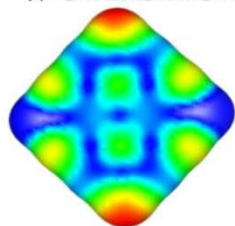


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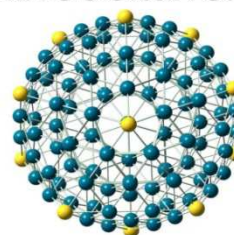
WORKSHOP ON COMPUTATIONAL NANOSCIENCE



30 MARCH - 5 APRIL 2014

Hosted by the Centre of Informatics
School of Natural Sciences.

2nd Announcement



Format of the Workshop:

The morning sessions will be devoted to introductory lectures, which will also provide participants exposure to recent developments in the field. The afternoons will be devoted to hands-on sessions, followed by discussions on results or specific questions. Research seminars and informal discussions are planned in the evenings. The participants will also have opportunity to present and discuss their own work.

Hands-on sessions:

Hands-on sessions, using the plane wave pseudopotential-based code *Quantum Espresso*, will be conducted by Prof. Stefano Baroni (SISSA, Trieste), Dr. Arrigo Calzolari (Istituto Nanoscienze, Modena) and Dr. Priya Johari (SNU). The TDDFT method will also be covered; as will the QM/MM Method, conducted by Prof. G. Narahari Sastry (ICT, Hyderabad). Exercises will involve static and dynamic calculations dealing with some electronic, optical, magnetic and vibrational properties. Transport properties will be treated using the *WanT* and *Quantumwise* codes, conducted by Dr. Arrigo Calzolari and Dr. Sitangshu Bhattacharya (SNU), respectively.

Topics to be covered:

- Materials at the nanoscale – Designing materials with tuneable properties
- Computational methods – Density functional theory
- Finite temperature *ab initio* molecular dynamics on nanomaterials
- Time dependent DFT & spectroscopy
- The Slater transition state
- Chemical properties derived from the electron density and its critical points
- The QM/MM method
- Electronic structures of 2D nanostructures
- Thermal and electric transport at the nanoscale
- Magnetic properties of Nanomaterials

Research seminars and Applications:

- Chemical bonding from local orbitals and plane waves
- Glassy Clusters: Dynamics and Landscape
- Nanoscale surface modifications for controlling wetting and adhesion properties
- Lithium & Beyond Lithium Battery Technology: Insights into Electrochemical & Nanostructural Properties
- Junctioned Semiconductor Quantum Structures for light harvesting & consumptions
- Organic and biomolecular interactions with carbon nanostructures
- Borons: A natural choice for nanosystems

List of confirmed speakers:

- Somobrata Acharya, (IACS, Kolkata)
- Stefano Baroni (SISSA, Trieste, Italy)
- Sitangshu Bhattacharya (SNU)
- Arrigo Calzolari (Istituto Nanoscienze, Modena, Italy)
- G.P. Das (IACS, Kolkatta)
- Richard Dronskowski (RWTH Aachen, Germany)
- D.G. Kanhere (Pune University)
- Vijay Kumar (SNU & VKF)

- Sagar Mitra (IIT, Mumbai)
- V. Ramgopal Rao (IIT, Mumbai)
- Susanta Sinha Roy (SNU)
- Sameer Sapra (IIT, Delhi)
- G. Narahari Sastry (IICT, Hyderabad)
- K.D. Sen (Central University of Hyderabad)
- Samarendra Pratap Singh (SNU)
- P. Srivastava (IITM, Gwalior)
- N. Sukumar (SNU)

Teaching Assistants

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Special programs:

- Sun.30th March, 5 PM: Inauguration
- Sun.30th March, 6:15 PM: Public Lecture “Steel *ab initio*” by Prof. Richard Dronskowski (RWTH Aachen)
- Tue.1st April, 5 PM: Public Lecture “Convergence of Bio-Nano-Information Technologies in the Nanoelectronics Era” by Prof. V.Ramgopal Rao (IIT, Mumbai)
- Wed.2nd April, 5 PM: Public Lecture “*Ab initio* colors” by Prof. Stefano Baroni (SISSA, Trieste)
- Wed.2nd April, 6 PM: Cultural evening by SNU students
- Sat.5th April, 10:30 AM: Participant presentations

Transportation and Accommodation: All invited speakers will be provided courtesy pick up and drop off from/to New Delhi airport and accommodations at a hotel in Greater NOIDA. Transportation will also be provided from the hotel to SNU campus in the morning and from SNU to the hotel in the evening. All Workshop students are expected to reach Delhi by around noon on Sunday 30th March 2014. Workshop students will be accommodated on the SNU campus. Shared transportation will be arranged from NOIDA Sector 16 Metro station to SNU at specific times on March 29th and 30th and back on April 5th. Please inform the Workshop Secretariat of your travel particulars, if you have not already done so. Further details regarding local transportation and accommodations will be sent to all confirmed participants prior to commencement of the Workshop.

We look forward to your participation in the Workshop.

With Best regards,

Workshop Co-chairs:

Vijay Kumar (E-mail: vijay.kumar@snu.edu.in)
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Shiv Nadar University is a multi-disciplinary research university, built in a spacious 256 acres fully-residential campus, in Chithera Village near Dadri, U.P., in the outskirts of Delhi. The University opened its doors in August 2011, and presently houses around a thousand students. Educational programs include leading to B.A., B.S., B.Tech., M.S., M.Tech., Ph.D. and M.B.A. degrees are offered in natural sciences, humanities, art and social sciences, engineering, analytics, education, business, management and entrepreneurship. The inter-disciplinary Center for Informatics includes faculty from the departments of physics, chemistry, life sciences and mathematics in the school of natural sciences, as well as faculty from the departments of computer science and engineering in the school of engineering, and visitors. Computational facilities at SNU include *Magus*, a 32-node, 512-core IBM HPC cluster, delivering a theoretical peak performance of 10.649 TF. Additionally several stand-alone Linux computers are used for teaching and research purposes, and as license servers. Our library, housed in a modern 5-storey building, provides online access, from anywhere in the campus, to thousands of electronic journals and databases, in addition to various books and e-books.

Supported by:

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