Mini-symposium B13
Accelerating the Discovery of Advanced Materials Using the Materials Genome Approach

Organizers:
Vijay Kumar
Dr. Vijay Kumar Foundation, India & Shiv Nadar University, India
Email: kumar@vkf.in & vijay.kumar@snu.edu.in

Miguel Dias Costa
National University of Singapore, Singapore
Email: phymdc@nus.edu.sg

Yuan Ping Feng
National University of Singapore, Singapore
Email: phyfyp@nus.edu.sg

Fri – 9 Jan 2015 | 16:00 – 18:00 | 04-35, Block S16

Chair: Vijay Kumar

16:00 B13-01 Keynote
In Silico Search for Heterogeneous Catalysts
Thomas Bligaard
SLAC National Accelerator Laboratory, 2575 Sand Hill Road, MS31, Menlo Park, CA 94025, USA

16:30 B13-02 Invited
First Principles Study and Design of Functional Materials for Energy Applications
Su-Huai Wei
National Renewable Energy Laboratory, Golden, CO, USA

17:00 B13-03 Invited
Computational Materials Design by Evolutionary Structure Prediction
Qiang Zhu, Artem R Oganov
Center of Materials by Design, Department of Geosciences, Stony Brook University, Stony Brook, NY, USA

17:30 B13-04 Invited
Materials informatics modeling for the design of advanced materials
N. Sukumar1,2,3, K. Wu1, P. Saha1, C. M. Breneman1, G. Pilania1, C. C. Wang1, G. Setzing2, R. Ramprasad3, B. L. Chittari4 and V. Kumar1,6
1Department of Chemistry and 2Center for Informatics, Shiv Nadar University, India, 3Department of Chemistry and RECCR Center, Rensselaer Polytechnic Institute, USA, 4Chemical, Materials, and Biomolecular Engineering and 5Department of Chemistry and Polymer Program, Institute of Materials Science, University of Connecticut, USA, 6Dr. Vijay Kumar Foundation, Gurgaon, India

Sat - 10 Jan 2015 | 11:00 – 12:45 | Room 04-35, Block S16

Chair: Miguel D. Costa

11:00 B13-05 Keynote
The Linking Data Driven Discoveries with ab initio approaches
Rajeev Ahuja
Department of Physics & Astronomy, Uppsala University, Box 516, 75120 Uppsala, Sweden

11:30 B13-06 Invited
Materials Discovery via CALYPSO Methodology
Yanchao Wang, Yanming Ma
State Key Lab of Superhard Materials, Jilin University, China

12:00 B13-07 Invited
Materials data in accelerating the process from materials design to mass production

14:00 B13-08 Invited
Design of Novel Magnetic Clusters from Genetic Algorithm
Jijun Zhao
Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China

14:30 B13-09 Invited
Study on the chemistry-structure-property relationship for new materials by a combined approach of artificial intelligence, physical based semi-empirical, first principles modeling and experiments
Ping Wu, Qing Xu, Mushtaq Sobhan, Franklin Anariba, Kostiantyn Sophia
Entropic Interface Group, Engineering Product Development, Singapore University of Technology and Design, Singapore 138682, Singapore

15:00 B13-10
Ab initio design of perovskite-type materials for photovoltaics
Arpan Krishna Deb1, Vijay Kumar1,2
1Center for Informatics, Shiv Nadar University, Chithera, Gautam Budh Nagar, Uttar Pradesh, India, 2Dr. Vijay Kumar Foundation, Gurgaon, Haryana, India

15:15 B13-11
Designing rare-earth-free strong magnets from ab initio calculations
Bheema Lingam Chittari1, Vijay Kumar1,2
1Dr. Vijay Kumar Foundation, 1969 Sector 4, Gurgaon 122001, Haryana, India, 2Center for Informatics, School of Natural Sciences, Shiv Nadar University, Chithera, Gautam Budh Nagar - 201320, U.P., India

15:30 B13-12
High-throughput screening for novel high-k dielectrics through first-principles calculation
Kanghoon Yim, Yong Youn, Joohye Lee, Kyuhyun Lee, Seungwu Han
Dept. of Materials Science and Engineering, Seoul National University, Seoul, Korea