



First National Conference on Mapping the “Materials Genome”

Organized by the Center for Informatics and the School of Natural Sciences

Shiv Nadar University, India

Dates: March 8-10, 2013

The First National Conference on Mapping the “Materials Genome” was the first conference on the campus of Shiv Nadar University, and also the first conference in India in the emerging research direction of the Materials Genome. 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. This conference brought some of the leading researchers in the country and a few from abroad in these areas and served to create awareness about this important emerging development in materials research.

Highlights of the Conference:

- 57 participants (invited speakers and poster presenters) from 30 different institutions
- 3 continents (North America, Europe and Asia) represented
- Inauguration of SNU’s 512-node High Performance Computing Cluster “*Magus*” by Mr. Shiv Nadar
- Cultural program by Shiv Nadar University students
- Cash Prizes and Awards to Best Poster (Amit A. Vernekar, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore) and Runner-Up (Zeenia Jagga and Shubham Kavishvar, Bioinformatics laboratory, Structural and Computational Biology Group, ICGEB, New Delhi)

The Conference started on the morning of March 8, 2013 with a welcome by Dr. Vijay Kumar, Conference Co-Chair. The Conference was inaugurated by Dr. Nikhil Sinha, Vice Chancellor of Shiv Nadar University, who welcomed the delegates to the University and outlined the idea of the Materials Genome in materials innovation. Following this, Dr. Rupamajari Ghosh, Director, School of Natural Sciences and Dean of Research and Graduate Studies, welcomed the delegates. Dr. N. Sukumar, Co-chair of the Conference and Director of the Center for Informatics and Head of the Department of Chemistry, then introduced the Materials Genome Initiative.

The technical sessions commenced with a talk by Dr. Saurav Pal, Director of CSIR-National Chemical Laboratory who introduced the quantum chemical computational approaches and their applications to a variety of materials. There were in all 57 participants from 30 institutions; and 3 continents were represented. The topics that were covered during the conference included various aspects of first principles molecular and materials modeling, 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. An evening social program of music and dance presented by the students of the university was appreciated by one and all. This was followed by a public lecture by Prof. D.G. Kanhere of the Central University of Rajasthan on "Computational science: Confluence of Mathematical Modeling, Computer Simulations and High Performance Computing".

A highlight of the conference was the inauguration of an IBM High Performance Computer "*Magus*" by Mr. Shiv Nadar, Founder of the University. This 32-node cluster delivering 332.8 Giga flops with each node and a peak performance of 10.649 TF is the first facility of its kind in any private university in India and will enable state-of-the art computational research at SNU. On this occasion Dr. Subram Natarajan, Director - IBM Deep Computing, India/SA gave a lecture on "High Performance Computing in a Smarter Planet".

Session on First Principles Based Materials Modelling:

- Dr. Sourav Pal, Director, CSIR-National Chemical Laboratory, Pune "**Computational simulation in Chemistry: Molecules to materials**"
- Prof. D. G. Kanhere, University of Rajasthan "**Finite temperature properties of finite size systems**"
- Prof. Saroj Nayak, Indian Institute of Technology, Bhubaneswar, Toshali Bhawan, Bhubaneswar and Director, Interconnect Focus Center at Rensselaer, Rensselaer Polytechnic Institute, Troy, NY "**Designing Next Generation Nanoelectronic using Large Scale Electronic Structure and Quantum Transport**"
- Dr. Nishant Sinha, Application Scientist, Accelrys "**Materials Genomics: A preview for future Material Innovation**"
- Prof. Yuan Ping Feng, Department of Physics, Faculty of Science, National University of Singapore, Singapore "**Carbon and Spintronics**"
- Prof. Indra Dasgupta, Department of Solid State Physics & Center for Advanced Materials, Indian Association for the Cultivation of Science, Jadavpur, Kolkata "**First Principles Study of Functional Nanomaterials**"
- Prof. Dr. Abhishek Kumar Singh, Materials Research Center, Indian Institute of Science, Bangalore "**Normal Pressure Induced Bandgap Tuning of 2D-materials**"
- Prof. Priya Johari, Shiv Nadar University "**Modulation of Properties of Nanomaterials: An Ab-Initio Study**"

- Prof. Pratim Chattaraj, Department of Chemistry and Institute for Theoretical Sciences, Indian Institute of Technology, Kharagpur **“All-metal aromaticity and hydrogen storage: A conceptual DFT approach”**
- Dr. G.Narahari Sastry, Molecular Modeling Group, Indian Institute of Chemical Technology, Hyderabad **“Molecular Aggregation: Insights from Database Analyses and Quantum Chemical Calculations”**
- Dr S. Auluck, National Physical Laboratory, New Delhi **“Thermoelectrics at CSIR@NPL”**
- Prof.P.Ravindran, Department of Physics, School of Basic and Applied Sciences, Central University of Tamil Nadu, Thiruvavur **“Design of hydrogen storage materials from ab-initio modeling”**

Session on Bio-Materials, Nanoinformatics, and the Nano-Bio Interface:

- Prof. G. Mugesh, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore **“Nanomaterials as Antioxidant Enzyme Mimetics”**
- Prof. Biswarup Pathak, Department of Chemistry, School of Basic Sciences, Indian Institute of Technology Indore, **“Solid Nanopores for Rapid DNA Sequencing”**
- Prof. Dipak Maity, Shiv Nadar University **“Magnetic Nanoparticles for Medical Diagnosis and Therapy”**
- Prof. N. Selvamurugan, SRM University, Kattankulathur **“Molecular Basis of Cell and Biomaterial Interactions for Bone Tissue Engineering”**
- Prof. Suman Chakraborty, Department of Mechanical Engineering, Indian Institute of Technology, Kharagpur **“Biomicrofluidics: A Journey with DNAs, Cells, and Painless Microneedles”**
- Prof. Soumyo Mukherji, Department of Biosciences and Bioengineering, Centre for Research in Nanotechnology and Sciences, Centre of Excellence in Nanoelectronics, Indian Institute of Technology, Bombay **“From Nanomaterials and Nanostructures to Optical Biosensors”**

Session on Systems and Network Approaches to Materials Informatics:

- Prof. Somdatta Sinha, Department of Biological Sciences, IISER Mohali **“Complexity in Genomic Patterns and Classification”**
- Dr. C. Suguna, Scientist, Centre for Cellular & Molecular Biology (CSIR), Habsiguda, Uppal Road, Hyderabad **“Network models of metabolic pathways of prokaryotes”**
- Prof. Ganesh Bagler, Scientist, Biotechnology Division, Institute of Himalayan Bioresource Technology (CSIR), Palampur (Himachal Pradesh) **“Modeling and control of complex diseases with an integrative network biology approach”**
- Dr. S.B. Rao, Professor Emeritus, C R Rao Advanced Institute of Mathematics, Statistics & Computer Science, University of Hyderabad Campus, Gachibowli, Hyderabad **“Application of Dempster-Shafer theory in ranking of nodes under various centrality measures in biological networks and systems”**
- Prof. Dhvani Raghav, Gautam Budh University, Greater NOIDA **“Role of genomics in identifying potential drug targets for cancer therapy”**

Session on Materials: Defects and Characterization:

- Prof. Sankar Dhar, Shiv Nadar University **“Novel functional materials by tailoring defects”**
- Dr. Vidya Ravindran, Center for Material Science & Nanotechnology, University of Oslo, Norway **“Understanding role of defects in semiconductors using density-functional calculations”**
- Prof. A. Kanjilal, M. Catalano, S. S. Harilal, and A. Hassanein. Shiv Nadar University **“The Role of Surface Chemistry on Extreme Ultraviolet Reflectivity of Ru Mirrors”**

Session on Data Visualization and Data Mining for Materials Informatics:

- Prof. Preston Macdougall, Pre-Pharmacy Coordinator and Assistant Chair, Department of Chemistry, Middle Tennessee State University, Murfreesboro, TN **“Hyperwall visualization technology for drug and materials design”**
- Dr. V.K.Jayaraman, Shiv Nadar University **“Support Vector Machines and its Applications to Materials Design”**
- Dr. Dinesh Gupta, Staff Research Scientist, Bioinformatics Laboratory, Structural and Computational Biology Group, International Centre for Genetic Engineering and Biotechnology, ICGEB Campus, Aruna Asaf Ali Marg, New Delhi **“Machine Learning based High throughput screening and drug design”**

Poster Session:

- Pradeep Kumar J, Lakshmi L, Jyothsna V, Prashanth Balaji D R, Saravanan S, Moorthi A and Selvamurugan N Department of Biotechnology, School of Bioengineering, SRM University, Kattankulathur 603 203, Tamil Nadu, India. **“Chitosan/Diopside scaffolds for Bone Tissue Engineering”**
- Amit A. Vernekar, G. Mugesh, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore **“Remarkable Peroxynitrite Scavenging Activity of Hemin Functionalized Graphene Nanosheets”**
- Neeraj K. Jaiswal and Pankaj Srivastava, Nanomaterials Research Group, ABV- Indian Institute of Information Technology and Management (IIITM), Gwalior- 474015, India. **“Enhanced metallicity in armchair graphene nanoribbons with Cu impurities”**
- Sandeep Kumar Jain and Pankaj Srivastava, Nanomaterials Research Group, Computational Nanoscience and Technology Lab (CNTL), ABV-Indian Institute of Information Technology & Management, Morena Link Road, Gwalior-474015 (MP) India **“First principles calculations for reflectivity of single walled boron nanotube”**
- C. P. Saini and S. Kasiviswanathan, Department of Physics, Indian Institute of Technology, Madras, India-600036. **“Growth and Characterization of $\text{CuIn}_{0.7}\text{Ga}_{0.3}\text{Se}_2$ and CdS Thin Films”**
- Ravi Kant Upadhyay, Sonali Bhandari and Susanta Sinha Roy, School of Natural Sciences, SNU. **“Synthesis of copper and copper oxide nanoparticles and their application as photocatalyst for water treatment”**
- Shameek Ghosh, Kalpesh Shelke, Srikant Jayaraman, Evolutionary Computing & Image Processing, Centre for Development of Advanced Computing, University of Pune, India **“ChaosPred: A Hybrid Chaos based Feature Selection and QSAR modelling approach for MHC Class-I Binding Peptide Therapeutic Design”**
- Shameek Ghosh, Vinay Nair, Monalisa Dutta and Sowmya Manian, Evolutionary Computing & Image Processing, Centre for Development of Advanced Computing, University of Pune, Pune, India. **“Classification of Penicillin-Binding Proteins using Support-Vector Machines”**
- Pradip B. Shelke and Vijay Kumar, Department of Physics, Ahmednagar College, Ahmednagar – 414001 and Dr. Vijay Kumar Foundation, 1969 Sector 4, Gurgaon - 122001, Haryana, India. **“Graphitic phase formation in a layer and in few layer ultrathin films of ZnO using ab initio calculations”**
- J. Karthikeyan, Vijay Kumar, P. Murugan, CSIR Central Electrochemical Research Institute, Karaikudi – 630 006, Tamil Nadu, India. **“Magnetism in MoS_{2+x} Parallelogram Platelets and Nanoribbons”**

- Vinay Randhawa and Ganesh Bagler, Biotechnology Division, CSIR-Institute of Himalayan Bioresource Technology, Palampur 176061, Himachal Pradesh, India. **“An integrative approach for modeling protein interactomes of complex diseases and in silico drug discovery”**
- Shivalika Pathania and Ganesh Bagler, Biotechnology Division, CSIR-Institute of Himalayan Bioresource Technology, Palampur 176061, Himachal Pradesh, India. **“A rational pharmacoinformatics framework to seek for natural compounds of therapeutic value”**
- Shikha Vashisht and Ganesh Bagler, Biotechnology Division, CSIR-Institute of Himalayan Bioresource Technology, Palampur 176061 Himachal Pradesh, India. **“Exploration of generic and specific cancer mechanisms by graph-theoretic analysis of Cancer Genes Network”**
- Zeenia Jagga, Shubham Kavishvar and Dinesh Gupta, Bioinformatics laboratory, Structural and Computational Biology Group, ICGEB, New Delhi **“Discovering potential Renal Cancer Biomarkers by Integrative Mining of cancer genome profiles”**
- Ganesh Prabhu, Sudepto Bhattacharya, Michael Krein, and N. Sukumar, Department of Chemistry, School of Natural Sciences and Center for Informatics, Shiv Nadar University, Tehsil Dadri, UP, India **“Network measures in polymer space”**
- Vivek Singh and Dhvani Raghav, School of Biotechnology, Gautam Buddha University, Greater Noida, UP. **“An informatics study of deleterious non-synonymous SNPs of ErbB3 kinase”**
- Sachin P. Nanavati, Shailaja Mahamuni, S. V. Ghaisas, and Vijay Kumar, CDAC, Pune University & SNU. **Atomic clusters of magic $(\text{ZnSe})_n$ ($n=13, 33$ and 34) clusters from first principles calculations.**
- A. Barman, A. P. Moon, C. Chattopadhyay, S.T. Aruna, N. Balaji, Gouthama, K. Mondal, Department of Material Science and Engineering, Indian Institute of Technology, Kanpur, India-208016, and Surface Engineering Division, CSIR-National Aerospace Laboratories, HAL Airport Road, Bangalore-560017 **“Corrosion Behavior of Ball Milled and Atmospheric Plasma Sprayed Ni-Ti Coating on Mild Steel”**
- Sweta Parashar , Pankaj Srivastava and Manisha Pattanaik, Nanomaterials Research Group, Computational Nanoscience & Technology Laboratory (CNTL), ABV-Indian Institute of Information Technology & Management (ABV-IIITM), Gwalior-474015, India **“Designing Biphenyl Based Rectification Devices with Ag Electrodes”**
- Muneendra Ojha, School of Engineering, SNU, Sangeetha R.G., School of Engineering, SNU, Arun Kumar, AITM, Amity University, Noida **“Realization of optical logic gates by trapping light in 1-D photonic band gap materials”**
- Swapnil Shukla, Kalpesh Shelke, Shameek Ghosh, Bimlesh Lochab, N. Sukumar, V. K. Jayaraman, Department of Chemistry, School of Natural Sciences, Shiv Nadar University, Greater Noida, District Gautam Budh Nagar, UP - 203207, Center for Modelling and Simulation, Pune University, Pune - 411007, Center for Development of Advanced Computing, Pune University Campus, Pune-411007, Centre of Informatics, School of Natural Sciences, Shiv Nadar University, Greater Noida, District Gautam Budh Nagar, UP – 203207 **“Modelling the Curing Characteristics of Monomers”**
- Rahul Agarwal, Dhvani Raghav and Ashutosh Singh, Department of Life Sciences, Shiv Nadar University, Greater Noida, UP, and Department of Biotechnology, Gautam Buddha University, Greater Noida **“Theoretical Identification of Differentially Expressed Genes in distinct Cervical Carcinoma stages”**
- Shashank Mishra, Gautam Buddha University, and Rahul Agarwal, Shiv Nadar University **“Nano-Robots In Medicine”**

- Priyanka Thakral & A K Bakhshi, Department of Chemistry, University of Delhi “**In-silico engineering of novel hetero-aromatic copolymers**”
- Prabhsharan Kaur, S. S. Sekhon, and Vijay Kumar, Dr. Vijay Kumar Foundation; Department of Physics, Guru Nanak Dev University, Amritsar; Department of Physics, The University of the West Indies, St. Augustine, Trinidad and Tobago; Center for Informatics, Shiv Nadar University “**Theoretical Study of Growth Behavior of III-N Compound Semiconductor Nanoparticles**”

Popular lectures:

- Prof. D. G. Kanhere, University of Rajasthan “**Computational science: Confluence of Mathematical Modeling, Computer Simulations and High Performance Computing**”
- Mr. Subram Natarajan, Director - IBM Deep Computing, India/SA “**High Performance Computing in a Smarter Planet**”

The organizers would like to thank all the participants from India and abroad who made this conference a success. We very warmly acknowledge and appreciate the whole hearted support we received from everybody ranging from our Vice Chancellor, Directors, the admin team, our esteem colleagues and the students who made every effort to make the visitors comfortable. We gratefully acknowledge sponsorship from IBM, Thermo Fisher and Waldner.

Conference Co-chairs

N. Sukumar

Vijay Kumar



Photo Gallery:

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