

THEME MEETING ON 2D NANOSTRUCTURES: GRAPHENE AND BEYOND

July 29-30, 2012

Materials Research Center, Indian Institute of Science, Bangalore-560012

SCIENTIFIC PROGRAM

July 29th, 2012 Sunday

(MRC Auditorium)

08:30-17:00

Registration Desk (MRC)

08:55-09:00

Welcome Address

A.K. Singh, G.P. Das

INAUGURAL PLENARY SESSION: Chair: **S.B. Krupanidhi**

09:00-09:45

PT-1

Graphene, graphene mimics and some of their fascinating properties

C.N.R. Rao

Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore

09:45-10:30

PT-2

Probing Graphene and MoS₂ transistors by Raman Spectroscopy

A. K. Sood

Department of Physics, Indian Institute of Science, Bangalore, India

10:30-11:00

COFFEE-BREAK

SESSION-1: Chair: **Swapan Ghosh**

11:00-11:25

Inv-1

A Pariser-Parr-Pople Model Hamiltonian based approach to the electronic structure and optical properties of graphene nanostructures

G. Kondeyya and **Alok Shukla**

Department of Physics, Indian Institute of Technology, Bombay, India

11:25-11:50

Inv -2

Phonon-limited transport coefficients in extrinsic Graphene

E. Muñoz

Instituto de Física, Pontificia Universidad Católica de Valparaíso, Avda. Brasil 2950, Valparaíso, Chile

- 11:50-12:15 Inv-3 Junctions of topological insulators
K. Sengupta
Indian Association for the Cultivation of Science, Kolkata, India
- 12:15-12:40 Inv-4 Jahn-Teller Effect and Magnetism in Graphene with a Substitutional Vacancy
B.R.K. Nanda
Department of Physics, Indian Institute of Technology, Madras, India
- 12:40-13:05 Inv-5 Strain Engineered Graphene: Current Trends and Prospects
Vitor M. Pereira
Graphene Research Centre and Department of Physics, National University of Singapore, Singapore
- 13:05-14:00 LUNCH BREAK
- 14:00-16:00 POSTER SESSION+COFFEE BREAK
- SESSION-2:** Chair: **Umesh V. Waghmare**
- 16:00-16:25 Inv-6 Graphitic-like Structures of Single and Multi-layers of Silicon Carbide
C.S. Jayanthi, S.Y. Wu and M. Yu
Department of Physics and Astronomy, University of Louisville, Louisville, KY 40292, USA
- 16:25-16:50 Inv-7 Magnetic Impurities in GNRS
D.G. Kanhere
Central University of Rajasthan, Kishangarh, Rajasthan, India
- 16:50-17:15 Inv-8 Polymer Dielectrics By Design
R. Ramprasad
University of Connecticut, Storrs, CT, USA
- 17:15-17:40 Inv-9 Graphene and graphitic analogues among binary semiconductors
Priya Mahadevan
Department of Condensed Matter Physics and Material Science, S.N. Bose National Centre for Basic Sciences, Kolkata, India

17:40-18:05 Inv-10 Defects and ad-atoms on hybrid h-BNC sheet
Prasenjit Sen, Pooja Srivastava and M. Deshpande
Harish-Chandra Research Institute, Chhatnag Road, Jhansi, Allahabad, India

18:05-18:30 Inv-11 Ammonia reaction mechanism over CNT – an ab initio study
Abhijit Chatterjee and Yoshiyuki Kawazoe
Material Science, Accelrys, Kasumigaseki 1-3-7, Tokyo, Japan

SPONSORS TALKS: Chair: **Arun M. Umarji**

18:30-19:00 Sp-1 Presentation from Dell/Intel

19:00 BANQUET (Hotel Sheraton, Bangalore)

July 30th, 2012 Monday

(MRC Auditorium)

PLENARY SESSION: Chair: **G. P. Das**

08:25-9:10 PT-3 Ab initio calculation to predict nanostructured materials
Yoshiyuki Kawazoe
New Industry Creation Hatchery Center, Tohoku University, Sendai 980-8579, Japan

09:10-09:15 BREAK

SESSION-3: Chair: **Kwang-Ryeol Lee**

09:15-09:40 Inv-12 Exploring Applications of Graphene in Spintronics, Hydrogen Storage,
Catalysis and Gas Sensing by First-principles Calculations
Minggang Zeng, Lei Shen, Miao Zhou, Xian Qin, Yunhao Lu, Chun Zhang,
Qingyuan Meng and **Yuan Ping Feng**
Department of Physics, National University of Singapore, Singapore

09:40-10:05 Inv-13 From semiconducting graphene to graphitic phase in layers of compound Semiconductors

Vijay Kumar

Dr. Vijay Kumar Foundation, Haryana, India

10:05-10:30 Inv-14 Electronic properties of Carbon and Boron Nitride based two-dimensional Nanomaterials: A first-principles study

Sugata Mukherjee

S.N. Bose National Centre for Basic Sciences, Kolkata, West Bengal, India

10:30-11:00

COFFEE BREAK

SESSION-4: Chair: **Vijay Kumar**

11:00-11:25 Inv-15 Exploring Hydrogen Storage Systems through Advanced Computational Materials Science

Rajeev Ahuja

Condensed Matter Theory Group, Department of Physics and Astronomy, Uppsala University, Sweden

11:25-11:50 Inv-16 Adsorption of clusters and organic molecules on graphene and 2D boron nitride

Biplab Sanyal

Department of Physics and Astronomy, Uppsala University, Sweden

11:50-12:15 Inv-17 Transport, magnetic and optical Properties of Decorated Graphenes and Graphene Nanoribbons

Swapan K. Pati

Theoretical Sciences Unit and New Chemistry Unit JNCASR, Bangalore, India

12:15-12:40 Inv-18 Ab-initio Study of Structural Stability of Ordered Long Periodic Structures In Al-rich Ti-Al System

A. Arya, P.S. Ghosh and G.K. Dey

Materials Science Division, Bhabha Atomic Research Centre, Mumbai, India

- 12:40-13:05 Inv-19 Coupling between quantum Hall state and electromechanics in suspended graphene resonator
Mandar M. Deshmukh, Vibhor Singh, Bushra Irfan, Ganesh Subramanian, Hari S. Solanki, Shamashis Sengupta, Sudipta Dubey, Anil Kumar and S. Ramakrishnan
DCMP and MS, TIFR, Homi Bhabha Road, Mumbai, India
- 13:05-14:00 LUNCH BREAK
- SESSION-5:** Chair: **Y. P. Feng**
- 14:00-14:25 Inv-20 The mechanism of graphene CVD growth
Feng Ding
Institute of Textiles and Clothing, Hong Kong Polytechnic University, Kowloon, Hong Kong
- 14:25-14:50 Inv-21 Graphene Sheets into Fullerene Molecules: Insights from DFTB based QM/MD Simulation
K.R.S. Chandrakumar
Theoretical Chemistry Section, Bhabha Atomic Research Center, Mumbai, India
- 14:50-15:15 Inv-22 Topological Defect Activation & Magnetism in Carbon Nanostructures
Tanusri Saha-Dasgupta
S.N. Bose National Centre for Basic Sciences, Kolkata, West Bengal, India
- 15:15-15:40 Inv-23 Tuning the Shape and Reactivity of Small Gold Clusters by Substrate Doping
Shobhana Narasimhan, Nisha Mammen and Stefano de Gironcoli
Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore, India
- 15:40-16:00 COFFEE-BREAK

SESSION-6: Chair: **Chiranjib Majumder**

- 16:00-16:25 Inv-24 First Principles Study of Strained 2-D Nanomaterials
Gyubong Kim, Mina Park, **Kwang-Ryeol Lee** and Yoshiyuki Kawazoe
Computational Science Center, Korea Institute of Science and Technology,
Seoul, Korea
- 16:25-16:50 Inv-25 Band gap engineering and other theoretical studies in graphene
K. Iyakutti, V. J. Surya and Y. Kawazoe
Department of Physics, Noorul Islam University, Kumaracoil, Kanyakumari,
TamilNadu, India
- 16:50-17:15 Inv-26 Cu-based spin-1/2 spin-gap tetramer and trimer system: complex
low-dimensional magnetic systems
Debjani Karmakar
Bhabha Atomic Research Centre, Trombay, Mumbai, India
- 17:15-17:40 Inv-27 Novel Nanostructures: Insights from first principles electronic structure
Calculations
Indra Dasgupta
Department of Solid State Physics & Center for Advanced Materials
Indian Association for the Cultivation of Science, Jadavpur, Kolkata, India
- 17:40-18:05 Inv-28 Ab-initio calculations of structural, electronic and magnetic properties of
 Mn_xTe_y Clusters
Anjali Kshirsagar and H. A. Shafiei Gol
Centre for Modeling and Simulation and Department of Physics,
University of Pune, Pune, India
- 18:05-19:00 CONCLUDING REMARKS **U.V. Waghmare, Y. Kawazoe**
- 19:00 SPECIAL DINNER (Centenary Visitors House Dining Hall)