Mini-symposium C10
Recent advances in the science of clusters

Organizers:

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Fri - 9 Jan 2015 | 11:00 – 12:30 | Room 04-37, Block S16

Chair: Biplab Sanyal

11:00 C10-01 Keynote
Predicting Properties of Clusters, Molecules and Nanocrystals Interacting with Static and Dynamic Fields
James R. Chelikowsky
Departments of Physics and Chemical Engineering, Center for Computational Materials, Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, Texas 78712-1229 USA

11:30 C10-02 Invited
Exploring and understanding the potential energy landscape of clusters
Stefan Goedecker
University of Basel, Switzerland

12:00 C10-08 Invited
Novel nanostructures of boron: Bowls, rings, tubes, cages, and sheets
Vijay Kumar
Dr. Vijay Kumar Foundation, 1969 Sector 4, Gurgaon 122001, Haryana, India, Center for Informatics, School of Natural Sciences, Shiv Nadar University, Chithera, Gautam Budh Nagar - 201307, UP, India

Fri - 9 Jan 2015 | 14:00 – 15:30 | Room 04-37, Block S16

Chair: Dilip Kanhere

14:00 C10-05 Invited
Chiral Spin Textures at Transition Metal Surfaces
Stefan Blügel
Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

14:30 C10-10 Invited
Correlated electronic structures of metalorganic molecules
Biplab Sanyal
Department of Physics and Astronomy, Uppsala University, Box-516, 75120, Uppsala, SWEDEN

15:00 C10-06
Feₙ (n = 1–6) clusters chemisorbed on vacancy defects in graphene: Stability, spin-dipole moment, and magnetic anisotropy.
S. Haldar¹, B. S. Pujari², S. Bhandary¹, F. Cossù³, O. Eriksson¹, D. Kanhere² and B. Sanyal¹
¹Div. of Materials Theory, Dept. of Physics and Astronomy, Uppsala University, Sweden; ²Centre for Modeling and Simulation, University of Pune, Pune, India; ³Materials Science Division, Department of Physical Science and Engineering, KAUST, Kingdom of Saudi Arabia

15:15 C10-07
Theoretical Studies of Thermodynamic Properties of Clusters

Fri - 9 Jan 2015 | 16:00 – 18:00 | Room 04-37, Block S16

Chair: James Chelikowsky

16:00 C10-03 Invited
Determining and Analyzing the Properties of Nanoparticles
Michael Springborg
Physical and Theoretical Chemistry, University of Saarland, 66123 Saarbrücken, Germany

16:30 C10-09 Invited
Structures and growth behavior of gas-phase and metal-supported boron clusters
Jijun Zhao
Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China

17:00 C10-12 Invited
Melting in finite size systems: A density functional perspective
Dilip Kanhere
University of Pune, India

17:30 C10-11 Invited
A computational study of Cu clusters within ferrite Fe matrix on atomic scale
Lin Zhang
Institute of Materials Physics and Chemistry, Northeastern University, Shenyang 110004, China

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