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

1 Summary

This Workshop followed the series started in Oxford (1983) and continued in Braunschweig (1984) and in Trieste (1987, 1989, 1991, 1993, 1995, 1997, 1999, 2001 and 2003). Following the tradition of the previous meetings, the Workshop has been devoted to recent advances in computational condensed matter physics and materials science, based on realistic calculations of the electronic structure of polyatomic systems.

The Workshop consisted of 28 invited talks, a special section on code development with 5 invited talks and a poster session with about 90 posters. The meeting was focused on methodological aspects, supplemented by sessions devoted to recent important applications. Its format was the one of a Workshop among specialists, with ample space for discussion and personal interaction. This edition, with a total attendance of 206 people, has seen a large number of young participants who could benefit from the interaction with more experienced scientists. Thanks to the ICTP funds we could also support (partially or in full) 9 participants from developing countries.

The Workshop has been followed by a one-week tutorial on the use of the Quantum ESPRESSO package, an open source package for electronic structure calculation. (See the web page `http://www.democritos.it/events/espresso-tutorial.php`). Many participants to this tutorial could follow the discussions at the Workshop and be exposed to the advanced applications of electronic structure methods presented here.

2 Description of the scientific content

The complete program of the Workshop is given at the end of this document. As can be seen from the program the addressed topics were very broad, ranging from formal theoretical developments in Quantum Monte-Carlo, ab-initio transport theory, ab-initio theory of superconductivity, linear scaling methods and density functional perturbation theory, to applications to nano and biological structures, to complex materials problems, and to surfaces and catalysis.

As in the tradition of the Workshop we had a section on the development of DFT beyond the local density formulation and related topics with contributions by S. Louie (US) and M. Head-Gordon (US).

We had a section devoted to the study of solids in an electric field (static and time dependent) and a related section devoted to density functional perturbation theory with contributions by I. Souza (US), O. Diéguez (US), F. Giustino (Switzerland), S.Y. Savrasov (US), M. Veithen (Belgium), and M. Lazzeri (France).

A section was devoted to linear scaling density functional theory calculations with contributions by M. Challacombe (US), M. Seijo (Spain) and J.L. Fattebert (US).

The ab-initio theory of superconductivity was illustrated by E.U.K. Gross (Germany) and applications were presented by S. Massidda (Italy).

Developments and applications of Quantum Monte Carlo methods were presented by C. Filippi (Netherlands), J.C. Grossman (US) and M. Fuchs (Germany).

Novel methods to deal with the ballistic transport in nanostructures were presented by N. Marzari (US) and by A. Smogunov (Italy).

Applications of the ab-initio methods to the study of nano and biological structures were presented by W. Andreoni (Switzerland), X. Blase (France), A. Oshiyama (Japan) and N. Manini (Italy).

Applications to complex material problems were presented by D. Alfè (UK), F. Willaime (France) and S.A. Bonev (Canada), while applications to surfaces and catalysis were presented by F. de Angelis (Italy), J.M. Soler (Spain) and N. Bonini (Italy).

Moreover, a special section was devoted to the modern methods for code development. Speakers in this section were P. Murray Rust (UK), A. Garcia and J. Wakelin (UK), P. Giannozzi (Italy), J. Junquera (Spain) and J.J.

Mortensen (Denmark).

A lively poster section with about 90 posters allowed young participants to present their work and to interact with more experienced scientists. The Workshop had a very international character and it contributed to strengthen contacts between scientists of US, Europe, Asia, and Africa and to continue the strong international attitude of this community. Speakers, committee members, organizers, and chairpersons (47 in total) were from North America (12), from Europe (33), and from Asia (2). Participants (159 in total) were from North America (10), Brasil (1), Europe (113), Eastern Europe (6), Asia (22), Africa (6), and New Zealand (1). 121 among the 159 participants were less than 35 years old.

More information on the event and a booklet of abstracts can be found at the address:
`http://cdsagenda5.ictp.trieste.it/full_display.php?smr=0&ida=a04178#`

3 Assessment of the results and impact of the event in the future direction of the field

The format of this Workshop has been tested and refined over the years, and the ICTP has provided the ideal framework for the meeting of scientists coming from all over the world, solving almost seamlessly the practical problems that arise in the organization of these meetings. This edition saw a very active and motivated participation of many researchers from several countries, witnessing the interest in many parts of the world to pursue, expand or also to start activities in computational condensed matter physics and materials science based on the electronic structure. This Workshop was a very good occasion for many young people to present their work and to meet more experienced scientists. The quality of the talks and of the posters was very high and very much appreciated. In particular, the number of young participants demonstrates the vitality of this field that is now a mature field that is helping to give a sound theoretical basis to many very rapidly developing areas such as the study of nano and biological structures, the study of complex materials and of materials at extreme conditions, and the microscopic understanding and control of chemical reactions. The Workshop gathered a very active community that struggle to improve and extend the numerical methods based on the electronic structure, increasing their accuracy and the number of properties that they can tackle. The participation of scientists from US, Europe, and Asia shows that these efforts are really international. The availability of open-source codes is a very important aspect for the growing of this community and this Workshop contributed to show the potentiality of these codes and to improve their future developments.

The Abdus Salam
International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organiza

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12th International Workshop on

Computational Physics and Materials Science:

Total Energy and Force Methods

Co-sponsored by:

- International School for Advanced Studies (SISSA)
- Lawrence Livermore National Laboratory (LLNL)
- European Science Foundation's Psi-k Programme (ESF)
- INFM DEMOCRITOS National Simulation Center
- Materials Computation Center (UIUC), Travel Program for Young Scientists

Organizers: G. Galli, E. Artacho, A. Dal Corso

Trieste - Italy, 13 - 15 January 2005
Venue: Main Building Lecture Hall

Final programme

THURSDAY, 13 JANUARY 2005

REGISTRATION AND OPENING REMARKS

08:00 - 09:00 --- Registration and administrative formalities ---

09:10 - 09:20 **Opening remarks**

BEYOND LOCAL DENSITY FORMULATIONS

Chairperson: S. de Gironcoli

09:20 - 10:00 **S. Louie** / *UC Berkeley & Lawrence Berkeley National Lab., USA*
Ab-initio study of the photo-excited state: nanotubes to self-trapped excitons

10:00 - 10:30 **M. Head-Gordon** / *UC Berkeley & Lawrence Berkeley National Lab., USA*
Fast electron correlation methods for molecules

10:30 - 11:00 --- --- Coffee break --- ---

AB-INITIO CALCULATIONS IN ELECTRIC AND MAGNETIC FIELDS

Chairperson: D. Vanderbilt

11:00 - 11:30 **I. Souza** / *UC Berkeley, USA*
Dynamics of Berry-phase polarization in time-dependent electric fields

11:30 - 11:50 **O. Diéguez** / *Rutgers University, USA*
First-principles simulations at constant electric polarization

11:50 - 12:10 **F. Giustino** / *EPFL & IRMMA, Switzerland*
Dielectric permittivity across interfaces in the atomic-scale limit

12:10 - 14:10 --- --- Break --- ---

LINEAR SCALING DENSITY FUNCTIONAL THEORY CALCULATIONS

Chairperson: G. Galli

14:10 - 14:40 **M. Challacombe** / *LANL, USA*
New developments in linear scaling electronic structure theory: the perturbed projector for ab-initio response theory and exact Hartree-Fock exchange in the condensed phase

14:40 - 15:10 **L. Seijo** / *UNAM, Spain*
Mosaico: a parallel, linear-scaling method for large molecules and embedded clusters

15:10 - 15:40 **J.-L. Fattebert** / *LLNL, USA*
Linear scaling first-principles molecular dynamics with controlled accuracy

15:40 - 16:10 --- --- Coffee break --- ---

SUPERCONDUCTIVITY WITHIN DENSITY FUNCTIONAL THEORY

Chairperson: R. Resta

16:10 - 16:40 **E.K.U. Gross** / *Freie Univ. Berlin, Germany*
DFT for superconductivity (theory)

16:40 - 17:10 **S. Massidda** / *INFM SLACS, Università di Cagliari, Italy*
DFT for superconductivity (applications)

SPECIAL SESSION ON CODES

Chairperson: E. Artacho

17:10 - 17:30 **P. Murray-Rust** / *University of Cambridge, UK*
Modular approaches to computational chemistry

17:30 - 18:00 **A. Garcia & J. Wakelin** / *Univ. del País Vasco, Bilbao, Spain & Cambridge Univ., UK*
Software tools for data interchange

18:00 - 18:20 **P. Giannozzi** / *Scuola Normale Superiore Pisa & DEMOCRITOS, Italy*
The Quantum-Espresso software distribution

18:20 - 18:35 **J. Junquera** / *Universidad de Cantabria, Spain*
Software tools for data interchange

18:35 - 18:55 **J.J. Mortensen** / *Technical University of Denmark*
An XML-format for atomic PAW setups

POSTER SESSION

FRIDAY, 14 JANUARY 2005

DENSITY FUNCTIONAL PERTURBATION THEORY

Chairperson: R. Resta

09:00 - 09:30 **S.Y. Savrasov** / *New Jersey Institute of Technology, USA*
Spectral density functionals for electronic structure calculations

09:30 - 09:50 **M. Veithen** / *University of Liege, Belgium*
Computation of non-linear optical properties from density functional theory

09:50 - 10:10 **M. Lazzeri** / *LMCP Paris, France*
Kohn anomalies and electron-phonon interactions in graphite

10:10 - 10:40 -- --- Coffee break --- ---

QUANTUM MONTE CARLO

Chairperson: R. Needs

10:40 - 11:10 **C. Filippi** / *Inst.-Lorentz Univ. Leiden, the Netherlands*
Excitation energies of photoactive molecules from Quantum Monte Carlo

11:10 - 11:40 **J.C. Grossman** / *LLNL, USA*
Efficient Quantum Monte Carlo energies for molecular dynamics simulations

11:40 - 12:10 **M. Fuchs** / *Max-Planck-Gesellschaft Berlin, Germany*
Diffusion Monte Carlo study of hydrogen bonded systems

12:10 - 14:10 --- --- Break --- ---

NANO AND BIO STRUCTURES

Chairperson: E. Tosatti

14:10 - 14:40 **W. Andreoni** / *IBM Research, Zürich, Switzerland*
The role of ab-initio molecular simulations in computational biology

14:40 - 15:10 **X. Blase** / *CNRS & Univ. Claude Bernard, Lyon, France*
From plastic to superconducting properties of covalent clathrates

15:10 - 15:40 **A. Oshiyama** / *University of Tsukuba, Japan*
Nano-shapes and electronic properties of carbon materials

15:40 - 16:10 **N. Manini** / *Università di Milano, Italy*
Jahn-Teller spectral fingerprint in molecular photoemission: C60

16:10 - 16:40 --- --- Coffee break --- ---

TRANSPORT PROPERTIES

Chairperson: J. Ihm

16:40 - 17:10 **N. Marzari** / *MIT, USA*
Electronic structure and quantum conductance of nanostructures: the case of functionalized nanotubes

17:10 - 17:30 **A.N. Smogunov** / *SISSA & INFM DEMOCRITOS, Trieste, Italy & Voronezh State University, Russia*
Electron transport in magnetic nanocontacts

17:30 - 19:00 **Free time - Posters up**

--- --- Conference dinner --- ---

SATURDAY, 15 JANUARY 2005

COMPLEX MATERIAL PROBLEMS

Chairperson: M. Gillan

09:20 - 09:40 **D. Alfe'** / *London, UK*
The melting curve of MgO from first principles calculations

09:40 - 10:00 **F. Willaime** / *CEA Saclay, France*
Kinetics of radiation defects in iron from first principles

10:00 - 10:20 **S.A. Bonev** / *Dalhousie University, Canada*
Ab-initio simulations of phase transitionds in dense hydrogen

10:20 - 10:50 --- --- Coffee break --- ---

SURFACES AND CATALYTIC PROCESSES

Chairperson: M. Bernasconi

10:50 - 11:10 **F. De Angelis** / *ISTM - CNR, Università di Perugia, Italy*
A time-dependent DFT study of [Fe(CN)6]4- sensitization of TiO2 nanoparticles

11:10 - 11:40 **J.M. Soler** / *UNAM, Spain*
Fast and reliable STM/STS simulations

11:40 - 12:00 **N. Bonini** / *SISSA & INFM DEMOCRITOS, Trieste, Italy*
Engineering the reactivity of metal catalysts: a model study of methane dehydrogenation on Rh(111)

12:00 - 12:00 **R. Martin** / *University of Illinois, Urbana, USA*
Closing remarks