The Abdus Salam International Centre for Theoretical Physics

14th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

Cosponsor(s): the International School for Advanced Studies (SISSA), the INFM DEMOCRITOS National Simulation Center, the International Center for Materials Research (ICMR), the Psi-k Network, and the Centre Européen de Calcul Atomique et Moléculaire (CECAM)
Organizer(s): R. Gebauer, F. Mauri, D. Vanderbilt
Trieste - Italy, 08 - 10 January 2009

Venue: Leonardo da Vinci Building Main Lecture Hall

Final programme

REGISTRATION AND WELCOME (Room:Leonardo da Vinci Building Main Lecture Hall)

8 January 2009

08:00 - 08:50 (Room: Leonardo da Vinci Building, Lobby)
--- REGISTRATION and ADMINISTRATIVE FORMALITIES ---

08:50 - 09:00 **K.R. Sreenivasan ICTP Director, and Organizers**
Welcoming Remarks

SESSION 1: Many-body Techniques for Real Materials (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Ralph Gebauer

8 January 2009

09:00 - 09:35 **Geoffrey Stenuit** / *CNR-INFM Democritos, Trieste, Italy*
Bridging the size gap between density-functional and many-body perturbation theory

09:35 - 10:10 **Giulia Galli** / *UC Davis, USA*
Efficient evaluation of dielectric matrices for ab-initio calculations of excited state properties and correlation energies

10:10 - 10:45 **Huy-Viet Nguyen** / *Hanoi National University of Education, Viet Nam and SISSA, Trieste, Italy*
Efficient and accurate calculation of exact exchange and RPA correlation energies in ACFD theory

10:45 - 11:30 --- Coffee Break + Registration ---

11:30 - 12:05 **Lucia Reining** / *École Polytechnique, Palaiseau, France*
Correlation in electronic excitations

12:05 - 12:40 **Claudio Attaccalite** / *U. del Pais Vasco, San Sebastian, Spain*
Electron correlation in graphene: band structure and electron-phonon interaction from GW

12:40 - 14:40 --- Lunch ---

SESSION 2: Simulations of Structural Properties (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Pablo Ordejon

8 January 2009

14:40 - 15:15 **Ismaila Dabo** / *INRIA and Université Paris-Est, France*
First-principles electrochemistry

15:15 - 15:50 **Chris Pickard** / *St. Andrews, UK*
Ab-initio random structure searching: A window on structure space

15:50 - 16:35 --- Coffee Break + Registration ---

16:35 - 17:10 **Ron Cohen** / *Carnegie Institution, USA*
Quantum Monte Carlo simulations of behavior at extreme conditions

POSTER SESSION 1 (Room:Adriatico Guest House (Lower Level 1))

8 January 2009

17:30 - 18:15 --- Poster setup at Adriatico Guest House (Lower level 1) ---

18:30 - 21:00 **Poster session / free discussions**
Informal buffet for all participants during the poster session

SESSION 3: 2008 ICTP Prize Ceremony (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Nicola Marzari

9 January 2009

08:50 - 09:35 **K.R. Sreenivasan** / *ICTP Director*
Welcoming Remarks and Presentation of the Award

09:35 - 10:10 **Zhong Fang** / *Center for Quantum Simulation Sciences, CAS, Beijing, China*
LDA+Gutzwiller method for correlated electron systems

10:10 - 10:55 --- Coffee Break ---

SESSION 4: Thermal and Electronic Transport (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Nicola Marzari

9 January 2009

10:55 - 11:30 **Davide Donadio** / *UC Davis, USA*
Thermal transport at the nanoscale

11:30 - 12:05 **Jeff Neaton** / *Molecular Foundry, LBNL, Berkeley, USA*
First-principles studies of single-molecule junction conductance: Links, length, and switching

12:05 - 14:40 --- Lunch ---

SESSION 5: Quantum Chemistry (Room:Leonardo da Vinci Building Main Lecture Hall)
Chairperson: Richard Martin

9 January 2009

14:40 - 15:15 **Ali Alavi** / *Cambridge, UK*
Fermion Quantum Monte Carlo in slater determinant spaces: A game of life, death and annihilation

15:15 - 15:50 **Beate Paulus** / *Freie Universität Berlin, Germany*
Explicitly correlated ab initio methods for metals

15:50 - 16:35 --- Coffee Break ---

16:30 - 17:05 **Troy Van Voorhis** / *MIT, Cambridge, USA*
Constrained DFT for electron transfer and reaction barrier heights

17:10 - 17:45 **Jose Soler** / *Universidad Autónoma de Madrid, Spain*
Efficient first-principles van der Waals density functional forces

POSTER SESSION 2 (Room:Adriatico Guest House (Lower Level 1))

9 January 2009

17:45 - 18:30 --- Poster setup at Adriatico Guest House (Lower Level 1) ---

18:30 - 21:00 **Poster session / free discussions**
Informal buffet for all participants during the poster session

SESSION 6: Carbon Nanostructures (Room:Leonardo da Vinci Building Main Lecture Hall) (**Saturday**)
Chairperson: Jisoon Ihm

10 January 2009

08:50 - 09:00 **Organizers**
Introduction of Keynote Speaker

09:00 - 09:50 **Alex Zettl** / *UC Berkeley, USA*
Exploiting the Electronic, Thermal, and Mechanical Properties of Carbon and BN Nanostructures
Keynote talk in honor of STEVEN LOUIE's 60th Birthday

09:50 - 10:25 **Gian-Marco Rignanese** / *Univ. Catholique de Louvain, Belgium*
Band offsets from many-body perturbation theory

10:25 - 11:00 **Young-Woo Son** / *KIAS, Seoul, Korea*
Energy gaps in graphene superstructures

11:00 - 11:45 --- Coffee Break ---

SESSION 7: Large-scale and Multi-scale Simulation (Room:Leonardo da Vinci Building Main Lecture Hall) (**Saturday**)
Chairperson: Giulia Galli

10 January 2009

11:45 - 12:20 **Karsten Reuter** / *FHI-MPG, Berlin, Germany*
Towards an error-controlled multi-scale catalysis modeling

12:20 - 12:55 **Rosa di Felice** / *INFM-CNR, Modena, Italy*
Computational investigation of DNA derivatives for nano-electronics

12:55 - 14:40 --- Lunch ---

SESSION 8: Functional Materials (Room:Leonardo da Vinci Building Main Lecture Hall) (**Saturday**)
Chairperson: Lucia Reining

10 January 2009

14:40 - 15:15 **Lilia Boeri** / *MPI-FKF, Stuttgart, Germany*
DFT studies of FeAs superconductors

15:15 - 15:50 **Gianni Profeta** / *Università degli Studi dell'Aquila, Italy*
Hydrogen superconductivity and other superconductors

15:50 - 16:35 --- Coffee Break ---

16:35 - 17:10 **Davide Ceresoli** / *MIT, Cambridge, USA*
Ab-initio pseudopotential calculations of the orbital magnetization

17:10 - 17:45 **Roberto Car** / *Princeton U., Princeton, USA*
Quantum protons in hydrogen bonded systems

17:45 - 17:55 **Concluding Remarks**