13th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

Directors:

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Summary

The "Total Energy" workshop is held traditionally in Trieste every two years, since 1987. The series has become one of the most important regular events of the international *ab-initio* electronic structure community. Meetings of similar format and contents are now held also regionally in North America and Asia. The workshop focuses on the most recent developments in the field of electronic structure methods. The choice of topics and lecturers is done in collaboration with the workshop's scientific committee. A preliminary meeting between the organizers and the scientific committee was held in Cambridge on January 13, 2006, to plan on the meeting program. For the 13th workshop, we extended the scientific areas traditionally covered by the workshop to include new areas such as spintronics, quantum chemistry, complex sampling methods, etc., where new exciting developments have taken place in the last couple of years. The workshop was structured in thematic sessions, as described in the Programme section. Also, three special plenary talks (given by three distinguished speakers) were organized, to celebrated the 60th birthday of A. Baldereschi (Univ. Trieste), R. Car (Princeton Univ.), and R. Resta (Univ. Trieste), and to acknowledge their contribution to the "Total energy" series of workshops. The workshop was highly successful, both scientifically and in attendance (with around 300 participants, about twice than in previous editions).

Scientific content and discussion at the event

The scientific focus of the workshop, as in previous editions, was put on both methodological/theoretical aspects and on specific applications, reflecting the fact that this is an area where theoretical and methodological developments are taking place at a fast pace, but which at the same time is contributing strongly to solving real problems related to applications.

One of the main characteristics of this area is the 'universal' applicability of the *ab-initio* electronic structures techniques to most or all condensed matter systems, be it an inorganic solid, a biomolecule, a liquid solution, or any form of matter in the condensed state. Therefore, it is making a real impact in fields like materials sciences, mineralogy, chemistry or biology. The workshop focused on particular applications in some specific areas, which are currently very active and specially promising. These included spin devices, biomolecules, alloys, amorphous semiconductors, supercritical CO_2, surfaces, interfaces, clusters, etc. As the areas of application diversify, also the range of properties that are becoming amenable to be computed with *ab-initio* techniques is becoming larger, and this is increasing the potential for real impact in other scientific disciplines.

The methodological aspects covered several areas in which rapid progress is being made. These involve both new methods to deal with different physical properties and processes using standard Density Functional Theory (DFT) (e.g., electron-phonon interactions, polarization and orbital magnetization in periodic solids), but also the development of new theories and methods to go beyond DFT, to be able to attack problems in which DFT (within its currently most common implementations) is not sufficiently accurate, or provides a completely wrong physical picture. This part of the workshop covered issues focusing on improving the current DFT implementations, like proposing new functionals able to describe weak van der Waals interactions within DFT, and developing time-dependend DFT approaches able, for instance, to provide accurate time evolution and excitation energies. Focus was also put into approaches to deal with strongly correlated systems, like SIC and LDA+U (both within the DFT framework), and linking DFT to advanced many body techniques like DMFT. Another focus of interest was post-DFT approaches (like GW and Bethe-Salpeter), able to describe excited states (including excitons). Finally, a session was devoted to Quantum Monte Carlo techniques, as a promising route to computing total energies, forces and electronic excitations (to mention a few properties) alternative to DFT, and which captures the full many-body complexity of the electronic (and even nuclear) wave functions.

A special methodological session was devoted to the general area of complexity in phase space and large time and space scales. This area concerns problems in which computing accurately the total energy (and its gradients) for a few fixed configurations is not enough to solve the problems posed. An example of this is the determination of the most favorable crystalline structures for a solid of a given chemical composition. This is a very complex problem, in which the number of possible structures to explore is enormous, and clever algorithms are being developed to learn from previous experience in known systems, to bring down the number of computations needed to a reasonable range, which can be tackled with

DFT techniques. Similarly, many problems in materials sciences (like crack propagation) involve a wide range of size and time scales, which makes it virtually impossible to deal with them with straightforward DFT approaches. Hybrid approaches in which DFT calculations are done only once in a while, and serve to refine classical force fields 'on the fly' are one possible route to solving these kinds of problems. Finally, focus was also put in trying to bring down the complexity of the DFT calculations to linear scaling in the number of degrees of freedom (number of electrons), in order to be able to extend these calculations to even larger systems.

As a final remark, we should stress that the Workshop served to celebrate the 60th birthday of three prominent scientists in our community: Profs. A. Bardereschi, R. Car and R. Resta. All three have left (and continue doing so!) a deep mark in the research in first-principles calculations. We paid recognition individually to each of them with a special Keynote Talk on topics related to the research of the three honorees. Federico Capasso (Harvard) presented a talk on Casimir Lifshitz forces and QED torques, in honor of A. Baldereschi; Joshua Zak (Haifa), talked about von Newmann Lattices and Wannier Functions, in honor of R. Resta; and M. L. Cohen (Berkeley) gave an overview of the evolution of the Pseudopotential method for Materials Sciences, in honor of R. Car.

Results and impact on the future direction of the field

The workshop was a great success, both in terms of the attendance (around twice the number of participants than in past editions), and of scientific interest.

The large number of participants in the workshop (around 300) is a sign of the good health of the field, with an increasing number of practitioners of first-principles calculations not only in the traditional areas like solid state physics and materials sciences, but also in other disciplines like mineralogy, biology, earth and atmospheric sciences, etc. Ab-initio techniques are making a real impact in these areas, and this shows in the number of people participating in workshops like this. Similar trends have been observed in other conferences, like the Psi-k Conference that has taken place in Schwabisch Gmünd (Germany), and which has experienced a similar increase in the number of participants, to the point that the next edition will take place in a different location offering more space to accommodate the growing audience.

We believe that the program put up by the Scientific Committee and the Organizers of the event has also been instrumental in attracting a large audience. The wide range of topics covered (from purely theoretical/methodological, to the very applied ones) makes the conference quite attractive for a wide audience. It must be noted, however, that the level of the conferences has been very high and that the topics were covered deeply and with a specialized audience in mind. This means that the community, even if it is growing quickly, maintains a very good scientific level and is able to follow the specialized discussion.

One of the most important facts about this area is the interaction with the experimental work. It gives the field its real importance and relevance. This is maturing to the extent that an increasing number of experimental groups are doing some first-principles modelling by themselves, in order to complement their experimental work and to improve their understanding of the processes studied experimentally. In the conference there were many good examples of interaction with experimental work, and we believe this joint venture between experiment and simulation is of paramount importance for the future of the field.

The community is in very good scientific health. The field is very imaginative and creative, and is experiencing a quick growth, both in terms of the capabilities of the techniques to deal with more complex problems and systems, and of their impact in other scientific areas. It is also a field in which its practitioners do not restrict themselves to the standard first principles techniques like DFT, but explore many other areas like model Hamiltonians for strongly correlated systems, semiempirical methods for large scale problems, hard-core quantum chemistry methods or field theoretical techniques for complicated many-body electronic states. This is very important in bringing new ideas and views into the mainstream, and this Conference is instrumental in their dissemination. It is also very important in giving this area a feeling of ‘community’, and we are sure that it will continue being very successful in future editions.

Final Program

THURSDAY, 11 January 2007

09:15 - 09:30 OPENING - Professor Katepalli R. SREENIVASAN – Director

09:30 - 10:30 Federico CAPASSO / *Harvard University, Cambridge, USA*
Harnessing quantum fluctuations: design, physics and nanomechanics of Casimir Lifshitz forces and QED torques
KEYNOTE TALK, in honor of Alfonso BALDERESCHI's 60th Birthday
Chairperson: M. Peressi

10:30 - 11:00 --- Coffee Break ---

SESSION 1: Electrons and Phonons - Chairperson: E. TOSATTI

11:00 - 11:30 Francesco MAURI / *Universite Pierre et Marie Curie, Paris, France*
Non-adiabatic vibrations in doped graphene

11:30 - 12:00 Aitor BERGARA / *Universidad del Pais Vasco, Bilbao, Spain*
Pressure Induced Complexity in Light Alkalies

12:00 - 12:30 Nicolas LORENTE / *Universite Paul Sabatier, Toulouse, France*
Vibronic effects in electron transport through atomic and molecular systems

12:30 - 12:50 Feliciano GIUSTINO / *University of California @ Berkeley, USA*
Electron-Phonon interaction with electron and lattice Wannier functions and superconductivity in Boron-doped diamond

12:50 - 14:30 --- Lunch Break ---

SESSION 2: Dispersion Forces in Density-Functional Theory - Chairperson: G. SCOLES

14:30 - 15:00 Bengt LUNDQVIST / *Chalmers University of Technology, Gothenburg, Sweden*
Promising path to DFT for sparse matter - a functional with Van der Waals interactions

15:00 - 15:30 Pablo GARCIA-GONZALEZ / *UNED, Madrid, Spain*
Many-body and time-dpendent DFT methods to evaluate electron total energies

15:30 - 15:50 Stefano de GIRONCOLI / *SISSA & DEMOCRITOS National Simulation Center*
van der Waals coefficients in DFT: a simple approximation for the polarizability

15:50 - 16:20 --- Coffee Break ---

SESSION 3: Excitations: GW and Bethe-Salpeter - Chairperson: L. REINING

16:20 - 16:50 Fabien BRUNEVAL / *Ecole Polytechnique, Palaiseau, France*
Self-consistent GW electronic structure of solids

16:50 - 17:20 Patrick RINKE / *Fritz-Haber-Institut, Berlin, Germany*
Exact-exchange based quasiparticle energy calculations applied to (transition) metal nitrides: ScN and InN

17:20 - 17:40 Paolo UMARI / *SISSA & DEMOCRITOS National Simulation Center*
Fast GW calculations using ultra-localized Wannier functions

17:40 - 19:00 --- POSTER SESSION I ---

FRIDAY, 12 January 2007

09:00 - 10:00 Joshua ZAK / *Technion, Haifa, Israel*
von Neumann Lattices and Wannier Functions
KEYNOTE TALK: in honor of Raffaele RESTA's 60th Birthday
Chairperson: D. Vanderbilt

SESSION 4: Polarization and Magnetization - Chairperson: X. GONZE

10:00 - 10:30 Timo THONHAUSER / *Rutgers University and MIT, USA*
Orbital magnetization in periodic solids and its connection to NMR

10:30 - 11:00 Umesh WAGHMARE / *JNCASR, Bangalore, India*
Geometric phases, distribution of electron charge centers, Wannier functions and bonding in materials

11:00 - 11:30 --- Coffee Break ---

SESSION 5: Time-Dependent Density-Functional Theory - Chairperson: R. GEBAUER

11:30 - 12:00 Kieron BURKE / *University of California, Irvine, USA*
Time-dependent density functional theory: An overview

12:00 - 12:30 Stefano BARONI / *SISSA & DEMOCRITOS National Simulation Center*
Turbocharging TDDFT using Lanczos chains

12:30 - 13:00 Ilya TOKATLY / *Moscow Instit. of Electronic Tech., Russia / Universitat Erlangen-Numberg, Germany*
Quantum mechanics in a commoving frame: An emergence of time-dependent deformation functional theory

13:00 - 14:30 --- Lunch Break ---

SESSION 6: Spintronics - Chairperson: J. IHM

14:30 - 15:00 Stefan BLUEGEL / *KFA, Julich, Germany*
Spin-dependent all-electron tunneling through junctions

15:00 - 15:30 Hadi AKBARZADEH / *Isfahan University of Technology, Iran*
Ab-initio study of Co_2MnSi (001) surface and Co_2MnSi/GaAs (001) interface

15:30 - 16:00 --- Coffee Break ---

SESSION 7: Surfaces, Interfaces and Clusters - Chairperson: J.M. SOLER

16:00 - 16:30 Annabella SELLONI / *Princeton University, USA*
Defects on TiO2 surfaces

16:30 - 17:00 Massimiliano STENGEL / *University of California @ Santa Barbara, USA*
First-principles calculations of capacitors at finite bias potential

17:00 - 17:30 Xin-gao GONG / *Fudan University, Shanghai, China*
Pressure Induced the Phase Transition in Nano-cluster and Nano-tubes

SESSION 8: From Inorganic to Bio - Chairperson: J.J. KOHANOFF

17:30 - 18:00 Dario ESTRIN / *University of Buenos Aires, Argentina*
Exploring Chemical Reactivity in Biological Systems with Hybrid QM/MM Methods

18:00 - 18:20 Moumita SAHARAY / *JNCASR, Bangalore, India*
Car-Parrinello Molecular Dynamics Simulation Studies on Supercritical Carbon Dioxide

19:30 - 21:30 --- POSTER SESSION II ---

SATURDAY, 13 January 2007

09:00 - 10:00 Marvin COHEN / *University of California, Berkeley, USA*
The Evolution of the Pseudopotential Method for Computational Materials Science
KEYNOTE TALK: in honor of Roberto CAR's 60th Birthday
Chairperson: S.G. Louie

SESSION 9: Complexity in Phase Space - Chairperson: A. GARCIA

10:00 - 10:30 Gerbrand CEDER / *MIT, Cambridge, USA*
The first principle prediction of crystal structure by combining knowledge methods with first principles energy methods

10:30 - 11:00 Thomas KUEHNE / *ETH Zurich, Lugano, Switzerland*
An efficient and accurate Car-Parrinello-like approach to Born-Oppenheimer molecular dynamics

11:00 - 11:30 Alessandro De VITA / *Universita di Trieste, Italy*
Mechanical properties of brittle solids studied with the "learn on the fly" hybrid MD scheme

11:30 - 12:00 --- Coffee Break ---

SESSION 10: Quantum Monte Carlo - Chairperson: M.J. GILLAN

12:00 - 12:30 David CEPERLEY / *University of Illinois @ Urbana-Champaign, USA*
Quantum Monte Carlo Simulations of Dense Hydrogen

12:30 - 13:00 Richard NEEDS / *Cambridge University, UK*
Equation of state and Raman frequency of diamond from quantum Monte Carlo

13:00 - 14:30 --- Lunch Break ---

SESSION 11: Functional Materials - Chairperson: S. NARASIMHAN

14:30 - 15:00 Igor ABRIKOSOV / *Linkoping University, Sweden*
Ab-initio theory of alloys: new possibilities for materials design

15:00 - 15:30 David DRABOLD / *Ohio University, Athens, USA*
Simulations of Hydrogenated Amorphous Silicon

SESSION 12: Strong Correlations: SIC, LDA+U and DMFT - Chairperson: M. FABRIZIO

15:30 - 16:00 Antoine GEORGES / *Ecole Polytechnique, Palaiseau, France*
Electronic structure of strongly correlated systems with dynamical mean-field theory: status report and perspectives

16:00 - 16:30 Igor MAZIN / *Naval Research Laboratory, Washington, USA*
Charge ordering as alternative to Jahn-Teller distortion

16:30 - 17:00 --- Coffee Break ---

17:00 - 17:30 Eva PAVARINI / *IFF, Juelich, Germany*
Electronic structure trends in transition metal oxides: the NMTO+DMFT approach

17:30 - 18:00 Axel SVANE / *University of Aarhus, Denmark*
Self-interaction correlation calculations of f-electron materials

18:00 - 18:15 CONCLUDING REMARKS : R. MARTÍN; Chairperson: P. ORDEJÓN