ram Sagar
Sankar Dhar	Muneendra Ojha	Seema Sehrawat
Krishna Jayadev	Ganesh Prabhu	Subhabrata Sen
V. K. Jayaraman	Vivek Rajput	Ashutosh Singh
Priya Johari	Gouriprasanna Roy	Samarendra Pratap Singh
	Susanta Sinha Roy	

The venue of the conference is the campus of Shiv Nadar University a multi-disciplinary research university, built in a sprawling 286 acres fully-residential campus, in Chithera Village near Dadri, U.P., in the outskirts of Delhi. The nearest airport, New Delhi, is about two hours from campus. The University opened its doors in August 2011, and now includes faculties in natural sciences, humanities and social sciences, engineering, education, business, art and design.