

## Workshop on Computational Nanoscience

Hosted by the Center for Informatics, School of Natural Sciences (SoNS)  
Shiv Nadar University  
30 March – 5 April, 2014

### PROGRAM

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**30 March 2014, Sunday**

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#### Session I: Inauguration

Venue: Seminar Hall 1, Ground Floor, C Wing, Academic Block

- 17:00**      **Welcome**  
*(Rupamanjari Ghosh, Director, SoNS; N. Sukumar, Director, Center for Informatics & HOD Chemistry; Vijay Kumar, Priya Johari)*
- 17:30**      **Materials at the nanoscale – Designing materials with tuneable properties**  
*Vijay Kumar (Shiv Nadar University and Dr. Vijay Kumar Foundation)*
- 18:15**      **Public Lecture: *Steel ab initio***  
*Richard Dronskowski (RWTH Aachen, Germany)*
- 19:30**      **Dinner**      (Venue: Cafeteria)
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**31 March 2014, Monday**

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#### Session II: Introductory Lectures -I

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

- 09:15**      **Computational methods – Density functional theory**  
*K.D. Sen (Central University of Hyderabad)*
- 10:45**      **Coffee break**
- 11:15**      **How to perform finite temperature *ab initio* molecular dynamics on nanomaterials**  
*D. G. Kanhere (Pune University)*
- 13:00**      **Lunch**      (Venue: Cafeteria)

### Session III: Hands-on session - I

Venue: Informatics Lab, 1<sup>st</sup> Floor, D Wing, Academic Block

**14:00**            **Introduction to plane wave total energy code - Installation of Quantum ESPRESSO code and ground-state calculations**

*Priya Johari (Shiv Nadar University), Arrigo Calzolari (Istituto Nanoscienze Modena, Italy), Stefano Baroni (International School of Advanced Studies - SISSA, Trieste, Italy)*

**16:00**            **Coffee break**

### Session IV: Research Seminars - I

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**17:00**            **Chemical bonding from local orbitals and plane waves**

*Richard Dronskowski, (RWTH Aachen, Germany)*

**17:45**            **Glassy Clusters: Dynamics and Landscape**

*D.G. Kanhere (Pune University)*

**19:30**            **Dinner**            (Venue: Cafeteria)

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**1 April 2014, Tuesday**

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### Session V: Introductory Lectures –II

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**09:15**            **Time dependent DFT & spectroscopy**

*Stefano Baroni (International School of Advanced Studies - SISSA, Trieste, Italy)*

**10:45**            **Coffee break**

**11:15**            **The Slater transition state: Some applications**

*K. D. Sen (Central University of Hyderabad, Hyderabad)*

**13:00**            **Lunch**            (Venue: Cafeteria)

### Session VI: Hands-on session - II

Venue: Informatics Lab, 1<sup>st</sup> Floor, D Wing, Academic Block

**14:00**            **Quantum ESPRESSO for excited-state calculations (turboTDDFT code)**

*Arrigo Calzolari & Stefano Baroni (International School of Advanced Studies - SISSA, Trieste, Italy)*

**16:00**            **Coffee break**

## Session VI: Research Seminars - II

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**17:00**            **Public Lecture: Convergence of Bio-Nano-Information Technologies in the Nanoelectronics Era**

*V. Ramgopal Rao (Indian Institute of Technology, Mumbai)*

**19:30**            **Dinner**            (Venue: Cafeteria)

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**2 April 2014, Wednesday**

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## Session VII: Introductory Lectures - III

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**09:15**            **Novel strategies for the evaluation of the electron and thermal transport in nanostructures**

*Arrigo Calzolari (Istituto Nanoscienze, Modena, Italy)*

**10:45**            **Coffee break**

**11:15**            **Chemical properties derived from the electron density and its critical points**

*N. Sukumar (Shiv Nadar University)*

**12:00**            **Nano-Heterostructures: Looking beyond the simple nanomaterials**

*Sameer Sapra (Indian Institute of Technology, Delhi)*

**13:00**            **Lunch**            (Venue: Cafeteria)

## Session VIII: Hands-on session - III

Venue: Informatics Lab, 1<sup>st</sup> Floor, D Wing, Academic Block

**14:00**            **The WanT code**

*Arrigo Calzolari (Istituto Nanoscienze, Modena, Italy)*

**16:00**            **Coffee break**

## Session IX: Research Seminars – III

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**17:00**            **Public Lecture: *Ab initio* colors**

*Stefano Baroni (International School of Advanced Studies - SISSA, Trieste, Italy)*

**18:00**            **Cultural evening by students of SNU**

Venue: Seminar Hall 1, Ground Floor, C Wing, Academic Block

**19:30**            **Dinner**            (Venue: Cafeteria)

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3 April 2014, Thursday

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**Session X: Introductory Lectures - IV**

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**09:15**            **QM/MM method**  
*G. Narahari Sastry (Indian Institute of Chemical Technology, Hyderabad)*

**10:45**            **Coffee break**

**11:15**            **Electronic structure of 2D nanostructures in the post-graphene era**  
*G.P. Das (Indian Association for Cultivation of Science, Kolkatta)*

**13:00**            **Lunch**            (Venue: Cafeteria)

**Session XI: Hands-on session - IV**

Venue: Informatics Lab, 1<sup>st</sup> Floor, D Wing, Academic Block

**14:00**            **QM/MM method**  
*G. Narahari Sastry (Indian Institute of Chemical Technology, Hyderabad)*

**16:00**            **Coffee break**

**Session XII: Research Seminars – IV**

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**17:00**            **Organic semiconductors: challenges and promises towards next generation electronic devices**  
*Samarendra Pratap Singh (Shiv Nadar University)*

**17:45**            **Phonon Engineering in Nanostructures: Controlling interfacial thermal resistance in fully inorganic and hybrid organic/inorganic nanojunction**  
*Arrigo Calzolari (Istituto Nanoscienze, Modena, Italy)*

**19:30**            **Dinner**            (Venue: Cafeteria)

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4 April 2014, Friday

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**Session XIII: Introductory Lectures - V**

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**09:15**            **Junctioned Semiconductor Quantum Structures for light harvesting & consumption**  
*Somobrata Acharya, (Indian Association for Cultivation of Science, Kolkatta)*

**10:45**            **Coffee break**

**11:15**            **Organic and biomolecular interactions with carbon nanostructures**  
*G. Narahari Sastry (Indian Institute of Chemical Technology, Hyderabad)*

**12:15**            **Magnetic properties of nanomaterials**  
*Vijay Kumar (Shiv Nadar University & Dr. Vijay Kumar Foundation)*

**13:00**            **Lunch**            (Venue: Cafeteria)

**Session XIV: Hands-on session - V**

Venue: Informatics Lab, 1<sup>st</sup> Floor, D Wing, Academic Block)

**14:00**            **Resistances of 2D materials**  
*Sitangshu Bhattacharya (Shiv Nadar University)*

**16:00**            **Coffee break**

**Session XV: Research Seminars – VI**

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**17:00**            **Borons: A natural choice for nanosystems**  
*P. Srivastava (Atal Bihari Vajpayee-Indian Institute of Information Technology and Management, Gwalior)*

**17:45**            **Nanoscale surface modifications for controlling wetting and adhesion properties**  
*Susanta Sinha Roy (Shiv Nadar University)*

**19:30**            **Dinner**            (Venue: Cafeteria)

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**5 April 2014, Saturday**

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**Session XVI: Research Seminars - VII**

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**09:15**            **Lithium and Beyond Lithium Battery Technology: Insights into Electrochemical and Nanostructural Properties**  
*Sagar Mitra (Indian Institute of Technology, Mumbai)*

**10:00**            **Coffee break**

**Session XVII: Research Seminars -VIII**

Venue: Seminar Hall, Lower Ground Floor, Library (E Wing)

**10:30**            **Presentations by participants**

**12:15**            **Closing**

**13:00**            **Lunch**            (Venue: Cafeteria)