

# 13<sup>th</sup> International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

## Abstract

The “Total Energy” workshop is held traditionally in Trieste every two years, since 1987. With 100-150 participants, the workshop is one of the most popular regular events of the international ab-initio electronic structure community. The workshop focuses on electronic structure methods and their applications in nanoscience, materials science, biochemistry, etc.

## Scientific Summary

### Directors:

Nicola Marzari (Dept of Materials Science and Engineering, MIT), Pablo Ordejon (ICMAB-CSIC, Barcelona), Sandro Scandolo (ICTP, Trieste)

### Motivation:

The “Total Energy” workshop is held traditionally in Trieste every two years, since 1987. The workshop has become one of the most important regular event 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 (see below). A preliminary meeting between the organizers and the scientific committee was held in Cambridge on January 13, 2006. For the 13th workshop we plan extend the scientific areas traditionally covered by the workshop, to include new areas such as electrochemistry, quantum chemistry, complex sampling methods, etc., where new exciting developments have taken place in the last couple of years.

Contributions are solicited from all areas of electronic structure theory, with particular emphasis on:

### Theory and Methods

- Density-functional theory 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 transport
- Response to external fields
- Simulations in realistic environments

## **Applications**

Nanoscience  
Biochemistry and Biomaterials  
Magnetism and spintronics  
Geophysics  
Functional Materials  
Surfaces  
Spectroscopies  
Catalysis and Electrochemistry  
Chemical reactions and kinetics  
Materials design

The workshop will be structured in thematic sessions, as described in the Programme section. A special session consisting of three plenary talks will celebrate the 60<sup>th</sup> birthday of A. Baldereschi (Univ. Trieste), R. Car (Princeton Univ.), and R. Resta (Univ. Trieste), and acknowledge their contribution to the “Total energy” series of workshops. The three plenary talks will be given by special guests (see Programme).

Expected number of participants:  
100-150 participants.

Duration of the meeting and dates:  
3 days, 11-13 January, 2007

## **Scientific Committee**

A. Baldereschi, EPF Lausanne, Switzerland  
S. Baroni, SISSA & DEMOCRITOS, Trieste, Italy  
G. Galli, Lawrence Livermore National Lab, USA  
M. Gillan, University College of London, UK  
X. Gonze, PCPM, Louvain-la-Neuve, Belgium  
E. Koch, Forschungszentrum Jülich, Germany  
J. Ihm, Seoul National University, Seoul, Korea  
S. Louie, University of California at Berkeley, USA  
N. Marzari, Massachusetts Institute of Technology, Cambridge, MA, USA  
L. Reining, Ecole Polytechnique Palaiseau, Paris, France  
R. Needs, University of Cambridge, UK  
P. Ordejon, ICMAB-CSIC, Barcelona, Spain  
M. Parrinello, ETHZ & CSCS, Zürich, Switzerland  
D. Vanderbilt, Rutgers University, Piscataway, USA

# Meeting Programme

## Meeting Program

The meeting program will consist of the following thematic sessions, each one featuring two to four speakers (40' per talk), for a total of about 30 speakers. A limited number of shorter (20') talks will also be included in the program.

Sessions:

1. Time-dependent Density-Functional Theory
2. Van der Waals interactions
3. GW and Bethe-Salpeter methods
4. Dynamical mean-field theory / LDA+U
5. Manganites
6. Quantum Monte Carlo
7. Complex sampling methods
8. Transport
9. Spintronics
10. Polarization and Magnetization
11. Functional Materials
12. Surfaces/Interfaces
13. Biochemistry

Besides the regular Workshop program, we will plan to have a session for the celebration of 60<sup>th</sup> birthday of Alfonso Baldereschi, Roberto Car and Raffaele Resta, where three distinguished speakers will give plenary talks in an area of interest of each honored individual.

# NICOLA MARZARI

## Associate Professor of Computational Materials Science

### Professional Preparation

University of Trieste, Italy	Laurea in Physics, <i>summa cum laude</i>	1992
University of Cambridge, UK	PhD in Physics	1993-1996
Department of Physics, Rutgers University	NSF-CISE Postdoctoral Fellow	1996-1998

### Appointments

Associate Professor of Computational Materials Science, DMSE, MIT		2005-to date
AMAX Assistant Professor of Computational Materials Science, DMSE, MIT		2002-2005
Assistant Professor of Computational Materials Science, DMSE, MIT		2001-2002
Research Staff, Department of Chemistry, Princeton University		1999-2001
Research Faculty, George Mason University and Naval Research Laboratory		1998-1999

### Honors

Human Capital and Mobility Doctoral Fellow	European Union	1993-1996
CISE Postdoctoral Fellow	NSF	1996-1998
AMAX Career Development Chair	MIT	2002-2005
Professeur Invitee	Institute Universitaire de France	2006

### Publications (5 most relevant, 5 recent); more than 100 invited talks

1. N. Marzari, D. Vanderbilt, and M. C. Payne, *Ensemble density-functional theory for ab-initio molecular dynamics of metals and finite-temperature insulators*, Phys. Rev. Lett., 79, 1337-40 (1997).
  2. N. Marzari, and D. Vanderbilt, *Maximally-localized generalized Wannier functions for composite energy bands*, Phys. Rev. B, 56, 12847-65 (1997).
  3. Y.-S. Lee, M. Buongiorno Nardelli, and N. Marzari, *Electronic-structure and quantum conductance of nanostructures from maximally-localized Wannier functions: the case of functionalized nanotubes*, Phys. Rev. Lett. 95, 076804 (2005).
  4. H.-L. Sit, M. Cococcioni, and N. Marzari, *Realistic, quantitative descriptions of electron-transfer reactions: diabatic surfaces from first-principles molecular dynamics*, Phys. Rev. Lett. 97, 028303 (2006).
  5. H. J. Kulik, M. Cococcioni, D. A. Scherlis, and N. Marzari, *Density-functional theory in transition metal chemistry: a self-consistent Hubbard U approach*, Phys. Rev. Lett. 97, 103001 (2006).
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1. M. Cococcioni, F. Mauri, G. Ceder, and N. Marzari, *Electronic-enthalpy functional for finite systems under pressure*, Phys. Rev. Lett. 94, 145501 (2005).
  2. P. Umari, A. Williamson, G. Galli, and N. Marzari, *Dielectric response of periodic systems from Quantum Monte Carlo calculations*, Phys. Rev. Lett. 95, 207602 (2005).
  3. B. Kozinski and N. Marzari, *Static dielectric properties of carbon nanotubes from first-principles*, Phys. Rev. Lett., 96, 166801 (2006)
  4. Y.-S. Lee and N. Marzari, *Fluxional handles for direct control of the conductance in functionalized nanotubes*, Phys. Rev. Lett. 97, 116801 (2006).
  5. B. Wood and N. Marzari, *Dynamical structure, bonding, and thermodynamics of the superionic sublattice in  $\alpha$ -AgI*, Phys. Rev. Lett. 97, in press (2006).

## Synergistic Activities

- Member and developer of the Quantum-Espresso consortium (*opEn Source Package for Research in Electronic Structure, Simulation, and Optimization*, [www.pwscf.org](http://www.pwscf.org) and [www.quantum-espresso.org](http://www.quantum-espresso.org)), a state-of-the-art integrated suite for electronic-structure simulations, freely available to researchers around the world under the terms of the GNU General Public License.
- Main author or the Wannier package ([www.wannier.org](http://www.wannier.org)), freely available under the terms of the GNU General Public License.
- Introduced novel computational methods now available both in public-domain and proprietary distributed packages: maximally-localized Wannier functions (CPMD, Quantum-ESPRESSO, CASTEP, FLAPW/Lausanne, JEEP), cold smearing (PWSCF, ABINIT, PARATEC, CASTEP), ensemble-DFT (Quantum-ESPRESSO, CASTEP, PARATEC, JEEP).
- Developed (in collaboration with Prof. Ceder) a distant-education graduate class in “Atomistic Modeling of Materials” now fully and freely available on the Web (lecture notes, lecture videos, homework assignments, computers codes), under the terms of the GNU General Public License: <http://ocw.mit.edu/OcwWeb/Materials-Science-and-Engineering/3-320Spring-2005/CourseHome/>
- Lecturer and organizer of electronic structure schools: (L) Asian/Pacific Regional School on Electronic Structure Methods and their Applications, ICTP/ICTS/NNSFC Beijing (P.R. China, 2004), (L) Asian/Pacific Regional School on Electronic Structure Methods and their Applications (Bangalore, 2006), (O) University of Illinois Urbana-Champaign (2006), (L) Asian/Pacific Regional College on Science at the Nanoscale, ICTP/ICTS/NNSFC Beijing (P.R. China, 2006).
- Developer and lecturer for a renovated materials science undergraduate curriculum (2003 start date), integrating in the sophomore year the teaching of quantum mechanics and thermodynamics, and supporting it with a mathematical core and experimental and computational labs. Presented framework at a invited talk at the TMS Annual Meeting “Educational strategies for computational materials science”.

## Collaborators and Other Affiliations

- 1) Collaborators (last 48 months) and co-editors (last 24 months), in alphabetical order:** P. M. Ajayan, A. Baldereschi, S. Bhattacharya, L. Blum, M. Buongiorno Nardelli, A. Calzolari, R. Car, G. Ceder, M. Cococcioni, J.-L. Fattebert, E. Kaxiras, G. Galli, F. Gygi, D. A. Huckaby, R. Cooke, E. Kaxiras, P. A. Kollman, M. Fornari, J. Gaillard, Y.-S. Lee, F. Mauri, T. J. Minehardt, C. Molteni, N. Mounet, S. Nayak, E. Pate, M. Peressi, A. M. Rao, B. Sadanadan, T. Savage, D. Scherlis H.-L. Sit, I. Souza, Y.-P. Sun, T. M. Tritt, B. Trout, D. Vanderbilt, B. G. Walker, S., Yip, A. Wieckowski, Y. Wu.
- 2) Graduate and postdoctoral advisors:** Michael C. Payne, University of Cambridge (UK), 1993-96 (graduate advisor); David Vanderbilt, Rutgers University (NJ) (NSF-CISE Fellowship Postdoctoral Advisor), 1996-98; David J. Singh, Naval Research Laboratory (DC), 1998-99; Roberto Car, Princeton University (NJ), 1999-2001.
- 3) Thesis advisor and postgraduate-scholar sponsor: Postdoctoral Scholars (9):** Damian Scherlis (2002- 2005); Matteo Cococcioni (2003 - 2006); Paolo Umari (2004 - 2005); Nicola Bonini (2005 - to date); Arash Mostofi (2005 - to date); Manu Sharma (2005), Francesca Baletto (2006 – to date), Oswaldo Dieguez (2006 – to date), Timo Thonhauser (2006 – to date). **Graduate Students (10):** Young-Su Lee, 2002 - to date; Brandon Wood, 2002 - to date; Hoi-Land Sit, 2002 - to date, Ismaila Dabo, 2003 - to date, Nicholas Miller, 2003 - to date, Boris Kozinsky, 2004 - to date, Nicolas Mounet (MSc, 2004-05), Heather Kulik (2004 – to date), Michael Tambe (2005 - to date), Nicolas Poilvert (2006 - to date). **Undergraduate Students (5):** Luke Shulenberg (Spring 2002), Mikael Rechtsman (Spring 2002- Spring 2003), Janet Ryu (Spring 2005 – Spring 2006), Adam Chao (Spring 2005 – Jan 2006), Chen Li (Fall 2006 –to date). **High-School Students (4):** Ann Chi, summer 2003, Caleb Ng, summer 2004, Giacomo Ferrari, summer 2005, Krzysztof Niemkiewicz, summer 2006.

## **SANDRO SCANDOLO**

Senior research scientist

The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy

### *Education:*

- 1993 – PhD in Physics (Scuola Normale Superiore, Pisa, Italy)

### *Employment history:*

- 2002-present – Senior research scientist, ICTP
- 2000-2002 – Visiting Research Staff, Dept. of Chemistry and Princeton Materials Institute, Princeton University
- 2002 – Associate Professor, International School for Advanced Studies, Trieste, Italy
- 1998-2002 – Assistant Professor, International School for Advanced Studies, Trieste, Italy

### *Brief track record:*

- Research interests: Ab-initio simulations with applications to high-pressure physics, materials science, geophysics and planetary science.
- 85 publications in refereed journals
- 50+ invited talks at international conferences
- Supervised 15 PhD and Diploma students
- Organizer of the CECAM/Psi-k workshop on Applications of First-Principle Methods to Geophysics, July 2001, Lyon, France
- Organizer of the CECAM/Psi-k workshop on Minerals Physics from Computation and Experiment, June 2006, Lyon, France
- Spokesperson of the working group on "Minerals" of the ESF network "Psi-K"
- Organizer of the 1998 ICTP Spring College on Computational Physics, of the 2000 ICTP Spring College on Electronic Structure Approaches to the Physics of Materials, Trieste, Italy, of the ICTP-ICTS Asian School on Electronic Structure Methods, Beijing, China, 2004, and of the ICTP-JNCASR-Democritos School on Computational Materials Science, July 2006, Bangalore, India.
- J. C. Jamieson award for high pressure physics. Awarded at the 1998 Gordon Research Conference on "Research at High-Pressure"

### *Five most relevant publications:*

- M. Santoro, F.A. Gorelli, R. Bini, G. Rocco, S. Scandolo, W.A. Crichton,  
*Amorphous silica-like carbon dioxide*  
Nature **441**, 857 (2006)
- A.F. Young, C. Sanloup, E. Gregoryanz, S. Scandolo, R.J. Hemley, and H.-k. Mao,  
*Synthesis of novel transition metal nitrides IrN<sub>2</sub> and OsN<sub>2</sub>*  
Phys. Rev. Lett. **96**, 155501 (2006)
- F. Baletto, C. Cavazzoni, S. Scandolo  
*Surface-trapped excess electrons on ice*  
Phys. Rev. Lett., **95**, 176801 (2005)
- X. Wang, S. Scandolo, R. Car  
*Carbon phase diagram from ab-initio molecular dynamics*  
Phys. Rev. Lett., **95**, 185701 (2005)
- V. De Renzi, R. Rousseau, D. Marchetto, R. Biagi, S. Scandolo, and U. del Pennino  
*Metal Work-Function Changes Induced by Organic Adsorbates: A Combined Experimental and Theoretical Study*  
Phys. Rev. Lett. **95**, 046804 (2005)

## **PABLO ORDEJÓN**

Research Professor

Instituto de Ciencia de Materiales de Barcelona, CSIC – Spain

### Education:

- PhD in Physics, Univ. Autónoma de Madrid. 1992.

### Employment History:

- 2005 – present: Research Professor, Inst. de Ciencia de Materiales de Barcelona, CSIC.
- 2003 – 2005: Senior Researcher, Inst. de Ciencia de Materiales de Barcelona, CSIC.
- 1999 – 2003: Permanent Researcher, Inst. de Ciencia de Materiales de Barcelona, CSIC.
- 1995 – 1999: Assistant Professor, Dpto. de Física, Universidad de Oviedo.
- 1994 – 1995: Postdoc. Res. Assoc., Dept. of Physics, Univ. of Illinois at Urbana-Champaign.
- 1992 – 1994: Visiting Scientist, Dept. of Physics, University of Illinois at Urbana-Champaign.
- 1990 – 1992: Research Assistant, Dpto. de Física de Materia Condensada, Univ. Autónoma Madrid.

### Visiting Professorships:

- June – August, 2003: Université Claude Bernard de Lyon (France).
- Sept. – Nov. 2003: Department of Physics and Astronomy, Ohio University, Athens, Ohio (USA).
- Nov. 2004: Université Paul Sabatier de Toulouse (France).
- July 2005: Donostia International Physics Center (Spain).

### Honors:

- Nov. 2005: Fellow of the American Physical Society,
- Dec. 2003: “Placa de Honor” of the Asociación Española de Científicos.

### Brief Track Record:

- Author of over 130 scientific papers and two patents, with nearly 5000 ISI citations
- 70+ invited talks
- Regional Editor of *physica status solidi*
- Member of the Physics Panel of the Spanish National Scientific Evaluation Agency, since 2004 (responsible for the area of Condensed Matter Physics).
- Member of numerous evaluations committees and panels.
- Spokesperson of the Working Group on Local Orbitals and Linear Scaling, ESF Psi-k Programme
- Organizer of four CECAM/Psi-k Workshops and Tutorials (1999, 2000, 2003, 2006), and several other workshops.
- IP in over ten research projects financed by the Spanish public funding agencies and the European Commission, and fourteen research contracts with industrial laboratories.

### Five most relevant publications during the past five years

- Soler, Artacho, Gale, García, Junquera, Ordejón, Sánchez-Portal. “The SIESTA method for ab initio order-N materials simulations”, *J. Phys. Cond. Matter* **14**, 2745 (2002)
- Brandbyge, Mozos, Ordejón, Taylor, Stokbro, “Density functional method for nonequilibrium electron transport” *Phys. Rev. B* **65**, 165401 (2002).
- Maultzsch, Reich, Thomsen, Requardt, Ordejón, “Phonon dispersion in graphite”, *Phys. Rev. Lett.* **92**, 075501 (2004)
- Fu, Willaime, Ordejón, “Stability and mobility of mono- and di-interstitials in  $\alpha$ -Fe”, *Phys. Rev. Lett.* **92**, 175503 (2004)
- Al-Brithen, Yang, Haider, Constantin, Lu, Smith, Sandler, Ordejón, “Scanning tunneling microscopy and surface simulation of zinc-blende GaN(001) intrinsic 4x reconstruction: Linear gallium tetramers?”, *Phys. Rev. Lett.* **95**, 146102 (2005).

## List of Invited Speakers

This is the list of proposed invited speakers for each of the Workshop Session:

1. Time-dependent Density-Functional Theory
  - Kieron Burke (Rutgers)
  - Stefano Baroni (SISSA)
  - Ilya Tokatly (Universität Erlangen-Nürnberg)
2. Van der Waals interactions
  - B. I. Lundqvist (Göteborg)
  - Pablo García Gonzalez (UNED-Madrid)
  - Stefano de Gironcoli (SISSA)
3. GW and Bethe-Salpeter methods
  - F. Bruneval (ETH)
  - P. Rinke (Fritz Haber Inst.)
  - Paolo Umari (MIT)
4. Dynamical mean-field theory / LDA+U
  - Antoine Georges (École Polytechnique)
  - Eva Pavarini (Univ. Pavia)
  - I. I. Mazin (NRL)
5. Manganites
  - Walter Temmermann (Daresbury Lab)
6. Quantum Monte Carlo
  - David Ceperley (UIUC)
  - Richard Needs (U. Cambridge)
  - M. Casula (SISSA)
7. Complex sampling methods
  - G. Ceder (MIT)
  - T. Kuehne (ETH)
  - A. De Vita (Kings College London)
8. Transport
  - Francesco Mauri (Université Pierre et Marie Curie)
  - Nicolas Lorente (Univ. Toulouse)
  - W.H. Duan (Tsinghua)
  - Aitor Bergara (Univ. Pais Vasco)
9. Spintronics
  - Patrick Bruno (MPI für Mikrostrukturphysik)
  - Stephan Bluegel (Julich)
  - Nagaosa (Univ. Tokyo)
  - H. Akbarzadeh (Univ. Isfahan)
10. Polarization and Magnetization
  - T. Thonhauser (Rutgers)
  - U. Waghmare (JNCASR Bangalore)
11. Functional Materials
  - I. Abrikosov (Linköping Univ.)
  - David Drabold (Ohio Univ.)
12. Surfaces/Interfaces
  - Jens Norkov (Tech. Univ. Denmark)
  - A. Selloni (Princeton)

- F. Baletto (ICTP)
13. Biochemistry
- Dario Estrin (Univ. Buenos Aires)

In the session of celebration for Alfonso Baldereschi, Roberto Car and Raffaele Resta, we will have the following distinguished speakers:

- Federico Capasso (Harvard)
- Marvin L. Cohen (Berkeley)
- Joshua Zak (Technion)