0.1 Report on 16th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

Trieste (Italy)

January 10-12th, 2013

The Abdus Salam International Centre for Theoretical Physics (ICTP)
Psi-k Network
International School for Advanced Studies (SISSA)
Centre Européen de Calcul Atomique et Moléculaire (CECAM)
CNR-IOM DEMOCRITOS National Simulation Center
Consorzio per la Fisica-Trieste
International Council for Science (ICSU)
Asia Pacific Center for Theoretical Physics (APCTP)

Organizers: C. Filippi, R. M. Martin, and N. Binggeli

http://cdsagenda5.ictp.trieste.it/full_display.php?ida=a12161

The "Total Energy" workshop took place at the ICTP in Trieste on 10-12 January 2013. It was the 16th in a very successful series of workshops, held every two years at the ICTP, and devoted to recent developments in the field of electronic structure methods and their applications to a fast growing range of materials and systems. The number of participants considerably increased over the years, with this year 248 participants from 46 different countries. The workshop was organized in 10 thematic sessions in which the oral presentations were by invitation only (28 invited speakers). The topics of the sessions included:

- Functional Materials and High-Throughput Materials Design
- Ab-initio and Quantum dynamics
- Non-adiabatic Processes in Molecular Systems
- Electronic Excitations
- RPA and Beyond
- DMFT and Strongly Correlated Materials
- Quantum Monte Carlo
- Search for New Phases and Classes of Materials
- Progress in Development of New Functionals

The taks were given by internationally recognized experts and featured some of the most significant advances in the past few years. They stimulated very lively scientific discussions and exchanges of ideas, which continued during the coffee and lunch breaks. All oral presentations were given in the ICTP Main Lecture Hall of the Leonardo da Vinci Building, and in view of the importance of this workshop, ICTP also elected to film it (the workshop videos can be downloaded at http://users.ictp.it/~video/2440/2440.htm).

The workshop had also two vibrant poster sessions (with more than 140 poster presentations). The poster sessions took place on the evenings of January 10 and 11 at the lower floor of the Adriatico Guesthouse. A buffet was served during these two poster sessions. Posters were organized by topics. On January 10, the general theme was: Theory and Methods. The posters were grouped and arranged according to the following topics: DFT beyond LDA, Time Dependent DFT, Many-Body Techniques for Real Materials, Quantum Monte Carlo, Ab-initio Molecular Dynamics, Large Scale and Multiscale Simulations, Activated Processes, Electronic and Thermal Transport, Response to External Fields, Simulations in Realistic Environments. On January 11, the general theme was: Applications. The topical divisions were: Nanoscience, Biochemistry and Biomaterials, Magnetism and Spintronics, Geophysics, Functional Materials, Surfaces and interfaces, Spectroscopies, Catalysis and Electrochemistry, Chemical Reactions and Kinetics, Materials Design. The high attendence and very lively discussions at these sessions until late in the nights confirmed the high success of this format.

The worshop was cosponsored by ICTP and also by several other institutions including the International School for Advanced Studies (SISSA), the Centre Européen de Calcul Atomique et Moléculaire (CECAM), the CNR-IOM DEMOCRITOS National Simulation Center, the Consorzio per la Fisica-Trieste, the International Council for Science (ICSU), and the Asia Pacific Center for Theoretical Physics (APCTP). The Psi-k contribution was used mainly to support the travel and accommodation of young invited European speakers/participants from the Psi-k community. This support was crucial for the success of the workshop. All the institutions that supported this workshop are warmly thanked by the organizers and participants.

Programme

	Thursday, 10 January 2013
08:00	Registration
08:50	Welcoming Remarks by F. Quevedo, ICTP Director, and Organizers
	SESSION 1: High-Throughput and Functional Materials Chairperson: Pablo Ordejón
09:00	*Atomic-scale design of energy materials* Kristian Thygesen - DTU, Denmark
09:30	*Simulation of phase change materials for data storage* Marco Bernasconi - University of Milano-Bicocca, Italy
10:00	Coffee Break + Registration
	SESSION 2: Exploring Functional Materials Chairperson: David Vanderbilt
10:30	*From transition metal oxides to cosmology with electronic structure calculations* Nicola Spaldin - ETHZ, Switzerland
11:00	*Field-lattice coupling in flexoelectrics and magnetoelectrics* Raffaele Resta - University of Trieste, Italy
11:30	*General model for spin-order induced polarization in multiferroics* Hong-jun Xiang - Fudan University, Shanghai, P. R. China
12:00	Lunch Break
	SESSION 3: Ab-Initio Dynamics Chairperson: Sandro Scandolo
14:00	*Water and its constituent ions under the microscope* Ali Hassanali - ETHZ, Switzerland
14:30	*Recent progress in multiscale molecular dynamics simulation* Bernd Ensing - University of Amsterdam, The Netherlands
15:00	*Efficient implementation of Hartree-Fock exchange, MP2, and RPA for periodic systems within the GPW Method* Jürg Hutter - University of Zurich, Switzerland
15:30	Coffee Break + Registration
	SESSION 4: Quantum Dynamics and Molecular Systems Chairperson: Ralph Gebauer
16:00	*Treating non-adiabatic dynamics with the MCTDH method - from grid-based to direct dynamics* Graham Worth - University of Birmingham, UK
16:30	*TDDFT-based non-adiabatic dynamics of complex molecular systems in external laser fields* Ivano Tavernelli - EPFL, Switzerland
17:00	*Quantum dynamics from classical trajectories: direct simulation of charge transfer in enzymes and molecular catalysts* Thomas Miller - California Institute of Technology, USA

	POSTER SESSION 1
17:30	Poster setup
19:00	Poster session / free discussions
	Friday, 11 January 2013
	SESSION 5: Electronic Excitations Chairperson: Richard Martin
09:00	*Electronic excitations in solids and nanostructures: GW, GW-BSE, and beyond* Steven Louie - University of California, Berkeley, USA
09:30	*A direct approach to the calculation of many-body Green's functions: beyond quasiparticles* Lucia Reining - Ecole Polytechnique, Palaiseau, France
10:00	Coffee Break
	SESSION 6: RPA and beyond Chairperson: Stefano Baroni
10:30	*Towards a unified description of ground and excited state properties: GW vs RPA and beyond* Patrick Rinke - Fritz Haber Institute, Germany
11:00	*RPA correlation potential in the adiabatic connection fluctuation-dissipation formalism* Stefano de Gironcoli - SISSA, Italy
11:30	*Competition between the electronic and phonon-mediated scattering channels in the out-of-equilibrium carrier dynamics of semiconductors: an ab initio approach* Andrea Marini - ISM, CNR, Italy
12:00	Lunch Break
	SESSION 7: DMFT and Strongly Correlated Materials Chairperson: Erik Koch
14:00	*Dynamical screening effects from first principles: implications for low-energy models and application to the iron pnictides* Michele Casula - Université Pierre et Marie Curie, France
14:30	*Mechanism for orbital ordering in transition-metal oxides* Eva Pavarini - Forschungszentrum Jülich, Germany
15:00	*Total energy and force calculations for correlated materials* Ivan Leonov - University of Augsburg, Germany
15:30	Coffee Break
	SESSION 8: Quantum Monte Carlo Chairperson: Sandro Sorella
16:00	*Towards a determinant space representation of the electronic wavefunction in the solid state* George Booth - Princeton University, USA
16:30	*Minimum energy pathways from Quantum Monte Carlo* Saverio Moroni - SISSA, Italy
17:00	*Total energy calculations: an auxiliary-field many-body perspective* Shiwei Zhang - College of William and Mary, USA

	POSTER SESSION 2
17:30	Poster setup
19:00	Poster session / free discussions
	Saturday, 12 January 2013
	SESSION 9: Search for New Phases and Classes of Materials Chairperson: Emilio Artacho
09:00	*Predicting the properties of ordinary matter under extreme conditions* Jeffrey M. McMahon - University of Illinois at Urbana-Champaign, USA
09:30	*New classes of piezoelectrics, ferroelectrics, and antiferroelectrics by first-principles high-throughput materials design* Joseph Bennett - Rutgers University, USA
10:00	Coffee Break
	SESSION 10: Progress in Development of New Functionals Chairperson: Michael Gillan
10:30	*A new generation of density-functional methods based on the adiabatic-connection dissipation-fluctuation theorem* Andreas Görling - University of Erlangen-Nürnberg, Germany
11:00	*Strong correlation in Kohn-Sham density-functional theory* Paola Gori Giorgi - Vrije Universiteit Amsterdam, The Netherlands
11:30	*Combining wave-function and density-functional theories: range-separated hybrids, multiconfigurational hybrids, and double hybrids* Julien Toulouse - Université Pierre et Marie Curie, France
12:00	*Bridging density-functional and many-body perturbation theory: orbital-density dependence in electronic-structure functionals* Andrea Ferretti - University of Modena, Italy
12:30	Closing remarks

The abstracts of the presented papers and the list of participants can be downloaded from the workshop website or from the psi-k portal.