

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

Francesco Mauri, Ralph Gebauer, and David Vanderbilt  
April 16, 2009

This workshop was the 14th in a very successful series of workshops, held every two years at the ICTP in Trieste, Italy. The workshop is devoted to exposing recent advances in computational condensed matter physics and materials science, based on realistic calculations of the electronic structure of complex systems. It was held this year on 8-10 January 2009, with three full days of oral presentations, and poster sessions on the evenings of 8 and 9 January. Attendance at the workshop has grown over the years, so that this year there were 230 participants, including 23 presenters of oral talks and 155 poster presenters.

This year the workshop focused on several specific scientific themes:

- Many-body, quantum-chemistry, and quasiparticle techniques for studying complex materials
- Separable representations of the dielectric function and related quantities
- Thermal and electrical transport at the nanoscale
- Graphene and BN-based nanostructures
- FeAs-based superconductors
- Simulations of properties of complex materials systems, including electrochemical reactions, catalysis, DNA, and momentum distributions in water

There were two special events at the workshop. The first was the award of the 2008 ICTP Prize, which this year went to two condensed-matter theorists, at the beginning of the morning session on January 9. ICTP Director K.R. Sreenivasan began with some remarks about the history and role of ICTP, and then announced the two prize winners: Zhong Fang, of the Center for Quantum Simulation Sciences, CAS, Beijing, China, and Abhishek Dhar of the Raman Research Institute, Bangalore, India. Dr. Fang then gave his prize talk on “LDA+Gutzwiller Method for Correlated Electron Systems.” Unfortunately, Dr. Dhar was unable to attend the workshop and so could not present his prize talk on the “Green-Kubo Formula for Heat Conduction in Open Systems.”

The second special event was a special session on the morning of January 10 to honor the upcoming 60th birthday of Steven Louie, of UC Berkeley, and to recognize his seminal contributions to quasiparticle methods and their application to nanostructures. To mark this event, Prof. Alex Zettl, also of UC Berkeley and a long-time

colleague of Louie's, presented a keynote talk on "Exploiting the Electronic, Thermal, and Mechanical Properties of Carbon and BN Nanostructures," in which he highlighted some of Louie's contributions.

The large attendance of the workshop led to some changes in the mechanics. Oral talks were given in the Main Lecture Hall of the Leonardo da Vinci Building as in past years, but in a break with past practice, the poster sessions were moved to the Lower Level of the Adriatico Guest House, where food and drinks were provided on buffet tables in order to avoid queues. Posters were organized and arranged by topic. On 8 January the general theme was "Theory and Methods" and the subtopics were 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 and Thermal Transport, Response to External Fields, Simulations in Realistic Environments, and Other Methods. On 9 January the general theme was "Applications" and the subtopics were Nanoscience, Biochemistry and Biomaterials, Magnetism and Spintronics, Geophysics, Functional Materials, Surfaces, Spectroscopies, Catalysis and Electrochemistry, Chemical Reactions and Kinetics, Materials Design, and Other Applications. Attendees seemed to feel that this format was very successful.

The workshop was cosponsored by ICTP and several other institutions: the International School for Advanced Studies (SISSA), the INFN 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). The organizers and participants of the workshop warmly thank these institutions for their support for the workshop.



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 / INFN-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**



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Activity SMR: **2014**

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

8 January 2009 - 10 January 2009  
Trieste - ITALY

*co-sponsored by:*

the International School for Advanced Studies (SISSA),  
the INFN 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)

**Total Number of Visitors: 230**

**Final List of Participants**

| No.             | NAME and INSTITUTE   | Nationality                             | Function   |
|-----------------|--|---|--|
| <b>DIRECTOR</b> |  | <b>Total number in this function: 3</b> |  |
| 1.              | <b>GEBAUER Ralph</b><br>Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b><br>Research Topic : <b>ELECTRONIC AND OPTICAL PROPERTIES</b><br><br>Permanent Institute:<br>The Abdus Salam International Centre for Theoretical Physics<br>Condensed Matter Section<br>Strada Costiera 11<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      rgebauer@ictp.it  | GERMANY                                 | <b>ORGANIZER</b>                                   |
| 2.              | <b>MAURI Francesco</b><br>Research Field :<br><br>Research Topic :<br><br>Permanent Institute:<br>Universite' Pierre et Marie Curie<br>Institut de Mineralogie et de Physique des Milieux Condenses<br>4, Place Jussieu<br>75252 Paris<br>FRANCE<br>Permanent Institute e mail      francesco.mauri@impmc.jussieu.fr   | ITALY                                   | <b>ORGANIZER</b>                                   |
| 3.              | <b>VANDERBILT David Hamilton</b><br>Research Field : <b>COMPUTATIONAL MATERIALS THEORY</b><br>Research Topic : <b>FERROELECTRIC, DIELECTRIC, AND MAGNETIC OXIDES</b><br><br>Permanent Institute:<br>Rutgers, The State University of New Jersey<br>Department of Physics & Astronomy<br>136 Frelinghuysen Road.<br>Piscataway NJ 08855-0849<br>UNITED STATES OF AMERICA<br>Permanent Institute e mail      dhv@physics.rutgers.edu | UNITED STATES OF AMERICA                | <b>ORGANIZER &amp; SCIENTIFIC COMMITTEE MEMBER</b> |



| No. | NAME and INSTITUTE | Nationality | Function |
|-----|--------------------|-------------|----------|
|-----|--------------------|-------------|----------|

**CONFERENCE SPEAKER**

**Total number in this function: 24**

4. **ALAVI Aii** UNITED KINGDOM **CONFERENCE SPEAKER**

Research Field : **ELECTRONIC STRUCTURE THEORY**

Research Topic : **QUANTUM MONTE CARLO METHODS**

Permanent Institute:

University of Cambridge  
 Department of Chemistry  
 Lensfield Road  
 Cambridge CB2 1EW  
 UNITED KINGDOM

Permanent Institute e mail asa10@cam.ac.uk

5. **ATTACCALITE Claudio** ITALY **CONFERENCE SPEAKER**

Research Field : **QMC, DFT AND MANY BODY PERTURBATION THEORY**

Research Topic : **GW APPROXIMATION TO DESCRIBE EXCITED STATES**

Permanent Institute:

Universidad del Pais Vasco  
 Facultad de Quimicas  
 Unidad de Fisica de Materiales  
 Centro Mixto CSIC, UPV, EHU  
 Edificio Korta  
 Avenida de Tolosa 72  
 E-20018 San Sebastian  
 SPAIN

Permanent Institute e mail claudio.attaccalite@gmail.com

6. **BOERI Lilia** ITALY **CONFERENCE SPEAKER**

Research Field : **DENSITY FUNCTIONAL STUDY OF NOVEL MATERIALS**

Research Topic : **FE-BASED SUPERCONDUCTORS**

Permanent Institute:

Max Planck Institut fuer Festkoerperphysik  
 Heisenbergstrasse 1  
 D-70569 Stuttgart  
 GERMANY

Permanent Institute e mail l.boeri@kf.mpg.de

| No. | NAME and INSTITUTE   | Nationality              | Function                  |
|-----|--|--------------------------|---------------------------|
| 7.  | <p><b>CAR Roberto</b></p> <p>Research Field :</p> <p>Research Topic :</p> <p>Permanent Institute:</p> <p>Princeton University<br/> Department of Chemistry<br/> Washington Road and William St.<br/> NJ 08544-1009 Princeton<br/> UNITED STATES OF AMERICA</p> <p>Permanent Institute e mail      rcar@princeton.edu</p>   | ITALY                    | <b>CONFERENCE SPEAKER</b> |
| 8.  | <p><b>CERESOLI Davide</b></p> <p>Research Field : <b>AB-INITIO SIMULATIONS</b></p> <p>Research Topic : <b>ORBITAL MAGNETISM; PHOTOVOLTAICS</b></p> <p>Permanent Institute:</p> <p>Massachusetts Institute of Technology<br/> Department of Materials Science and Engineering<br/> 77 Massachusetts Ave.<br/> Cambridge MA 02139-4307<br/> UNITED STATES OF AMERICA</p> <p>Permanent Institute e mail      ceresoli@mit.edu</p> | ITALY                    | <b>CONFERENCE SPEAKER</b> |
| 9.  | <p><b>COHEN Ronald E.</b></p> <p>Research Field :</p> <p>Research Topic :</p> <p>Permanent Institute:</p> <p>Carnegie Institution for Science<br/> Geophysical Laboratory<br/> 5251 Broad Branch Road, N.W.<br/> 20015 Washington<br/> UNITED STATES OF AMERICA</p> <p>Permanent Institute e mail      cohen@gl.ciw.edu</p>  | UNITED STATES OF AMERICA | <b>CONFERENCE SPEAKER</b> |

| No. | NAME and INSTITUTE  | Nationality | Function                  |
|-----|---|-------------|---------------------------|
| 10. | <p><b>DABO Ismaila</b><br/>           Research Field : <b>ELECTRONIC-STRUCTURE CALCULATIONS</b><br/><br/>           Research Topic : <b>QUANTUM ELECTROCHEMISTRY</b><br/><br/>           Permanent Institute:<br/>           CERMICS, ENPC<br/>           Universite' Paris Est<br/>           6 et 8, Avenue Blaise Pascal<br/>           Cite' Descartes<br/>           Champs sur Marne<br/>           F-77455 Marne La Vallee Cedex 2<br/>           FRANCE<br/>           Permanent Institute e mail      dabo@cermics.enpc.fr</p> | FRANCE      | <b>CONFERENCE SPEAKER</b> |
| 11. | <p><b>DI FELICE Rosa</b><br/>           Research Field :<br/><br/>           Research Topic :<br/><br/>           Permanent Institute:<br/>           INFM CNR S3 Centre<br/>           c/o Dipartimento di Fisica<br/>           Universita' di Modena e Reggio Emilia<br/>           Via Campi, 213/A<br/>           41100 Modena<br/>           ITALY<br/>           Permanent Institute e mail      ROSA@UNIMORE.IT</p>   | ITALY       | <b>CONFERENCE SPEAKER</b> |
| 12. | <p><b>DONADIO Davide</b><br/>           Research Field : <b>CONDENSED MATTER THEORY AND MATERIALS SCIENCE</b><br/>           Research Topic : <b>THERMOELECTRIC PROP. OF NANOSCALE, NANOSTR. MAT.</b><br/><br/>           Permanent Institute:<br/>           University of California<br/>           Department of Chemistry<br/>           One Shields Avenue<br/>           Davis CA 95616-8677<br/>           UNITED STATES OF AMERICA<br/>           Permanent Institute e mail      ddonadio@ucdavis.edu</p>                      | ITALY       | <b>CONFERENCE SPEAKER</b> |

| No. | NAME and INSTITUTE  | Nationality                | Function   |
|-----|---|----------------------------|--|
| 13. | <b>FANG Zhong</b>   | PEOPLE'S REPUBLIC OF CHINA | <b>CONFERENCE SPEAKER</b>                            |
|     | Research Field :  |                            |  |
|     | Research Topic :  |                            |  |
|     | Permanent Institute:  |                            |  |
|     | Center for Quantum Simulation Sciences                                    |                            |  |
|     | Institute of Physics  |                            |  |
|     | Chinese Academy of Sciences   |                            |  |
|     | P.O. Box 603  |                            |  |
|     | Beijing 100080  |                            |  |
|     | PEOPLE'S REPUBLIC OF CHINA  |                            |  |
|     | Permanent Institute e mail      zfang@aphy.iphy.ac.cn                     |                            |  |
| 14. | <b>GALLI Giulia</b>   | ITALY                      | <b>CONFERENCE SPEAKER &amp; SCIENTIFIC COMMITTEE</b> |
|     | Research Field : <b>COND. MATT., PHYSICAL CHEMISTRY, MATERIALS SCI.</b>   |                            |  |
|     | Research Topic : <b>NANOSCI., MATERIALS FOR ENERGY, AQUEOUS SOLUTIONS</b> |                            |  |
|     | Permanent Institute:  |                            |  |
|     | University of California  |                            |  |
|     | Department of Chemistry   |                            |  |
|     | One Shields Avenue  |                            |  |
|     | Davis CA 95616-8677   |                            |  |
|     | UNITED STATES OF AMERICA  |                            |  |
|     | Permanent Institute e mail      gagalli@ucdavis.edu                       |                            |  |
| 15. | <b>NEATON Jeffrey B.</b>  | UNITED STATES OF AMERICA   | <b>CONFERENCE SPEAKER</b>                            |
|     | Research Field : <b>ELECTRONIC STRUCT. THEORY, COMPUTAT. NANOSCIENCE</b>  |                            |  |
|     | Research Topic : <b>CHARGE TRANSPORT, HYBRID INTERFACES EXCIT. STATES</b> |                            |  |
|     | Permanent Institute:  |                            |  |
|     | Lawrence Berkeley National Laboratory                                     |                            |  |
|     | Material Science Division   |                            |  |
|     | Molecular Foundry   |                            |  |
|     | 1 Cyclotron Road  |                            |  |
|     | Berkeley CA 94720   |                            |  |
|     | UNITED STATES OF AMERICA  |                            |  |
|     | Permanent Institute e mail      jboneaton@lbl.gov                         |                            |  |

| No. | NAME and INSTITUTE  | Nationality    | Function                                  |
|-----|---|----------------|---|
| 16. | <b>NGUYEN Viet Huy</b><br>Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b><br>Research Topic : <b>DFT BEYOND LDA</b>  | VIET NAM       | <b>CONFERENCE SPEAKER</b>                 |
|     | Permanent Institute:<br>Hanoi University of Education<br>Faculty of Physics<br>136 Xuan-Thuy Street<br>Cau-Giay District<br>Hanoi<br>VIET NAM<br>Permanent Institute e mail      nhviet@sissa.it              |                | nhviet@sissa.it<br><b>31 October 2008</b> |
| 17. | <b>PAULUS Beate</b><br>Research Field : <b>THEORETICAL AND QUANTUM CHEMISTRY</b><br>Research Topic : <b>WAVE FUNCTION-BASED CORREL. METH. FOR EXT. SYTEMS</b>   | GERMANY        | <b>CONFERENCE SPEAKER</b>                 |
|     | Permanent Institute:<br>Freie Universitat Berlin<br>Physical and Theoretical Chemistry<br>Institute of Chemistry and Biochemistry<br>Takustr. 3<br>D-14195 Berlin<br>GERMANY                                  |                |   |
| 18. | <b>PICKARD Christopher James</b><br>Research Field : <b>ELECTRONIC STRUCTURE THEORY</b><br>Research Topic : <b>MAGNETIC RESONANCE AND STRUCTURE PREDICTION</b>  | UNITED KINGDOM | <b>CONFERENCE SPEAKER</b>                 |
|     | Permanent Institute:<br>University of St Andrews<br>School of Physics and Astronomy<br>North Haugh<br>Fife<br>KY16 9SS St Andrews<br>UNITED KINGDOM<br>Permanent Institute e mail      cjp10@st-andrews.ac.uk |                |   |

| No. | NAME and INSTITUTE   | Nationality | Function   |
|-----|--|-------------|--|
| 19. | <b>PROFETA Gianni</b><br>Research Field : <b>COMPUTATIONAL CONDENSED MATTER THEORY</b><br>Research Topic : <b>SUPERCONDUCTIVITY</b>  | ITALY       | <b>CONFERENCE SPEAKER</b>                            |
|     | Permanent Institute:<br>Universita' degli Studi dell'Aquila<br>Dipartimento di Fisica<br>Via Vetoio, 10<br>Coppito<br>67010 L'Aquila<br>ITALY<br>Permanent Institute e mail      gianni.profeta@aquila.infn.it |             |  |
| 20. | <b>REINING Lucia</b><br>Research Field : <b>CONDENSED MATTER THEORY AND AB INITIO CALCULATIONS</b><br>Research Topic : <b>THEORETICAL SPECTROSCOPY</b>   | GERMANY     | <b>CONFERENCE SPEAKER &amp; SCIENTIFIC COMMITTEE</b> |
|     | Permanent Institute:<br>Ecole Polytechnique<br>Laboratoire des Solides Irradies<br>Route de Saclay<br>F-91128 Palaiseau Cedex<br>FRANCE<br>Permanent Institute e mail      lucia.reining@polytechnique.fr      |             |  |
| 21. | <b>REUTER Karsten</b><br>Research Field : <b>THEORETICAL SURFACE SCIENCE</b><br>Research Topic : <b>MULTI-SCALE MODELING APPROACHES</b>  | GERMANY     | <b>CONFERENCE SPEAKER</b>                            |
|     | Permanent Institute:<br>Fritz-Haber-Institut Der Max-Planck-Gesellschaft<br>Department of Theory<br>Faradayweg 4-6<br>D-14195 Berlin<br>GERMANY<br>Permanent Institute e mail      reuter@FHI-Berlin.mpg.de    |             |  |

| No. | NAME and INSTITUTE  | Nationality       | Function                  |
|-----|---|-------------------|---------------------------|
| 22. | <b>RIGNANESE Gian-Marco</b><br>Research Field : <b>COMPUTATIONAL PHYSICS</b><br><br>Research Topic : <b>MANY-BODY PERTURBATION THEORY</b><br><br>Permanent Institute:<br>Universite Catholique de Louvain<br>Unite de Physico-Chimie et Physique des Materiaux<br>Batiment Boltzmann<br>Place Croix Du Sud 1<br>B-1348 Louvain La Neuve<br>BELGIUM<br>Permanent Institute e mail      gian-marco.rignanese@uclouvain.be | BELGIUM           | <b>CONFERENCE SPEAKER</b> |
| 23. | <b>SOLER Jose Maria</b><br>Research Field :<br><br>Research Topic :<br><br>Permanent Institute:<br>Universidad Autonoma de Madrid<br>Dep.To de Fisica Teorica de La Materia Condensada<br>Facultad de Ciencias<br>Ciudad Universitaria<br>Cantoblanco<br>E-28049 Madrid<br>SPAIN<br>Permanent Institute e mail      JOSE.SOLER@UAM.ES   | SPAIN             | <b>CONFERENCE SPEAKER</b> |
| 24. | <b>SON Young-Woo</b><br>Research Field :<br><br>Research Topic :<br><br>Permanent Institute:<br>Korea Institute for Advanced Study KIAS<br>School of Computational Sciences<br>87 Hoegiro<br>Dongdaemun-gu<br>Seoul 130-722<br>REPUBLIC OF KOREA<br>Permanent Institute e mail      hand@kias.re.kr   | REPUBLIC OF KOREA | <b>CONFERENCE SPEAKER</b> |

| No. | NAME and INSTITUTE  | Nationality   | Function                                      |
|-----|---|---|---|
| 25. | <b>STENUIT Geoffrey</b><br>Research Field : <b>COMPUTATIONAL PHYSICS</b><br><br>Research Topic : <b>MANY-BODY PERTURBATION THEORY</b>   | BELGIUM   | <b>CONFERENCE SPEAKER</b>                     |
|     |   | Present institute:<br>CNR-INFM Democritos<br>c/o SISSA<br>via Beirut 2-4<br>34014 Trieste<br>Italy<br>Present Institute e mail<br>Until when: | stenuit@sissa.it<br><br><b>31 August 2009</b> |
| 26. | <b>VAN VOORHIS Troy</b><br>Research Field : <b>THEORETICAL CHEMISTRY</b><br><br>Research Topic : <b>ELECTRONIC EXCITED STATES, ELECTRON TRANSFER</b>  | UNITED STATES OF AMERICA  | <b>CONFERENCE SPEAKER</b>                     |
|     | Permanent Institute:<br>Massachusetts Institute of Technology<br>Department of Chemistry<br>77 Massachusetts Avenue<br>MA 02139 Cambridge<br>UNITED STATES OF AMERICA<br>Permanent Institute e mail | tvan@mit.edu  |   |
| 27. | <b>ZETTL Alex</b><br>Research Field :<br><br>Research Topic :   | UNITED STATES OF AMERICA  | <b>CONFERENCE SPEAKER</b>                     |
|     | Permanent Institute:<br>University of California<br>Department of Physics<br>366 Le Conte Hall<br>Berkeley CA 94720-7300<br>UNITED STATES OF AMERICA<br>Permanent Institute e mail                  | azettl@physics.berkeley.edu,<br>geesqrd@berkeley.edu  |   |



| No.                | NAME and INSTITUTE  | Nationality                               | Function                |
|--------------------|---|---|-------------------------|
| <b>PARTICIPANT</b> |   | <b>Total number in this function: 203</b> |                         |
| 28.                | <b>ACHILLI Simona</b><br>Research Field : <b>THEORETICAL SURFACE PHYSICS</b><br><br>Research Topic : <b>SURFACES AB-INIT.ELECTR.PROP. DFT EMBEDD.APPROACH</b><br><br>Permanent Institute:<br>Universita' degli Studi di Milano Bicocca<br>Dip. Scienza dei Materiali<br>Via R. Cozzi 53<br>20125 Milano<br>ITALY<br>Permanent Institute e mail      simona.achilli@mater.unimib.it  | ITALY                                     | <b>PARTICIPANT</b>      |
| 29.                | <b>ADEBAYO Gboyega Augustine</b><br>Research Field :<br><br>Research Topic :<br><br>Permanent Institute:<br>University of Agriculture<br>Department of Physics<br>P.M.B. 2240<br>Abeokuta<br>Ogun State<br>NIGERIA<br>Permanent Institute e mail      adebayo@unaab.skannet.com,<br>adebayo@daad-alumni.de  | NIGERIA                                   | <b>JUNIOR ASSOCIATE</b> |
| 30.                | <b>AGUADO PUENTE Pablo</b><br>Research Field : <b>FIRST PRINCIPLES, FERROELECTRICS, 2DEG, SCREENING</b><br>Research Topic : <b>NEW PHENOMENA IN OXIDE INTERFACES</b><br><br>Permanent Institute:<br>Universidad de Cantabria<br>Ciencias de la Tierra y Fisica de la Materia Condensada<br>Avda. de Los Castros s/n<br>39005 Santander<br>SPAIN<br>Permanent Institute e mail      paguado@gmail.com,<br>pablo.aguado@unican.es | SPAIN                                     | <b>PARTICIPANT</b>      |

| No. | NAME and INSTITUTE  | Nationality              | Function                |
|-----|---|--------------------------|-------------------------|
| 31. | <b>AKBARZADEH Hadi</b><br>Research Field :<br><br>Research Topic :<br><br>Permanent Institute:<br>Isfahan University of Technology<br>Department of Physics<br>84156 Isfahan<br>ISLAMIC REPUBLIC OF IRAN<br>Permanent Institute e mail      akbarzad@cc.iut.ac.ir   | ISLAMIC REPUBLIC OF IRAN | <b>SENIOR ASSOCIATE</b> |
| 32. | <b>AL-KELSH Abdalla Mohamed</b><br>Research Field : <b>COND. MATTER, SOLID STATE, SOLAR ENERGY</b><br>Research Topic : <b>DFT DEFECTS, DIFFUSION, SOLAR ENERGY</b><br><br>Permanent Institute:<br>Al Fateh University<br>Faculty of Science<br>Department of Physics<br>P.O. Box 13102<br>Tripoli<br>LIBYAN ARAB JAMAHIRIYA<br>Permanent Institute e mail      alkesh@yahoo.com | LIBYAN ARAB JAMAHIRIYA   | <b>PARTICIPANT</b>      |
| 33. | <b>ALAM Md. Sahabul</b><br>Research Field : <b>MATERIAL SCIENCE, NANOSCIENCE</b><br><br>Research Topic : <b>NANO-MATERIALS CHARACTERIZATION BY SPM</b><br><br>Permanent Institute:<br>Dhaka University<br>Department of Physics<br>1000 Dhaka<br>BANGLADESH<br>Permanent Institute e mail      alam@univdhaka.edu   | BANGLADESH               | <b>PARTICIPANT</b>      |

| No. | NAME and INSTITUTE  | Nationality | Function           |
|-----|---|-------------|--------------------|
| 34. | <p><b>ALFE' Dario</b><br/>           Research Field : <b>CONDENSED MATTER PHYSICS</b><br/>           Research Topic : <b>ELECTRONIC STRUCTURE METHODS</b></p> <p>Permanent Institute:<br/>           University College London<br/>           Department of Earth Sciences<br/>           Gower Street<br/>           London WC1E CBT<br/>           UNITED KINGDOM<br/>           Permanent Institute e mail      d.alf@ucl.ac.uk</p>  | ITALY       | <b>PARTICIPANT</b> |
| 35. | <p><b>AMADON Bernard</b><br/>           Research Field : <b>ELECTRONIC STRUCTURE</b><br/>           Research Topic : <b>CORRELATIONS, ELECTRONIC EXCITATIONS, DFT</b></p> <p>Permanent Institute:<br/>           CEA, Département de Physique Théorique et Appliquée<br/>           Service de Physique de la Matière Condensée<br/>           BP 12<br/>           91680 Bruyeres Le Chatel<br/>           FRANCE<br/>           Permanent Institute e mail      bernard.amadon@cea.fr</p> | FRANCE      | <b>PARTICIPANT</b> |
| 36. | <p><b>ANDREUSSI Oliviero</b><br/>           Research Field : <b>COMPUTATIONAL MATERIAL SCIENCE</b><br/>           Research Topic : <b>IONIC LIQUID</b></p> <p>Permanent Institute:<br/>           Massachusetts Institute of Technology<br/>           77 Massachusetts Avenue<br/>           Cambridge MA 02139-4307<br/>           UNITED STATES OF AMERICA<br/>           Permanent Institute e mail      oliviero@mit.edu</p>   | ITALY       | <b>PARTICIPANT</b> |

| No. | NAME and INSTITUTE   | Nationality   | Function           |
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| 37. | <b>ANGIOLETTI-UBERTI Stefano</b><br>Research Field : <b>ALLOY THERMODYNAMICS &amp; KINETICS,ATOMISTIC MODELING</b><br>Research Topic : <b>INTERFACIAL FREE ENERGIES</b>  | ITALY   | <b>PARTICIPANT</b> |
|     |  | Present institute:<br>Imperial College of Science and Technology<br>Prince Consort Road<br>South Kensington<br>SW7 2AZ London<br>United Kingdom<br>Present Institute e mail      sangiole@imperial.ac.uk<br>Until when: <b>1 October 2010</b> |                    |
| 38. | <b>ARTACHO Emilio</b><br>Research Field : <b>CONDENSED MATTER PHYSICS</b><br>Research Topic : <b>CONDENSED MATTER PHYSICS</b>  | SPAIN   | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>University of Cambridge<br>Department of Earth Sciences<br>Downing Street<br>CB2 3EQ Cambridge<br>UNITED KINGDOM<br>Permanent Institute e mail      emilio@esc.cam.ac.uk   |   |                    |
| 39. | <b>ASLAM Farzana</b><br>Research Field : <b>LASER PHOTONICS AND PHOTONIC MATERIALS</b><br>Research Topic : <b>NANOPARTICLES AND PHOTONICS MATERIALS</b>  | PAKISTAN  | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>Coventry University<br>Department of Mathematics, Statistics and Engineering Sciences<br>Armstrong Siddeley Building<br>Coventry CV1 5FB<br>UNITED KINGDOM<br>Permanent Institute e mail      farzana.aslam@coventry.ac.uk,<br>farzana.aslam@gmail.com |   |                    |

| No. | NAME and INSTITUTE  | Nationality              | Function  |
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| 40. | <b>BAFTIZADEH BAGHAL Fahimeh</b><br>Research Field : <b>MOLECULAR DYNAMICS-BIOLOGICAL SYSTEMS-DFT THEORY</b><br>Research Topic : <b>STATISTICAL AND MOLECULAR BIOPHYSICS</b><br><br>Permanent Institute:<br>Ferdowsi University of Mashhad<br>Physics Department<br>School of Sciences<br>Mashhad 91775-1436<br>ISLAMIC REPUBLIC OF IRAN<br>Permanent Institute e mail      fbaftizadeh@yahoo.com | ISLAMIC REPUBLIC OF IRAN | <b>PARTICIPANT</b><br><br>Present institute:<br>S.I.S.S.A. - International School for Advanced Studies<br>Via Beirut 2-4<br>34014 Trieste<br>Italy<br><br>Present Institute e mail      fbafti@sissa.it<br>Until when: <b>31 October 2009</b> |
| 41. | <b>BARONI Stefano</b><br><br>Research Field :<br><br>Research Topic :<br><br>Permanent Institute:<br>SISSA & DEMOCRITOS National Simulation Center<br>Via Beirut 6<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      baroni@sissa.it   | ITALY                    | <b>SCIENTIFIC COMMITTEE MEMBER</b>  |
| 42. | <b>BARUSELLI Pier Paolo</b><br>Research Field : <b>THEORETICAL CONDENSED MATTER PHYSICS</b><br>Research Topic : <b>TRANSPORT IN NANOSYSTEMS, ELECTRONIC STRUCTURE</b><br><br>Permanent Institute:<br>S.I.S.S.A. - International School for Advanced Studies<br>Via Beirut 2-4<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      pierpaolobaruselli@libero.it                           | ITALY                    | <b>PARTICIPANT</b>  |

| <b>No.</b> | <b>NAME and INSTITUTE</b>   | <b>Nationality</b> | <b>Function</b>    |
|------------|---|--------------------|--------------------|
| 43.        | <b>BAUMEISTER Paul</b><br>Research Field : <b>MOLECULARDYNAMICS REALSPACE SURFACES BIOMOLECULES</b><br>Research Topic : <b>PAW METHOD</b><br><br>Permanent Institute:<br>Forschungszentrum Julich Gmbh<br>Institut für Festkörperforschung<br>Theorie 1<br>Leo-Brand-Strasse<br>D-52425 Julich<br>GERMANY<br>Permanent Institute e mail        p.baumeister@fz-juelich.de                               | GERMANY            | <b>PARTICIPANT</b> |
| 44.        | <b>BEDOYA MARTINEZ Olga Natalia</b><br>Research Field : <b>ELECTRONIC AND THERMODYNAMIC PROP. OF MATERIALS</b><br>Research Topic : <b>DFT AND THERMODYNAMIC PROPERTIES</b><br><br>Permanent Institute:<br>Institut de Ciencia de Materials de Barcelona (ICMAB)<br>C.S.I.C.<br>Campus Universitario de la UAB<br>E-08193 Bellaterra<br>SPAIN<br>Permanent Institute e mail        natalia@icmab.es      | COLOMBIA           | <b>PARTICIPANT</b> |
| 45.        | <b>BENNECER Badis</b><br>Research Field : <b>CONDENSED MATTER</b><br><br>Research Topic : <b>OPTICAL VIBRATIONAL PROPERTIES OF SEMICONDUCTORS</b><br><br>Permanent Institute:<br>University 08 May 1945 Guelma<br>Physics Laboratory<br>Department of Exact Sciences<br>P.O. Box 401<br>Guelma 24000<br>ALGERIA<br>Permanent Institute e mail        b_bennacer@hotmail.com,<br>bennecer@univ-guelma.dz | ALGERIA            | <b>PARTICIPANT</b> |

| No. | NAME and INSTITUTE   | Nationality | Function           |
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| 46. | <b>BERNASCONI Marco</b><br>Research Field : <b>AB-INITIO MOLECULAR DYNAMICS SIMULATIONS</b><br>Research Topic : <b>AMORPHOUS MATERIALS FOR MICROELECTR. AND PHOTONICS</b><br><br>Permanent Institute:<br>Universita' degli Studi di Milano Bicocca<br>Dip. Scienza dei Materiali<br>Via R. Cozzi 53<br>20125 Milano<br>ITALY<br>Permanent Institute e mail      marco.bernasconi@mater.unimib.it                     | ITALY       | <b>PARTICIPANT</b> |
| 47. | <b>BETRANHANDY Emmanuel</b><br>Research Field : <b>DFT, STRUCTURES, PHYSICAL PROPERTIES OF MATERIALS</b><br>Research Topic : <b>BORON CARBIDES, MECHANICAL PROPERTIES</b><br><br>Permanent Institute:<br>Ecole Polytechnique<br>Laboratoire des Solides Irradies<br>Route de Saclay<br>F-91128 Palaiseau Cedex<br>FRANCE<br>Permanent Institute e mail      emmanuel.betranhandy@polytechnique.edu                   | FRANCE      | <b>PARTICIPANT</b> |
| 48. | <b>BIDDAU Giulio</b><br>Research Field : <b>SURFACE CATALYSIS</b><br><br>Research Topic : <b>SURFACE INDUCED CYCLODEHYDROGENATION OF PAHS</b><br><br>Permanent Institute:<br>Universidad Autonoma de Madrid<br>Dep.To de Fisica Teorica de La Materia Condensada<br>Facultad de Ciencias<br>Ciudad Universitaria<br>Cantoblanco<br>E-28049 Madrid<br>SPAIN<br>Permanent Institute e mail      giulioenrico@gmail.com | ITALY       | <b>PARTICIPANT</b> |

| No. | NAME and INSTITUTE   | Nationality    | Function           |
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| 49. | <p><b>BINDER Felix</b></p> <p>Research Field : <b>SOLID STATES PHYSICS, DFT AND CAR-PARINELLO</b></p> <p>Research Topic : <b>SIMULATION OF SEMICONDUCTOR STRUCTURES</b></p> <p>Permanent Institute:</p> <p>Ecole Polytechnique Federale de Lausanne<br/> CSEA ITP SB EPFL<br/> Batiment PPH, Station 13<br/> 1015 Lausanne<br/> SWITZERLAND</p> <p>Permanent Institute e mail      janfelix.binder@epfl.ch</p> | GERMANY        | <b>PARTICIPANT</b> |
| 50. | <p><b>BINNIE Simon John</b></p> <p>Research Field : <b>DFT, DMC, QMC, SURFACE ENERGY</b></p> <p>Research Topic : <b>DFT, DMC SURFACE ENERGIES</b></p> <p>Permanent Institute:</p> <p>University College London<br/> Dept. Physics &amp; Astronomy<br/> Gower Street<br/> WC1E 6BT London<br/> UNITED KINGDOM</p> <p>Permanent Institute e mail      s.binnie@ucl.ac.uk</p>                                     | UNITED KINGDOM | <b>PARTICIPANT</b> |
| 51. | <p><b>BORGHI Giovanni</b></p> <p>Research Field : <b>CONDENSED MATTER</b></p> <p>Research Topic : <b>DENSITY FUNCTIONAL THEORY</b></p> <p>Permanent Institute:</p> <p>S.I.S.S.A. - International School for Advanced Studies<br/> Via Beirut 2-4<br/> 34014 Trieste<br/> ITALY</p> <p>Permanent Institute e mail      borghi@sissa.it</p>  | ITALY          | <b>PARTICIPANT</b> |



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| 52. | <b>BOWLER David Robert</b><br>Research Field : <b>O(N) DFT, SEMICONDUCTOR SURFACES, NANOWIRES</b><br>Research Topic : <b>O(N) DFT</b>   | UNITED KINGDOM | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>University College London<br>Dept. Physics & Astronomy<br>Gower Street<br>WC1E 6BT London<br>UNITED KINGDOM<br>Permanent Institute e mail      david.bowler@ucl.ac.uk                                   |                |                    |
| 53. | <b>BRAKO Radovan</b><br>Research Field : <b>SOLID STATE THEORY, DF CALCULATIONS</b><br>Research Topic : <b>GRAPHENE ON SURFACES, NON LOCAL CORRELATION</b>  | CROATIA        | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>Rudjer Boskovic Institute<br>Bijenicka Cesta 54<br>P.O. Box 180<br>HR-10002 Zagreb<br>CROATIA<br>Permanent Institute e mail      radovan@thphys.irb.hr  |                |                    |
| 54. | <b>BRANCOLINI Giorgia</b><br>Research Field : <b>ELECTRONIC PROPERTIES, DNA</b><br>Research Topic : <b>ELECTRONIC STRUCTURE OF METAL-MODIFIED DNA BP</b>  | ITALY          | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>INFM CNR S3 Centre<br>c/o Dipartimento di Fisica<br>Universita' di Modena e Reggio Emilia<br>Via Campi, 213/A<br>41100 Modena<br>ITALY<br>Permanent Institute e mail      giorgia.brancolini@unimore.it |                |                    |

| No. | NAME and INSTITUTE   | Nationality | Function           |
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| 55. | <b>BURNUS Tobias</b><br>Research Field : <b>ELECTR.STRUCTURE, COND.MATTER &amp; DOWN TO MOLECULES</b><br>Research Topic : <b>(TIME-DEPEND.) DFT, SPECTROSCOPY, MANY-BODY TECH.</b>   | GERMANY     | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>Universitat Zu Koln<br>II Physikalisches Institut<br>Zulpicher Str. 77<br>D-50937 Cologne<br>GERMANY<br>Permanent Institute e mail      burnus@net-b.de,<br>burnus@ph2.uni-koeln.de  |             |                    |
| 56. | <b>CALZOLARI Arrigo</b><br>Research Field :<br>Research Topic : <b>SURFACES</b>  | ITALY       | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>Universita' di Modena e Reggio Emilia<br>Center on Nanostructures & Biosystems at Surfaces<br>Department of Physics<br>Via Campi 213/A<br>41100 Modena<br>ITALY<br>Permanent Institute e mail      calzolari.arrigo@unimore.it |             |                    |
| 57. | <b>CAZORLA SILVA Claudio</b><br>Research Field : <b>MATERIALS, CONDENSED MATTER PHYICS</b><br>Research Topic : <b>HIGH PRESSURES AND TEMPERATURES</b>  | SPAIN       | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>University College London<br>Department of Physics & Astronomy<br>London Centre for Nanotechnology<br>17-19 Gordon Street<br>London WC1H 0AH<br>UNITED KINGDOM<br>Permanent Institute e mail      c.silva@ucl.ac.uk            |             |                    |

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| 58. | <b>COBIAN GONZALEZ Manuel</b><br>Research Field : <b>DFT "ELECTRONIC STRUCTURE" "MOLECULAR DYNAMICS"</b><br>Research Topic : <b>DENSITY FUNCTIONAL THEORY ELECTRONIC TRANSPORT</b><br><br>Permanent Institute:<br>Institut de Ciencia de Materials de Barcelona (ICMAB)<br>C.S.I.C.<br>Campus Universitario de la UAB<br>E-08193 Bellaterra<br>SPAIN<br>Permanent Institute e mail      cobian@icmab.es   | SPAIN       | <b>PARTICIPANT</b> |
| 59. | <b>COSTA Bismarck Vaz</b><br>Research Field : <b>SIMULATION: MONTE CARLO AND MOLECULAR DYNAMICS</b><br>Research Topic : <b>SURFACE AND SPIN DYNAMICS</b><br><br>Permanent Institute:<br>Universidade Federal de Minas Gerais,<br>Instituto de Ciencias Exactas<br>Departamento de Fisica<br>Laboratory for Simulation in Physics<br>Av. Antonio Carlos 6627<br>Pampulha<br>30123-970 Belo Horizonte<br>M.G.<br>BRAZIL<br>Permanent Institute e mail      bvc@fisica.ufmg.br | BRAZIL      | <b>PARTICIPANT</b> |
| 60. | <b>CUNY Jerome</b><br>Research Field : <b>SOLID-STATE NMR, CALCULATION OF NMR PARAMETERS</b><br>Research Topic : <b>APPLICATION OF GIPAW TO MO CLUSTER COMPOUNDS</b><br><br>Present institute:<br>Ecole Nationale Supérieure de Chimie<br>Avenue du General Leclerc<br>35700 Rennes<br>France<br>Present Institute e mail      jerome.cuny@ensc-rennes.fr<br>Until when: <b>1 October 2010</b>  | FRANCE      | <b>PARTICIPANT</b> |

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| 61. | <p><b>DA COSTA E SILVA Jusciane</b><br/>           Research Field : <b>MAGNETISM AND SPINTRONICS, NANOSCIENCE</b><br/>           Research Topic : <b>ELECTRONIC AND THERMAL TRANSPORT</b></p> <p>Permanent Institute:<br/>           Universidade Federal do Ceara<br/>           Departamento de Fisica<br/>           Campus do Pici<br/>           Caixa Postal 6030<br/>           60455-970 Fortaleza<br/>           Ceara<br/>           BRAZIL<br/>           Permanent Institute e mail      juscianec@gmail.com</p>   | BRAZIL      | <b>PARTICIPANT</b> |
| 62. | <p><b>DA PIEVE Fabiana</b><br/>           Research Field : <b>SPECTROSCOPY, STRONGLY CORRELATED MATERIALS</b><br/>           Research Topic : <b>ELECTRONIC EXCITATIONS,LATTICE DYNAMICS</b></p> <p>Permanent Institute:<br/>           Universite' Catholique de Louvain (UCL)<br/>           Unite' de Physico-Chimie et de Physique des Materiaux (PCPM)<br/>           Sciences des Materiaux et des Procedes (MAPR)<br/>           Batiment Boltzmann<br/>           1 Place Croix du Sud<br/>           1348 Louvain La Neuve<br/>           BELGIUM<br/>           Permanent Institute e mail      fabiana.dapieve@uclouvain.be</p> | ITALY       | <b>PARTICIPANT</b> |
| 63. | <p><b>DAL CORSO Andrea</b><br/>           Research Field : <b>SOLID STATE PHYSICS</b><br/>           Research Topic : <b>ELECTRONIC STRUCTURE THEORY</b></p> <p>Permanent Institute:<br/>           S.I.S.S.A. - International School for Advanced Studies<br/>           Via Beirut 2-4<br/>           34014 Trieste<br/>           ITALY<br/>           Permanent Institute e mail      dalcorso@sissa.it</p>  | ITALY       | <b>PARTICIPANT</b> |

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| 64. | <b>DE GIRONCOLI Stefano Maria</b><br>Research Field : <b>ELECTRONIC STRUCTURE</b><br><br>Research Topic : <b>VDW IN DFT, CATALYSIS, SURF.SCI., ELECTROCHEMISTRY</b><br><br>Permanent Institute:<br>SISSA & DEMOCRITOS National Simulation Center<br>Via Beirut 6<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      degironc@sissa.it  | ITALY  | <b>PARTICIPANT</b> |
| 65. | <b>DE PAIVA Rosangela</b><br>Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b><br>Research Topic : <b>METAL-SEMICONDUCTOR INTERFACES</b><br><br>Permanent Institute:<br>Laboratory MDM Materiali e Dispositivi per la Microelettronica INFM,<br>CNR<br>Via C. Olivetti, 2<br>20041 Agrate Brianza, Milano<br>ITALY<br>Permanent Institute e mail      alberto.debernardi@mdm.infm.it                  | BRAZIL   | <b>PARTICIPANT</b> |
|     |  | Present institute:<br>Universita' di Modena e Reggio Emilia<br>Center on Nanostructures & Biosystems at Surfaces<br>Department of Physics<br>Via Campi 213/A<br>41100 Modena<br>Italy<br>Present Institute e mail      rosangela.depaiva@unimore.it<br>Until when: <b>7 April 2009</b> |                    |
| 66. | <b>DEBERNARDI Alberto</b><br>Research Field : <b>DFT, PLANE-WAVE PSEUDOPOTENTIAL TECHNIQUES</b><br>Research Topic : <b>PHONON LIFETIME, HIGH-K OXIDES, BAND OFFSET</b><br><br>Permanent Institute:<br>Laboratory MDM Materiali e Dispositivi per la Microelettronica INFM,<br>CNR<br>Via C. Olivetti, 2<br>20041 Agrate Brianza, Milano<br>ITALY<br>Permanent Institute e mail      alberto.debernardi@mdm.infm.it | ITALY  | <b>PARTICIPANT</b> |

| No. | NAME and INSTITUTE  | Nationality | Function               |
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| 67. | <b>DEKURA Haruhiko</b><br>Research Field : <b>HIGH-PRESSURE PHYSICS, PHONON,<br/>SUPERCONDUCTIVITY</b><br>Research Topic : <b>SUPERCONDUCTIVITY IN BORON SYSTEMS</b><br><br>Permanent Institute:<br>the Institute of Scientific and Industrial Research<br>Osaka University<br>8-1 Mihogaoka<br>Ibaraki<br>567 Osaka<br>JAPAN<br>Permanent Institute e mail      dekura@cmp.sanken.osaka-u.ac.jp                        | JAPAN       | <b>PARTICIPANT</b>     |
|     |   |             | <b>30 January 2009</b> |
| 68. | <b>DIEGUEZ LOPEZ Oswaldo</b><br>Research Field : <b>ELECTRONIC STRUCTURE METHODS</b><br><br>Research Topic : <b>DENSITY FUNCTIONAL THEORY,<br/>FERROELECTRICS</b><br><br>Permanent Institute:<br>Institut de Ciencia de Materials de Barcelona (ICMAB)<br>C.S.I.C.<br>Campus Universitario de la UAB<br>E-08193 Bellaterra<br>SPAIN<br>Permanent Institute e mail      odiequez@icmab.es                                | SPAIN       | <b>PARTICIPANT</b>     |
| 69. | <b>DUGAN Nazim</b><br>Research Field : <b>QUANTUM MONTE CARLO METHODS GENETIC<br/>ALGORITHMS</b><br>Research Topic : <b>EXACT QUANTUM MONTE CARLO METHODS<br/>FERMION NODES</b><br><br>Permanent Institute:<br>Middle East Technical University<br>Department of Physics<br>Inonu Bul.<br>Cankaya<br>06531 Ankara<br>TURKEY<br>Permanent Institute e mail      ndugan@metu.edu.tr,<br>ndugan@photon.physics.metu.edu.tr | TURKEY      | <b>PARTICIPANT</b>     |

| No. | NAME and INSTITUTE  | Nationality | Function           |
|-----|---|-------------|--------------------|
| 70. | <b>EL HAJ HASSAN Fouad</b><br>Research Field : <b>PHYSICS OF CONDENSED MATTER</b><br><br>Research Topic : <b>DFT, LDA, FP-LAPW SEMICONDUCTORS</b><br><br>Permanent Institute:<br>Lebanese University<br>Faculty of Science I<br>LPM Laboratoire de Physique des Materiaux<br>El Hadath<br>Beirut<br>LEBANON<br>Permanent Institute e mail      hassan.f@ul.edu.lb                     | LEBANON     | <b>PARTICIPANT</b> |
| 71. | <b>ESHET Hagai</b><br>Research Field : <b>COMPUTATIONAL PHYSICS</b><br><br>Research Topic : <b>MOLECULAR DYNAMICS</b><br><br>Permanent Institute:<br>Computational Science Laboratory<br>Department of Chemistry & Applied Biosciences<br>ETH Zurich<br>USI Campus<br>Via Giuseppe Buffi 13<br>CH-6900 Lugano<br>SWITZERLAND<br>Permanent Institute e mail      hagai.eshet@gmail.com | ISRAEL      | <b>PARTICIPANT</b> |
| 72. | <b>FARNESI Matteo</b><br>Research Field : <b>SURFACE SCIENCE</b><br><br>Research Topic : <b>CATALYSIS</b><br><br>Permanent Institute:<br>S.I.S.S.A.<br>International School for Advanced Studies<br>Via Beirut 2-4<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      matteo.farnesi@gmail.com  | ITALY       | <b>PARTICIPANT</b> |

| <b>No.</b> | <b>NAME and INSTITUTE</b>   | <b>Nationality</b> | <b>Function</b>    |
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| 73.        | <b>FERRETTI Andrea</b><br>Research Field : <b>ELEC. AND TH. TRANSPORT, CORRELATIONS, METHODS</b><br>Research Topic : <b>HYBRID SYSTEMS, GW METHOD, WANNIER FUNCTIONS</b><br><br>Permanent Institute:<br>Universita' di Modena e Reggio Emilia<br>Center on Nanostructures & Biosystems at Surfaces<br>Department of Physics<br>Via Campi 213/A<br>41100 Modena<br>ITALY<br>Permanent Institute e mail      andrea.ferretti@unimore.it                             | ITALY              | <b>PARTICIPANT</b> |
| 74.        | <b>FOULKES William Matthew Colwyn</b><br>Research Field : <b>CONDENSED MATTER PHYSICS, MATERIALS PHYSICS</b><br>Research Topic : <b>ELECTRONIC STRUCTURE THEORY</b><br><br>Permanent Institute:<br>Imperial College London<br>Blackett Laboratory<br>Condensed Matter Theory Group<br>Department of Physics<br>Prince Consort Road<br>SW7 2AZ London<br>UNITED KINGDOM<br>Permanent Institute e mail      wmc.foulkes@imperial.ac.uk,<br>m.foulkes@imperial.ac.uk | UNITED KINGDOM     | <b>PARTICIPANT</b> |
| 75.        | <b>FRATESI Guido</b><br>Research Field : <b>THEORETICAL CONDENSED MATTER PHYSICS</b><br>Research Topic : <b>SURFACE ADSORPTION DIFFUSION AND SPECTROSCOPY</b><br><br>Permanent Institute:<br>Universita' degli Studi di Milano<br>Dipartimento di Fisica<br>Via Celoria, 16<br>20133 Milano<br>ITALY<br>Permanent Institute e mail      fratesi@mater.unimib.it   | ITALY              | <b>PARTICIPANT</b> |



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| 76.        | <b>GARCIA ARRIBAS Alberto</b><br>Research Field : <b>COMPUTATIONAL MATERIALS SCIENCE</b><br><br>Research Topic : <b>NEW METHODS</b><br><br>Permanent Institute:<br>Institut de Ciencia de Materials de Barcelona (ICMAB)<br>C.S.I.C.<br>Campus Universitario de la UAB<br>E-08193 Bellaterra<br>SPAIN<br>Permanent Institute e mail      albertog@icmab.es                             | SPAIN              | <b>PARTICIPANT</b> |
| 77.        | <b>GARCIA DE GURTUBAY Idoia</b><br>Research Field : <b>CONDENSED MATTER PHYSICS</b><br><br>Research Topic : <b>QUANTUM MONTE CARLO, DFT, ELECTRONIC STRUCTURE</b><br><br>Permanent Institute:<br>Universidad del Pais Vasco<br>Facultad de Ciencias<br>Dep. de La Materia Condensada<br>Apt. 644<br>48080 Bilbao<br>SPAIN<br>Permanent Institute e mail      idoia.gurtubay@ehu.es     | SPAIN              | <b>PARTICIPANT</b> |
| 78.        | <b>GARCIA GIL Sandra</b><br>Research Field : <b>CONDENSED MATTER, ELECTRONIC TRANSPORT, SURFACES</b><br>Research Topic : <b>DFT</b><br><br>Permanent Institute:<br>Institut de Ciencia de Materials de Barcelona (ICMAB)<br>C.S.I.C.<br>Campus Universitario de la UAB<br>E-08193 Bellaterra<br>SPAIN<br>Permanent Institute e mail      sandragil@gmail.com,<br>sandra.garcia@cin2.es | SPAIN              | <b>PARTICIPANT</b> |

| No. | NAME and INSTITUTE   | Nationality  | Function           |
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| 79. | <p><b>GELMAN Alexander</b></p> <p>Research Field : <b>QUANTUM OPTICS, QUANTUM INFORMATION, SQUEEZED LIGHT</b></p> <p>Research Topic : <b>QUANTUM MEMORY, QUANTUM NOISE, ENTANGLED STATES</b></p> <p>Permanent Institute:</p> <p>Institute of Applied Physics<br/> Russian Academy of Sciences<br/> 46 Ulyanov Street<br/> 603095 Nizhny Novgorod<br/> RUSSIAN FEDERATION</p> <p>Permanent Institute e mail      <a href="mailto:gelman@appl.sci-nnov.ru">gelman@appl.sci-nnov.ru</a></p> | RUSSIAN FEDERATION   | <b>PARTICIPANT</b> |
| 80. | <p><b>GIACOMAZZI Luigi</b></p> <p>Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b></p> <p>Research Topic : <b>VIBRATIONAL SPECTRA OF GLASSES AND CRYSTALS</b></p> <p>Permanent Institute:</p> <p>CNR-INFM Democritos<br/> c/o SISSA<br/> via Beirut 2-4<br/> 34014 Trieste<br/> ITALY</p>  | ITALY  | <b>PARTICIPANT</b> |
|     |  | <p>Present institute:</p> <p>The Abdus Salam International Centre for Theoretical Physics<br/> Condensed Matter Section<br/> Strada Costiera 11<br/> 34014 Trieste<br/> Italy</p> <p>Present Institute e mail      <a href="mailto:giacomaz@ictp.it">giacomaz@ictp.it</a></p> <p>Until when:                      <b>14 March 2010</b></p> |                    |
| 81. | <p><b>GIANNOZZI Paolo</b></p> <p>Research Field : <b>CONDENSED MATTER PHYSICS</b></p> <p>Research Topic : <b>CARBON NANOSTRUCTURES</b></p> <p>Permanent Institute:</p> <p>Universita' di Udine<br/> Dipartimento di Fisica<br/> via delle Scienze 208<br/> 33100 Udine<br/> ITALY</p> <p>Permanent Institute e mail      <a href="mailto:p.giannozzi@fisica.uniud.it">p.giannozzi@fisica.uniud.it</a></p>  | ITALY  | <b>PARTICIPANT</b> |

| No. | NAME and INSTITUTE   | Nationality | Function           |
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| 82. | <b>GIDOPOULOS Nikitas Ioannis</b><br>Research Field : <b>THEORETICAL AND COMPUTATIONAL PHYSICS<br/>CHEMISTRY</b><br>Research Topic : <b>CONDENSED MATTER ATOM MOLECULAR<br/>NEUTRON SCATTERING</b><br><br>Permanent Institute:<br>ISIS Facility<br>Rutherford Appleton Laboratory<br>Chilton<br>Didcot<br>OX11 0QX Oxon<br>UNITED KINGDOM<br>Permanent Institute e mail      N.Gidopoulos@rl.ac.uk           | GREECE      | <b>PARTICIPANT</b> |
| 83. | <b>GIL REBAZA Arles Victor</b><br>Research Field : <b>PHYSIC OF SOLID STATE</b><br><br>Research Topic : <b>ELECTRONIC STRUCTURE, MAGNETIC<br/>PROPERTIES</b><br><br>Permanent Institute:<br>Universidad Nacional De La Plata<br>Facultad De Ciencias Exactas<br>Departamento de Fisica<br>Calle 49 y 115<br>1900 CC 67<br>La Plata<br>ARGENTINA<br>Permanent Institute e mail      arlesv@fisica.unlp.edu.ar | PERU        | <b>PARTICIPANT</b> |
| 84. | <b>GIUSTINO Feliciano</b><br>Research Field : <b>COMPUTATIONAL MATERIALS SCIENCE</b><br><br>Research Topic : <b>FIRST-PRINCIPLES MATERIALS MODELING</b><br><br>Permanent Institute:<br>University of Oxford<br>Department of Materials<br>Parks Road<br>OX1 3PH Oxford<br>UNITED KINGDOM<br>Permanent Institute e mail      feliciano.giustino@materials.ox.ac.uk  | ITALY       | <b>PARTICIPANT</b> |

| No. | NAME and INSTITUTE  | Nationality                | Function           |
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| 85. | <b>GONG Xin-gao</b><br>Research Field : <b>CONDENSED MATTER</b><br>Research Topic :<br><br>Permanent Institute:<br>Fudan University<br>Department of Physics<br>220 Handan Road<br>200433 Shanghai<br>PEOPLE'S REPUBLIC OF CHINA<br>Permanent Institute e mail      xggong@fudan.edu.cn   | PEOPLE'S REPUBLIC OF CHINA | <b>PARTICIPANT</b> |
| 86. | <b>GONZALEZ HERNANDEZ Rafael Julian</b><br>Research Field : <b>DENSITY-FUNCTIONAL THEORY BEYOND LDA</b><br>Research Topic : <b>STUDY OF MAGNETIC SEMICONDUCTORS</b><br><br>Permanent Institute:<br>Universidad Nacional de Colombia<br>Facultad de Ciencias<br>Departamento de Fisica<br>Apartado Aereo 5997<br>Cra.30, Cll. 45<br>Ciudad Universitaria<br>Bogota<br>COLOMBIA<br>Permanent Institute e mail      rgonzalezh@unal.edu.co,<br>rafaelgonzalezh@gmail.com | COLOMBIA                   | <b>PARTICIPANT</b> |
| 87. | <b>GONZALEZ VAZQUEZ Otto Emiliano</b><br>Research Field : <b>COMPUTATIONAL PHYSICS IN CONDENSED MATTER</b><br>Research Topic : <b>ABINITIO CALCULATION, MULTIFERROICS</b><br><br>Permanent Institute:<br>Institut de Ciencia de Materials de Barcelona (ICMAB)<br>C.S.I.C.<br>Campus Universitario de la UAB<br>E-08193 Bellaterra<br>SPAIN<br>Permanent Institute e mail      otto@icmab.es  | CUBA                       | <b>PARTICIPANT</b> |

| No. | NAME and INSTITUTE  | Nationality | Function           |
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| 88. | <b>GRAU CRESPO Ricardo</b><br>Research Field : <b>DFT, STATISTICAL MECHANICS, MATERIALS, SURFACES</b><br>Research Topic : <b>DFT MODELLING OF SITE-DISORDERED MATERIALS</b><br><br>Permanent Institute:<br>University College London<br>Department of Chemistry<br>Christopher Ingold Laboratories<br>20 Gordon Street<br>WC1H 0AJ London<br>UNITED KINGDOM<br>Permanent Institute e mail      rgrauc@gmail.com | CUBA        | <b>PARTICIPANT</b> |
| 89. | <b>GREULING Andreas</b><br>Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b><br><br>Research Topic : <b>ELECTRONIC STRUCTURE OF TiO2</b><br><br>Permanent Institute:<br>Universitat Osnabrueck<br>Fachbereich Physik<br>Barbarastrasse 7<br>D-49069 Osnabrueck<br>GERMANY<br>Permanent Institute e mail      agreulin@uos.de   | GERMANY     | <b>PARTICIPANT</b> |
| 90. | <b>GUEORGUIEV Gueorgui Kostov</b><br>Research Field : <b>AB INITIO CALCULATIONS, DFT, MOLECULAR DYNAMICS</b><br>Research Topic : <b>CLUSTER-ASSEMBLED, FULLERENE-LIKE MATERIALS</b><br><br>Permanent Institute:<br>Linkoping University<br>Department of Physics, IFM<br>58183 Linkoping<br>SWEDEN<br>Permanent Institute e mail      gekos@ifm.liu.se  | BULGARIA    | <b>PARTICIPANT</b> |

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|-----|--|-------------|--------------------|
| 91. | <b>GUPTA Dinesh Chandra</b><br>Research Field : <b>MATERIAL SCIENCE BAND STRUCTURE,<br/> PHASE TRANSITION</b><br>Research Topic : <b>BANDS IN SOLID, NANO UNDER PRESSURE,<br/> TEMPERATURE</b><br><br>Permanent Institute:<br>Jiwaji University<br>School of Studies In Physics<br>474 011 (M.P.) Gwalior<br>INDIA<br>Permanent Institute e mail      soszix@yahoo.co.in                     | INDIA       | <b>PARTICIPANT</b> |
| 92. | <b>GUPTA Sanjeev Kumar</b><br>Research Field : <b>VIBRATIONAL PROPERTIES OF<br/> NANOPARTICLES</b><br>Research Topic : <b>DENSITY FUNCTIONAL CALCULATION OF<br/> NANOSTRUCTURES</b><br><br>Permanent Institute:<br>University of Bhavnagar<br>Department of Physics<br>364002 Bhavnagar<br>INDIA<br>Permanent Institute e mail      sanjeev0302@rediffmail.com,<br>skgupta.physics@gmail.com | INDIA       | <b>PARTICIPANT</b> |
| 93. | <b>HAMDI Ilyes</b><br>Research Field : <b>AB-INITIO TOTAL ENERGY CALCULATIONS</b><br><br>Research Topic : <b>THERMAL PROPERTIES OF SEMICONDUCTORS</b><br><br>Permanent Institute:<br>University of Tunis<br>Faculty of Sciences<br>Dept. of Physics<br>2092 EL MANAR Tunis<br>TUNISIA<br>Permanent Institute e mail      ilyeshamdi@yahoo.fr   | TUNISIA     | <b>PARTICIPANT</b> |

| No. | NAME and INSTITUTE   | Nationality    | Function           |
|-----|--|----------------|--------------------|
| 94. | <b>HARL Judith</b><br>Research Field : <b>RPA CORRELATION ENERGIES, OPTICAL SPECTRA</b><br>Research Topic : <b>RARE GAS SOLIDS, RPA ATOMIZATION ENERGIES</b>   | AUSTRIA        | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>University of Vienna<br>Institute For Material Physics<br>Sensengasse 8/12<br>1090 Vienna<br>AUSTRIA<br>Permanent Institute e mail <a href="mailto:judith.harl@univie.ac.at">judith.harl@univie.ac.at</a>    |                |                    |
| 95. | <b>HASNIP Philip James</b><br>Research Field : <b>ELECTRONIC STRUCTURE</b><br>Research Topic : <b>DENSITY FUNCTIONAL THEORY, ESPECIALLY FOR METALS</b>   | UNITED KINGDOM | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>University of York<br>Department of Physics<br>Heslington YO10 5DD<br>UNITED KINGDOM<br>Permanent Institute e mail <a href="mailto:pjh503@york.ac.uk">pjh503@york.ac.uk</a>                                  |                |                    |
| 96. | <b>HAYNES Peter David</b><br>Research Field : <b>FIRST-PRINCIPLES ELECTRONIC STRUCTURE METHODS</b><br>Research Topic : <b>LINEAR SCALING DENSITY-FUNCTIONAL THEORY</b>   | UNITED KINGDOM | <b>PARTICIPANT</b> |
|     | Permanent Institute:<br>Imperial College London<br>Department of Materials<br>Exhibition Road<br>London SW7 2AZ<br>UNITED KINGDOM<br>Permanent Institute e mail <a href="mailto:p.haynes@imperial.ac.uk">p.haynes@imperial.ac.uk</a> |                |                    |

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| 97. | <p><b>HE Lixin</b></p> <p>Research Field : <b>O(N) METHODS, QUANTUM DOTS, MULTIFERROICS</b></p> <p>Research Topic : <b>SPIN-LATTICE COUPLING IN MULTIFERROICS</b></p> <p>Permanent Institute:</p> <p>University of Science and Technology of China<br/> Key Laboratory of Quantum Information<br/> 96 Jinzhai Rd<br/> Hefei 230026<br/> Anhui<br/> PEOPLE'S REPUBLIC OF CHINA<br/> Permanent Institute e mail helx@ustc.edu.cn</p> | PEOPLE'S REPUBLIC OF CHINA   | <b>PARTICIPANT</b> |
| 98. | <p><b>HERNANDEZ Eduardo Robert Rafael</b></p> <p>Research Field : <b>MOLECULAR DYNAMICS, ELECTRONIC STRUCTURE</b></p> <p>Research Topic : <b>COEXISTENCE OF PHASES; ELECTRONIC STRUCTURE</b></p> <p>Permanent Institute:</p> <p>Institut de Ciencia de Materials de Barcelona (ICMAB)<br/> C.S.I.C.<br/> Campus Universitario de la UAB<br/> E-08193 Bellaterra<br/> SPAIN<br/> Permanent Institute e mail ehe@icmab.es</p>        | UNITED KINGDOM   | <b>PARTICIPANT</b> |
| 99. | <p><b>HINE Nicholas Daniel Mark</b></p> <p>Research Field : <b>DFT, QMC, DEFECTS</b></p> <p>Research Topic : <b>LINEAR-SCALING DFT, METAL OXIDES, PEROVSKITES</b></p>  | UNITED KINGDOM   | <b>PARTICIPANT</b> |
|     |  | <p>Present institute:</p> <p>Imperial College London<br/> Department of Materials<br/> Exhibition Road<br/> London SW7 2AZ<br/> United Kingdom<br/> Present Institute e mail nicholas.hine@imperial.ac.uk<br/> Until when: <b>1 April 2009</b></p> |                    |



| No.  | NAME and INSTITUTE   | Nationality       | Function                           |
|------|--|-------------------|------------------------------------|
| 100. | <b>HUG Gilles</b><br>Research Field : <b>EELS, XAFS, PHASE DIAGRAMS, TRANSPORT PROPERTIES</b><br>Research Topic : <b>METALS, CARBIDES, MAX PHASES, CHALCOPYRITES</b><br><br>Permanent Institute:<br>ONERA<br>The French Aerospace Lab<br>BP 72 - 29 avenue de la Division Leclerc<br>92322 Chatillon<br>FRANCE<br>Permanent Institute e mail      gilles.hug@onera.fr        | FRANCE            | <b>PARTICIPANT</b>                 |
| 101. | <b>IAZZI Mauro</b><br>Research Field : <b>CONDENSED MATTER</b><br><br>Research Topic : <b>ELECTRONIC TRANSPORT PROPERTIES AND CORRELATION</b><br><br>Permanent Institute:<br>S.I.S.S.A. - International School for Advanced Studies<br>Via Beirut 2-4<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      iazzi@sissa.it  | ITALY             | <b>PARTICIPANT</b>                 |
| 102. | <b>IHM Jisoon</b><br>Research Field : <b>CONDENSED MATTER THEORETICAL PHYSICS</b><br>Research Topic : <b>CARBON NANOTUBES, HYDROGEN STORAGE MATERIALS</b><br><br>Permanent Institute:<br>Seoul National University<br>Department of Physics<br>San 56-1<br>Shillim-Dong<br>Kwanak-Gu<br>151 747 Seoul<br>REPUBLIC OF KOREA<br>Permanent Institute e mail      jihm@snu.ac.kr | REPUBLIC OF KOREA | <b>SCIENTIFIC COMMITTEE MEMBER</b> |

| No.  | NAME and INSTITUTE   | Nationality | Function           |
|------|--|-------------|--------------------|
| 103. | <b>INIGUEZ GONZALEZ Jorge</b><br>Research Field : <b>FIRST-PRINCIPLES SIMULATIONS, MATERIALS SCIENCE</b><br>Research Topic : <b>NANOSTRUCTURED MULTIFUNCTIONAL MATERIALS</b>                               | SPAIN       | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Institut de Ciencia de Materials de Barcelona - CSIC<br>Campus de La U.A.B.<br>Bellaterra<br>08193 Barcelona<br>SPAIN<br>Permanent Institute e mail      jiniguez@icmab.es         |             |                    |
| 104. | <b>IORI Federico</b><br>Research Field : <b>STRONG CORRELATION, SPECTROSCOPIES, OPTICS</b><br>Research Topic : <b>SI NANOSTRUCTURES, VXOY OPTOELECTRONIC PROPERTIES</b>                                    | ITALY       | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Ecole Polytechnique<br>Laboratoire des Solides Irradies<br>Route de Saclay<br>F-91128 Palaiseau Cedex<br>FRANCE<br>Permanent Institute e mail      federico.iori@polytechnique.edu |             |                    |
| 105. | <b>JAKUBAS Pawel</b><br>Research Field : <b>NANOSCIENCE, SPINTRONICS, DFT</b><br>Research Topic : <b>DEFECT PHYSICS IN II-VIS AND III-VS</b>   | POLAND      | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Polish Academy of Sciences<br>Institute For Theoretical Physics<br>Al. Lotnikow 32/46<br>O2-668 Warsaw<br>POLAND<br>Permanent Institute e mail      jakubas@ifpan.edu.pl           |             |                    |

| No.  | NAME and INSTITUTE   | Nationality | Function           |
|------|--|-------------|--------------------|
| 106. | <b>KHALIULLIN Rustam</b><br>Research Field : <b>ELECTRONIC STRUCTURE, STATISTICAL MECHANICS</b><br>Research Topic : <b>SOLID STATE, PHASE TRANSITIONS</b>  | BELARUS     | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>ETH Zurich<br>Department of Chemistry and Applied Biosciences<br>USI Campus<br>Via Buffi, 13<br>6900 Lugano<br>SWITZERLAND<br>Permanent Institute e mail      rustam@berkeley.edu,<br>rustam@phys.chem.ethz.ch |             |                    |
| 107. | <b>KHOMYAKOV Petr Alexandrovich</b><br>Research Field : <b>CONDENSED MATTER AND COMPUTATIONAL PHYSICS</b><br>Research Topic : <b>DFT, TRANSPORT THROUGH NANOWIRES, GRAPHENE</b>  | BELARUS     | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>University of Twente<br>Computational Materials Science<br>Faculty of Science and Technology<br>P.O. Box 217<br>7500 AE Enschede<br>NETHERLANDS<br>Permanent Institute e mail      p.khomyakov@tnw.utwente.nl  |             |                    |
| 108. | <b>KIRIN Davor</b><br>Research Field : <b>RAMAN SPECTROSCOPY, LATTICE DYNAMICS CALCULATIONS</b><br>Research Topic : <b>DFT CALC.OF CRYSTAL PROPERTIES AT HIGH PRESSURES</b>  | CROATIA     | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Rudjer Boskovic Institute<br>Bijenicka Cesta 54<br>P.O. Box 180<br>HR-10002 Zagreb<br>CROATIA<br>Permanent Institute e mail      Davor.Kirin@irb.hr  |             |                    |

| No.  | NAME and INSTITUTE   | Nationality     | Function                           |
|------|--|-----------------|------------------------------------|
| 109. | <b>KOCH Erik</b><br><br>Research Field : <b>CONDENSED MATTER PHYSICS</b><br><br>Research Topic : <b>ELECTRONIC STRUCTURE, STRONG CORRELATIONS</b><br><br>Permanent Institute:<br>Forschungszentrum Julich Gmbh<br>Institut fur Festkorperforschung<br>Theorie 1<br>Leo-Brand-Strasse<br>D-52425 Julich<br>GERMANY<br>Permanent Institute e mail      e.koch@fz-juelich.de  | GERMANY         | <b>SCIENTIFIC COMMITTEE MEMBER</b> |
| 110. | <b>KOHANOFF Jorge Jose</b><br><br>Research Field : <b>CONDENSED MATTER PHYSICS</b><br><br>Research Topic : <b>ELECTRONIC STRUCTURE. COMPUTATIONAL METHODS</b><br><br>Permanent Institute:<br>The Queen's University of Belfast<br>School of Mathematics and Physics<br>Atomistic Simulation Group<br>Northern Ireland<br>BT7 1NN Belfast<br>UNITED KINGDOM<br>Permanent Institute e mail      j.kohanoff@qub.ac.uk | UNITED KINGDOM  | <b>PARTICIPANT</b>                 |
| 111. | <b>KORYTAR Richard</b><br><br>Research Field : <b>MANY-BODY TECHN. FOR NANOSCIENCE, ELEC. CORREL</b><br><br>Research Topic : <b>SIM. OF KONDO EFFECT IN STM OF ADSORBATES</b><br><br>Permanent Institute:<br>Institut de Ciencia de Materials de Barcelona (ICMAB)<br>C.S.I.C.<br>Campus Universitario de la UAB<br>E-08193 Bellaterra<br>SPAIN<br>Permanent Institute e mail      rk21419@decef.elf.stuba.sk      | SLOVAK REPUBLIC | <b>PARTICIPANT</b>                 |

| No.  | NAME and INSTITUTE   | Nationality | Function           |
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| 112. | <p><b>KOTAKOSKI Jani</b><br/>           Research Field : <b>DFT, MD, MC</b></p> <p>Research Topic : <b>FREE ENERGY CALCULATIONS OF SOLID NITROGEN</b></p> <p>Permanent Institute:<br/>           Technische Universitat Darmstadt<br/>           FB Material und Geowissenschaften<br/>           Fachgebiet Strukturforschung<br/>           Petersenstr. 23<br/>           D-64287 Darmstadt<br/>           GERMANY<br/>           Permanent Institute e mail      jani.kotakoski@iki.fi</p> | FINLAND     | <b>PARTICIPANT</b> |
| 113. | <p><b>KSHIRSAGAR Anjali</b><br/>           Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b></p> <p>Research Topic : <b>PURE AND DOPED II-VI SEMICONDUCTOR CLUSTERS</b></p> <p>Permanent Institute:<br/>           University of Pune<br/>           Department of Physics<br/>           Ganeshkhind<br/>           411 007 Pune<br/>           Maharashtra<br/>           INDIA<br/>           Permanent Institute e mail      ANJALI@PHYSICS.UNIPUNE.ERNET.INDIA</p>           | INDIA       | <b>PARTICIPANT</b> |
| 114. | <p><b>KUNC Karel</b><br/>           Research Field : <b>COMPUTATIONAL PHYSICS</b></p> <p>Research Topic : <b>SEMICONDUCTOR OVERLAYERS</b></p> <p>Permanent Institute:<br/>           Universite' de Paris VI Pierre et Marie Curie<br/>           Institut des Nanosciences de Paris<br/>           UMR et CNRS<br/>           140, rue de Lourmel<br/>           75015 Paris<br/>           FRANCE<br/>           Permanent Institute e mail      karel.kunc@upmc.fr</p>                      | FRANCE      | <b>PARTICIPANT</b> |

| No.  | NAME and INSTITUTE  | Nationality | Function           |
|------|---|-------------|--------------------|
| 115. | <p><b>LAI O Alessandro</b><br/>           Research Field : <b>MOLECULAR SIMULATIONS</b><br/>           Research Topic : <b>RARE EVENTS TECHNIQUES</b></p> <p>Permanent Institute:<br/>           S.I.S.S.A.<br/>           International School for Advanced Studies<br/>           Via Beirut 2-4<br/>           34014 Trieste<br/>           ITALY<br/>           Permanent Institute e mail      laio@sissa.it</p>   | ITALY       | <b>PARTICIPANT</b> |
| 116. | <p><b>LANI Giovanna</b><br/>           Research Field : <b>MANY BODY PERTURBATION THEORY</b><br/>           Research Topic : <b>BEYOND THE GWA FOR STRONGLY CORRELATED SYSTEMS</b></p> <p>Permanent Institute:<br/>           Ecole Polytechnique<br/>           Laboratoire des Solides Irradies<br/>           Route de Saclay<br/>           F-91128 Palaiseau Cedex<br/>           FRANCE<br/>           Permanent Institute e mail      giovanna.lani@polytechnique.edu</p>          | ITALY       | <b>PARTICIPANT</b> |
| 117. | <p><b>LATHIOTAKIS Nektarios</b><br/>           Research Field : <b>DFT, STRONGLY CORRELATED SYSTEMS</b><br/>           Research Topic : <b>DENSITY MATRIX FUNCTIONAL THEORY</b></p> <p>Permanent Institute:<br/>           National Hellenic Research Foundation<br/>           Theoretical and Physical Chemistry Institute<br/>           48 Vas. Constantinou Ave.<br/>           11635 Athens<br/>           GREECE<br/>           Permanent Institute e mail      lathiot@eie.gr</p> | GREECE      | <b>PARTICIPANT</b> |

| No.  | NAME and INSTITUTE   | Nationality  | Function                |
|------|--|--|-------------------------|
| 118. | <p><b>LAZIC Predrag</b><br/>           Research Field : <b>DFT, ELECTRONIC STRUCTURE</b></p> <p>Research Topic : <b>NONLOCAL CORRELATIONS, VAN DER WAALS INTERACTION</b></p> <p>Permanent Institute:<br/>           Rudjer Boskovic Institute<br/>           Division of Theoretical Physics<br/>           Bijenicka Cesta 54<br/>           P.O. Box 180<br/>           10002 Zagreb<br/>           CROATIA<br/>           Permanent Institute e mail      plazic@thphys.irb.hr</p>              | CROATIA  | <b>PARTICIPANT</b>      |
|      |  | Present institute:<br>Forschungszentrum Julich GmbH<br>Institut fur Festkorperforschung (IFF)<br>D-52425 Julich<br>Germany |                         |
|      |  | Until when:  | <b>31 December 2009</b> |
| 119. | <p><b>LEE Mal-Soon</b><br/>           Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b></p> <p>Research Topic :</p> <p>Permanent Institute:<br/>           Michigan State University<br/>           Department of Physics<br/>           4208 BPS Bldg.<br/>           MI 48824 East Lansing<br/>           UNITED STATES OF AMERICA<br/>           Permanent Institute e mail      mslee@pa.msu.edu</p>  | REPUBLIC OF KOREA  | <b>PARTICIPANT</b>      |
| 120. | <p><b>LEONOV Ivan</b><br/>           Research Field : <b>STRONGLY CORRELATED ELECTRON SYSTEMS</b></p> <p>Research Topic : <b>STRUCTURAL RELAXATION IN PM CORRELATED SYSTEMS</b></p> <p>Permanent Institute:<br/>           Universitat Augsburg<br/>           Theoretische Physik III<br/>           EKM Elektronische Korrelationen und Magnetismus<br/>           D-86135 Augsburg<br/>           GERMANY<br/>           Permanent Institute e mail      ivan.leonov@physik.uni-augsburg.de</p> | RUSSIAN FEDERATION   | <b>PARTICIPANT</b>      |

| No.  | NAME and INSTITUTE   | Nationality                   | Function  |
|------|--|-------------------------------|---|
| 121. | <b>LI Yanli</b><br><br>Research Field : <b>ELECTROCHEMICAL FIELD, MAGNETISM</b><br><br>Research Topic : <b>FIRST-PRINCIPLES</b><br><br><br><br><br><br><br><br><br><br>liyanli128@163.com  | PEOPLE'S REPUBLIC OF<br>CHINA | <b>PARTICIPANT</b><br><br><br><br><br><br><br><br><br><br>Present institute:<br>CERMICS, ENPC<br>Universite' Paris Est<br>6 et 8, Avenue Blaise Pascal<br>Cite' Descartes<br>Champs sur Marne<br>F-77455 Marne La Vallee Cedex 2<br>France<br><br>Until when: <b>1 January 2010</b> |
| 122. | <b>LOPEZ PEREZ Jorge</b><br><br>Research Field : <b>MATERIAL SCIENCE</b><br><br>Research Topic : <b>AB-INITIO FERROELECTRICS</b><br><br><br><br><br>Permanent Institute:<br>Institut de Ciencia de Materials de Barcelona (ICMAB)<br>C.S.I.C.<br>Campus Universitario de la UAB<br>E-08193 Bellaterra<br>SPAIN<br>Permanent Institute e mail <b>jjp@icmab.es</b>   | SPAIN                         | <b>PARTICIPANT</b>  |
| 123. | <b>LOUIE Steven Gwon Sheng</b><br><br>Research Field : <b>CONDENSED MATTER PHYSICS AND NANOSCIENCE</b><br><br>Research Topic : <b>ELECTRONIC PROPERTIES OF SOLIDS AND NANOSTRUCTURES</b><br><br><br><br>Permanent Institute:<br>University of California<br>Department of Physics<br>366 Le Conte Hall<br>Berkeley CA 94720-7300<br>UNITED STATES OF AMERICA<br>Permanent Institute e mail <b>sglouie@berkeley.edu</b> | UNITED STATES OF AMERICA      | <b>SCIENTIFIC COMMITTEE MEMBER</b>  |



| No.  | NAME and INSTITUTE  | Nationality                | Function           |
|------|---|----------------------------|--------------------|
| 124. | <p><b>LUKACEVIC Igor</b></p> <p>Research Field : <b>DFT, DFPT, TDDFT, CONDENSED MATTER, SPECTROSCOPY</b></p> <p>Research Topic : <b>CALCULATIONS OF HIGH-PRESSURE PHASE TRANSITIONS</b></p> <p>Permanent Institute:</p> <p>University of J. J. Strossmayer<br/> Department of Physics<br/> Trg Ljudevita Gaja 6,<br/> 31000 Osijek<br/> CROATIA</p> <p>Permanent Institute e mail      ilukacevic@fizika.unios.hr</p>         | CROATIA                    | <b>PARTICIPANT</b> |
| 125. | <p><b>M'PASSI-MABIALA Bernard</b></p> <p>Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b></p> <p>Research Topic : <b>ELECTRONIC STRUCTURE OF NANOSTRUCTURES</b></p> <p>Permanent Institute:</p> <p>Universite Marien Ngouabi<br/> Faculte des Sciences<br/> Departement de Physique<br/> B.P. 69<br/> Brazzaville<br/> PEOPLE'S REPUBLIC OF CONGO</p> <p>Permanent Institute e mail      mpassi_b@yahoo.com</p> | PEOPLE'S REPUBLIC OF CONGO | <b>PARTICIPANT</b> |
| 126. | <p><b>MA Yanming</b></p> <p>Research Field : <b>HIGH PRESSURE; SUPERHARD MATERIALS</b></p> <p>Research Topic : <b>HIGH PRESSURE STRUCTURE AND SUPERCONDUCTIVITY.</b></p> <p>Permanent Institute:</p> <p>Jilin University<br/> State Key Laboratory For Superhard Material<br/> 2699 Qianjin Road<br/> 130012 Changchun<br/> PEOPLE'S REPUBLIC OF CHINA</p> <p>Permanent Institute e mail      mym@jlu.edu.cn</p>              | PEOPLE'S REPUBLIC OF CHINA | <b>PARTICIPANT</b> |

| No.  | NAME and INSTITUTE   | Nationality                   | Function           |
|------|--|-------------------------------|--------------------|
| 127. | <b>MA Yuchen</b><br><br>Research Field : <b>DENSITY-FUNCTIONAL THEORY BEYOND LDA</b><br><br>Research Topic : <b>MANY-BODY TECHNIQUES FOR REAL MATERIALS</b><br><br>Permanent Institute:<br>Universitat Osnabrueck<br>Fachbereich Physik<br>Barbarastrasse 7<br>D-49069 Osnabrueck<br>GERMANY<br>Permanent Institute e mail      yuma@uos.de  | PEOPLE'S REPUBLIC OF<br>CHINA | <b>PARTICIPANT</b> |
| 128. | <b>MACHADO CHARRY Fabio Eduardo</b><br><br>Research Field : <b>ELECTRONIC STRUCTURE OF MATERIALS</b><br><br>Research Topic : <b>LOW DIMENSIONAL MATERIALS</b><br><br>Permanent Institute:<br>CEA Centre d'Etudes de Saclay<br>DEN DANS DMN SRMP<br>F-91191 Gif sur Yvette<br>FRANCE<br>Permanent Institute e mail      eduardo.machado@cea.fr  | COLOMBIA                      | <b>PARTICIPANT</b> |
| 129. | <b>MANCERA RODRIGUEZ Luis Alberto</b><br><br>Research Field : <b>NANOSCIENCE AND FUNCTIONAL MATERIALS</b><br><br>Research Topic : <b>AB-INITIO METHODS,AB-INITIO MOLECULAR DYNAMICS</b><br><br>Permanent Institute:<br>Universitat Ulm<br>1. Nachwuchsgruppe Theorie<br>Albert-Einstein-Allee 11<br>D-89081 Ulm<br>GERMANY<br>Permanent Institute e mail      luis.mancera@uni-ulm.de,luismanc@ho<br>tmail.com | COLOMBIA                      | <b>PARTICIPANT</b> |

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|------|---|-------------|--------------------|
| 130. | <b>MARCHI Mariapia Corrada</b><br>Research Field : <b>CONDENSED MATTER</b><br><br>Research Topic : <b>QMC SIMULATIONS</b>   | ITALY       | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>SISSA & DEMOCRITOS National Simulation Center<br>Via Beirut 6<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      marchi@ts.infn.it, marchi@sissa.it   |             |                    |
| 131. | <b>MARMODORO Alberto</b><br>Research Field : <b>THEORETICAL CONDENSED MATTER PHYSICS</b><br><br>Research Topic : <b>AB-INITIO METHODS FOR DMS</b>   | ITALY       | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>University of Warwick<br>Department of Physics<br>Gibbet Hill Road<br>CV4 7AL Coventry<br>UNITED KINGDOM<br>Permanent Institute e mail      a.marmodoro@warwick.ac.uk   |             |                    |
| 132. | <b>MARSMAN Martijn</b><br>Research Field : <b>DFT, MANY-BODY PERTURBATION THEORY</b><br><br>Research Topic : <b>MANY-BODY PERTURBATION THEORY</b>   | NETHERLANDS | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Institut fur Material Physics &<br>Centre for Computational Materials Science<br>University of Vienna<br>Sensengasse 8/12<br>A-1090 Vienna<br>AUSTRIA<br>Permanent Institute e mail      martijn.marsman@univie.ac.at |             |                    |

| No.  | NAME and INSTITUTE  | Nationality   | Function                               |
|------|---|---|--|
| 133. | <b>MARTIN Richard Mc Fadden</b><br>Research Field : <b>THEORY OF CONDENSED MATTER,<br/>ELECTRONIC STRUCTURE</b><br>Research Topic : <b>STRONGLY CORRELATED SYSTEMS</b>  | UNITED STATES OF AMERICA  | <b>PARTICIPANT</b>                     |
|      | Permanent Institute:<br>University of Illinois at Urbana Champaign<br>Department of Physics<br>1110 West Green Street<br>Urbana IL 61801-3080<br>UNITED STATES OF AMERICA<br>Permanent Institute e mail      rmartin@uiuc.edu                       |   |  |
| 134. | <b>MARZARI Nicola</b><br>Research Field : <b>COMPUTATIONAL MATERIALS SCIENCE</b><br>Research Topic : <b>ELECTRONIC-STRUCTURE THEORY</b>   | ITALY   | <b>SCIENTIFIC COMMITTEE<br/>MEMBER</b> |
|      | Permanent Institute:<br>Massachusetts Institute of Technology<br>Department of Materials Science and Engineering<br>77 Massachusetts Ave.<br>Cambridge MA 02139-4307<br>UNITED STATES OF AMERICA<br>Permanent Institute e mail      marzari@mit.edu |   |  |
| 135. | <b>MCNELLIS Erik</b><br>Research Field : <b>ELECTRONIC CORRELATION SOLID STATE<br/>TDDFT</b><br>Research Topic : <b>MOLECULAR SWITCHES AT SOLID SURFACES</b>  | SWEDEN  | <b>PARTICIPANT</b>                     |
|      | mcnellis@fhi-berlin.mpg.de  | Present institute:<br>Fritz-Haber-Institut Der Max-Planck-Gesellschaft<br>Faradayweg 4-6<br>D-14195 Berlin<br>Germany | Until when: <b>1 April 2009</b>        |

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| 136. | <p><b>MEDEIROS Subenia Karine</b><br/>           Research Field : <b>FIRST PRINCIPLES STUDY USING DFT</b><br/> <br/>           Research Topic : <b>AB-INITIO MOLECULAR DYNAMICS</b></p> <p>Permanent Institute:<br/>           Universidade do Estado do Rio Grande do Norte UERN<br/>           Departamento de Fisica<br/>           Rua Almino Afonso, 478<br/>           59.610-210 Mossoro<br/>           RN<br/>           BRAZIL<br/>           Permanent Institute e mail      skmedeiros@gmail.com</p>          | BRAZIL      | <b>PARTICIPANT</b> |
| 137. | <p><b>MEYER Joerg</b><br/>           Research Field : <b>ADSORPTION, SURFACE DYNAMICS</b><br/> <br/>           Research Topic : <b>ENERGY DISSIPATION DURING ADSORPTION PROCESSES</b></p> <p>Permanent Institute:<br/>           Fritz-Haber-Institut Der Max-Planck-Gesellschaft<br/>           Department of Theory<br/>           Faradayweg 4-6<br/>           D-14195 Berlin<br/>           GERMANY<br/>           Permanent Institute e mail      meyer@fhi-berlin.mpg.de</p>                                      | GERMANY     | <b>PARTICIPANT</b> |
| 138. | <p><b>MIRANDA Caetano Rodrigues</b><br/>           Research Field : <b>COMP. PHYS., PHYS. OF COND. MATTER, ENERGY SCIENCE</b><br/>           Research Topic : <b>DFT, MOLECULAR DYNAMICS, INTERFACES</b></p> <p>Permanent Institute:<br/>           Kyoto University<br/>           Department of Civil and Earth Resources Engineering<br/>           Kyotodaigaku, Katsura, Nishikyoku<br/>           Kyoto 615-8540<br/>           JAPAN<br/>           Permanent Institute e mail      caetano.miranda@gmail.com</p> | BRAZIL      | <b>PARTICIPANT</b> |

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|------|--|----------------|--------------------|
| 139. | <b>MIYAZAKI Tsuyoshi</b><br>Research Field : <b>LARGE-SCALE DFT SIMULATIONS</b><br><br>Research Topic : <b>DNA, ORGANIC SOLIDS, NANOSTRUCTURED MATERIALS</b>   | JAPAN          | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>National Research Institute for Metals (NIMS)<br>1-2-1 Sengen<br>Tsukuba<br>Ibaraki 305-0047<br>JAPAN<br>Permanent Institute e mail      miyazaki.tsuyoshi@nims.go.jp                                  |                |                    |
| 140. | <b>MOHACEK-GROSEV Vlasta</b><br>Research Field : <b>VIBRATIONAL SPECTROSCOPY, MOLECULAR CRYSTALS</b><br>Research Topic : <b>RAMAN SPECTROSCOPY</b>   | CROATIA        | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Rudjer Boskovic Institute<br>Bijenicka Cesta 54<br>P.O. Box 180<br>HR-10002 Zagreb<br>CROATIA<br>Permanent Institute e mail      mohacek@irb.hr  |                |                    |
| 141. | <b>MORRIS Andrew James</b><br>Research Field : <b>ELECTRONIC STRUCTURE, DFT, QMC, GW APPROXIMATION</b><br>Research Topic : <b>DEFECTS IN SEMICONDUCTORS</b>  | UNITED KINGDOM | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Cambridge University<br>Theory of Condensed Matter Group<br>Cavendish Laboratory<br>19, J.J. Thomson Avenue<br>Cambridge CB3 0HE<br>UNITED KINGDOM<br>Permanent Institute e mail      ajm255@cam.ac.uk |                |                    |

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|------|---|---|---------------------|
| 142. | <b>MOSTOFI Arash Abolhassan</b><br>Research Field : <b>COMPUTATIONAL ELECTRONIC STRUCTURE</b><br><br>Research Topic :<br><br><br>Permanent Institute:<br>Imperial College London<br>Department of Materials<br>Exhibition Road<br>London SW7 2AZ<br>UNITED KINGDOM<br>Permanent Institute e mail      a.mostofi@imperial.ac.uk  | UNITED KINGDOM  | <b>PARTICIPANT</b>  |
| 143. | <b>MUNOZ GARCIA Ana Belen</b><br>Research Field : <b>SOLID STATE LIGHTING, LINEAR SCALING METHODS</b><br>Research Topic : <b>YTTRIUM ALUMINIUM GARNET, ORDER N METHODS</b><br><br><br><br><br><br><br><br><br><br>Permanent Institute:<br>Technische Universitaet Chemnitz<br>Institut Fuer Physik<br>Reichenhainer Strasse 70<br>D-09126 Chemnitz<br>GERMANY<br>Permanent Institute e mail      ebn@hrz.tu-chemnitz.de | SPAIN   | <b>PARTICIPANT</b>  |
|      |   | Present institute:<br>Universidad Autonoma de Madrid<br>Facultad de Ciencias<br>Departamento de Quimica<br>c/ Francisco Tomas y Valente, 7<br>Campus Universitario de<br>Cantoblanco<br>28049 Madrid<br>Spain |                     |
|      |   | Until when:   | <b>1 March 2011</b> |
| 144. | <b>NADIMI Ebrahim</b><br>Research Field : <b>DFT, ELECTRONIC PROPERTIES, ELECTRONIC TRANSPORT</b><br>Research Topic : <b>AB INITIO CALCULATION OF ELECTRONIC TRANSPORT</b><br><br><br>Permanent Institute:<br>Technische Universitaet Chemnitz<br>Institut Fuer Physik<br>Reichenhainer Strasse 70<br>D-09126 Chemnitz<br>GERMANY<br>Permanent Institute e mail      ebn@hrz.tu-chemnitz.de                             | ISLAMIC REPUBLIC OF IRAN  | <b>PARTICIPANT</b>  |

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|------|--|----------------|---|
| 145. | <b>NARASIMHAN Shobhana</b><br>Research Field : <b>AB INITIO DENSITY FUNCTIONAL THEORY CALCULATIONS</b><br>Research Topic : <b>SURFACES, CLUSTERS, CATALYSIS, GAS STORAGE</b><br><br>Permanent Institute:<br>Jawaharlal Nehru Centre for Advanced Scientific Research<br>Theoretical Sciences Unit<br>Jakkur Campus<br>560064 Bangalore<br>INDIA<br>Permanent Institute e mail      shobhana@jncasr.ac.in | INDIA          | <b>PARTICIPANT</b>  |
| 146. | <b>NEEDS Richard James</b><br><br>Research Field : <b>ELECTRONIC STRUCTURE COMPUTATIONS</b><br>Research Topic : <b>QMC AND DENSITY FUNCTIONAL METHODS</b><br><br>Permanent Institute:<br>Cavendish Laboratory<br>University of Cambridge<br>JJ Thompson Avenue<br>Cambridge CB3 0HE<br>UNITED KINGDOM<br>Permanent Institute e mail      rn11@cam.ac.uk  | UNITED KINGDOM | <b>SCIENTIFIC COMMITTEE MEMBER</b>  |
| 147. | <b>NEGRI Carlotta</b><br>Research Field : <b>CONDENSED MATTER</b><br>Research Topic : <b>NANOFRICTION &amp; TRIBOLOGY</b><br><br>Permanent Institute:<br>Universita' degli Studi di Milano<br>Via Festa del Perdono 7<br>20122 Milano<br>ITALY<br>Permanent Institute e mail      carlotta.negri@studenti.unimi.it   | ITALY          | <b>PARTICIPANT</b><br><br><br>Present institute:<br>S.I.S.S.A. - International School for Advanced Studies<br>Via Beirut 2-4<br>34014 Trieste<br>Italy<br><br>Until when: <b>30 June 2009</b> |



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| 148. | <p><b>NGUYEN Thuong Manh</b><br/>           Research Field : <b>SURFACE SCIENCE, QUANTUM CHEMISTRY</b><br/>           Research Topic : <b>MOLECULE/METAL , ORGANIC MOLECULAR SEMICONDUCTORS</b></p> <p>Permanent Institute:<br/>           Swiss Federal Laboratories For Materials Testing &amp; Research<br/>           Empa<br/>           Ueberlandstrasse 129<br/>           CH-8600 Duebendorf<br/>           SWITZERLAND<br/>           Permanent Institute e mail      manhthuongvietnam@gmail.com</p>                             | VIET NAM    | <b>PARTICIPANT</b> |
| 149. | <p><b>NOVAES Frederico Dutilh</b><br/>           Research Field : <b>CONDENSED MATTER PHYSICS</b><br/>           Research Topic : <b>COMPUTER SIMULATION, DFT, ELECTRONIC TRANSPORT</b></p> <p>Permanent Institute:<br/>           Institut de Ciencia de Materials de Barcelona (ICMAB)<br/>           C.S.I.C.<br/>           Campus Universitario de la UAB<br/>           E-08193 Bellaterra<br/>           SPAIN<br/>           Permanent Institute e mail      fdnovaes@icmab.es</p>   | BRAZIL      | <b>PARTICIPANT</b> |
| 150. | <p><b>O'REGAN David D.</b><br/>           Research Field : <b>LINEAR-SCALING, DFT+U, TDDFT, COMPUTATIONAL BIOLOGY</b><br/>           Research Topic : <b>ENERGETIC &amp; OPTICAL RESPONSE OF BIOMOLECULES</b></p> <p>Permanent Institute:<br/>           Cambridge University<br/>           Theory of Condensed Matter Group<br/>           Cavendish Laboratory<br/>           19, J.J. Thomson Avenue<br/>           Cambridge CB3 0HE<br/>           UNITED KINGDOM<br/>           Permanent Institute e mail      ddo20@cam.ac.uk</p> | IRELAND     | <b>PARTICIPANT</b> |

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|------|--|--------------------------|--------------------|
| 151. | <p><b>OGUZIE Emeka Emmanuel</b></p> <p>Research Field : <b>METAL CORROSION AND PROTECTION; ORGANIC INHIBITORS</b></p> <p>Research Topic : <b>DFT/IMAGING BASED MODELS FOR CORROSION INHIBITORS</b></p> <p>Permanent Institute:</p> <p>Federal University of Technology, Owerri FUTO<br/> P.M.B. 1526<br/> Owerri<br/> Imo State<br/> NIGERIA</p> <p>Permanent Institute e mail      oguziemeka@yahoo.com</p> | NIGERIA                  | <b>PARTICIPANT</b> |
| 152. | <p><b>OLEYNIK Ivan</b></p> <p>Research Field : <b>DFT MODELING OF MATERIALS</b></p> <p>Research Topic : <b>DFT MODELING OF MATERIALS</b></p> <p>Permanent Institute:</p> <p>University of South Florida<br/> Department of Physics<br/> 4202 East Fowler Avenue<br/> Tampa FL 33620-5700<br/> UNITED STATES OF AMERICA</p> <p>Permanent Institute e mail      ioleyenik@gmail.com</p>                        | UNITED STATES OF AMERICA | <b>PARTICIPANT</b> |
| 153. | <p><b>ONO Tomoya</b></p> <p>Research Field : <b>FIRST-PRINCIPLES CALCULATION</b></p> <p>Research Topic : <b>LARGE SCALE CALCULATION, TRANSPORT</b></p> <p>Permanent Institute:</p> <p>Graduate School of Engineering<br/> Prec. Sci. Tech. Department<br/> Osaka University<br/> 2-1, Yamada-oka, Suita<br/> Osaka 565-0871<br/> JAPAN</p> <p>Permanent Institute e mail      ono@prec.eng.osaka-u.ac.jp</p> | JAPAN                    | <b>PARTICIPANT</b> |

| No.  | NAME and INSTITUTE   | Nationality | Function                           |
|------|--|-------------|------------------------------------|
| 154. | <b>ORDEJON RONTOME Pablo Jesus</b><br><br>Research Field : <b>CONDENSED MATTER PHYSICS</b><br><br>Research Topic : <b>FIRST-PRINCIPLES METHODS FOR ELECTRONIC STRUCTURE</b><br><br>Permanent Institute:<br>Institut de Ciencia de Materials de Barcelona - CSIC<br>Campus de La U.A.B.<br>Bellaterra<br>08193 Barcelona<br>SPAIN<br>Permanent Institute e mail      ordejon@icmab.es | SPAIN       | <b>SCIENTIFIC COMMITTEE MEMBER</b> |
| 155. | <b>OTSUKA Takao</b><br><br>Research Field : <b>THEORETICAL CHEMISTRY, QUANTUM CHEMISTRY</b><br><br>Research Topic : <b>DFT, GREEN'S FUNCTION, ORDER-N, EXCITED STATE</b><br><br>Permanent Institute:<br>National Institute for Materials Science<br>1-2-1 Sengen<br>Tsukuba<br>Ibaraki 305-0047<br>JAPAN<br>Permanent Institute e mail      OOTSUKA.Takao@nims.go.jp                 | JAPAN       | <b>PARTICIPANT</b>                 |
| 156. | <b>PASTORE Giorgio</b><br><br>Research Field : <b>LIQUID AND AMORPHOUS STATE, AB-INITIO MD</b><br><br>Research Topic : <b>MOLTEN SALTS, PATCHY COLLOIDS, LIQUID WATER</b><br><br>Permanent Institute:<br>Universita' degli Studi di Trieste<br>Dipartimento di Fisica Teorica<br>Strada Costiera 11<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      pastore@ts.infn.it  | ITALY       | <b>PARTICIPANT</b>                 |

| No.  | NAME and INSTITUTE  | Nationality              | Function           |
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| 157. | <b>PAULATTO Lorenzo</b><br>Research Field : <b>ELECTRONIC STRUCTURE, CHEMICAL PHYSICS, CATALYSIS</b><br>Research Topic : <b>DFT SIMULATION OF SURFACE NANOCATALYSIS</b><br><br>Permanent Institute:<br>S.I.S.S.A.<br>International School for Advanced Studies<br>Via Beirut 2-4<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      paulatto@sissa.it   | ITALY                    | <b>PARTICIPANT</b> |
| 158. | <b>PAYAMI SHABESTAR Mahmoud</b><br>Research Field : <b>ELECTRONIC STRUCTURE CALCULATION, CONDENSED MATTER</b><br>Research Topic : <b>METAL CLUSTERS, SURFACES INTERFACES, ADSORPTION</b><br><br>Permanent Institute:<br>Atomic Energy Organization of Iran, AEOI<br>Nuclear Science & Technology Research Institute<br>Kargar Shomali<br>P.O.Box 14395-836<br>Tehran<br>ISLAMIC REPUBLIC OF IRAN<br>Permanent Institute e mail      mpayami@aeoi.org.ir | ISLAMIC REPUBLIC OF IRAN | <b>PARTICIPANT</b> |
| 159. | <b>PEKOZ Rengin</b><br>Research Field : <b>STRUCTURAL AND ELECTRONIC PROP. OF NANOSYSTEMS</b><br>Research Topic : <b>DFT CALCULATIONS OF BULK PROP. OF CONDENSED MATTER</b><br><br>Permanent Institute:<br>Middle East Technical University<br>Department of Physics<br>Inonu Bul.<br>Cankaya<br>06531 Ankara<br>TURKEY<br>Permanent Institute e mail      rpekoz@newton.physics.metu.edu.tr  | TURKEY                   | <b>PARTICIPANT</b> |

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| 160. | <p><b>PERESSI Maria</b></p> <p>Research Field : <b>SOLID STATE PHYSICS; COMPUTATIONAL PHYSICS</b></p> <p>Research Topic : <b>ELECTRONIC STRUCTURE; SEMICONDUCTORS; SURFACES</b></p> <p>Permanent Institute:</p> <p>Universita' degli Studi di Trieste<br/> Dipartimento di Fisica Teorica<br/> Strada Costiera 11<br/> 34014 Trieste<br/> ITALY</p> <p>Permanent Institute e mail      peressi@ts.infn.it</p> | ITALY       | <b>PARTICIPANT</b> |
| 161. | <p><b>PETZOLD Vivien</b></p> <p>Research Field : <b>CATALYSIS, DFT</b></p> <p>Research Topic : <b>AMMONIA DECOMPOSITION, ERROR ESTIMATION FOR GGAS</b></p> <p>Permanent Institute:</p> <p>Technical University of Denmark<br/> Fyskvej<br/> Building 307<br/> 2800 Kongens Lyngby<br/> DENMARK</p> <p>Permanent Institute e mail      petzold@fysik.dtu.dk</p>  | GERMANY     | <b>PARTICIPANT</b> |
| 162. | <p><b>PICCININ Simone</b></p> <p>Research Field : <b>COMPUTATIONAL PHYSICS</b></p> <p>Research Topic : <b>HETEROGENOUS CATALYSIS</b></p> <p>Permanent Institute:</p> <p>University of Sydney<br/> Dept. of Theoretical Physics<br/> (N.S.W. 2006)<br/> Sydney<br/> AUSTRALIA</p> <p>Permanent Institute e mail      piccinin@physics.usyd.edu.au</p>  | ITALY       | <b>PARTICIPANT</b> |

| No.  | NAME and INSTITUTE   | Nationality | Function           |
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| 163. | <b>PISTOL Mats-Erik</b><br>Research Field : <b>DENSITY FUNCTIONAL THEORY, PAIR DENSITIES</b><br>Research Topic : <b>N-REPRESENTABILITY, EXCHANGE-CORRELATION HOLES</b><br><br>Permanent Institute:<br>Solid State Physics<br>Lund University<br>Box 118<br>S-221 00 Lund<br>SWEDEN<br>Permanent Institute e mail      mats-erik.pistol@ff.lth.se   | SWEDEN      | <b>PARTICIPANT</b> |
| 164. | <b>POHL Johan</b><br>Research Field : <b>COMPUTATIONAL CATALYSIS, DFT, MULTI SCALE MODELING</b><br>Research Topic : <b>THERMODYNAMICS AND KINETICS OF NANOALLOYS</b><br><br>Permanent Institute:<br>Technische Universitat Darmstadt<br>FB Material und Geowissenschaften<br>Fachgebiet Strukturforschung<br>Petersenstr. 23<br>D-64287 Darmstadt<br>GERMANY<br>Permanent Institute e mail      johanpohl@web.de     | GERMANY     | <b>PARTICIPANT</b> |
| 165. | <b>POLONI Roberta</b><br>Research Field : <b>VIRTUAL CRYSTAL APPROXIMATION; HIGH PRESSURE</b><br>Research Topic : <b>VIRTUAL CRYSTAL APPROXIMATION (VCA)</b><br><br>Present institute:<br>Institut de Ciencia de Materials de Barcelona (ICMAB)<br>C.S.I.C.<br>Campus Universitario de la UAB<br>E-08193 Bellaterra<br>Spain<br>Present Institute e mail      rpoloni@icmab.es<br>Until when: <b>5 November 2009</b> | ITALY       | <b>PARTICIPANT</b> |

| No.  | NAME and INSTITUTE  | Nationality    | Function           |
|------|---|----------------|--------------------|
| 166. | <b>PRASONGKIT Jariyane</b><br>Research Field : <b>DFT, ELECTRON TRANSPORT PROPERTIES</b><br><br>Research Topic : <b>MOLECULAR ELECTRONICS THEORY</b>  | THAILAND       | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>University of Uppsala<br>Condensed Matter Theory Group<br>Department of Physics<br>P.O. Box 530<br>S-75121 Uppsala<br>SWEDEN<br>Permanent Institute e mail      jariyane.prasongkit@fysik.uu.se   |                |                    |
| 167. | <b>PROBERT Matthew Ian James</b><br>Research Field : <b>THEORETICAL CONDENSED MATTER PHYSICS</b><br><br>Research Topic : <b>TOTAL ENERGY METHODS AND GENETIC ALGORITHMS</b>   | UNITED KINGDOM | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>University of York<br>Department of Physics<br>Heslington<br>York YO10 5DD<br>UNITED KINGDOM<br>Permanent Institute e mail      mjp1@york.ac.uk   |                |                    |
| 168. | <b>RAUGEI Simone</b><br>Research Field : <b>BIOPHYSICS</b><br><br>Research Topic : <b>PROTEINS FUNCTION</b>   | ITALY          | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>S.I.S.S.A.<br>International School For Advanced Studies<br>Statistical and Biological Physics Sector<br>Via Beirut 4<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      raugai@sissa.it |                |                    |

| No.  | NAME and INSTITUTE  | Nationality | Function           |
|------|---|-------------|--------------------|
| 169. | <p><b>RICHARD Nicolas Antoine Daniel</b><br/>           Research Field : <b>AB INITIO, DFT, GW, OXIDES, DEFECTS</b><br/>           Research Topic : <b>OPTICAL PROPERTIES OF DEFECTS SILICON OXIDATION</b></p> <p>Permanent Institute:<br/>           Commissariat a l'Energie Atomique<br/>           Bruyeres Le Chatel<br/>           B.P. 12<br/>           F-91297 Arpajon Cedex<br/>           FRANCE<br/>           Permanent Institute e mail      nicolas.richard@cea.fr</p>                           | FRANCE      | <b>PARTICIPANT</b> |
| 170. | <p><b>RIZZI Michele</b><br/>           Research Field : <b>COMPUTATIONAL CONDENSED MATTER</b><br/>           Research Topic : <b>TRANSITION METALS SURFACE REACTIVITY</b></p> <p>Permanent Institute:<br/>           Universita' degli Studi di Trieste<br/>           Dipartimento di Fisica Teorica<br/>           Strada Costiera 11<br/>           34014 Trieste<br/>           ITALY<br/>           Permanent Institute e mail      rizzi@ts.infn.it</p>   | ITALY       | <b>PARTICIPANT</b> |
| 171. | <p><b>RODRIGUEZ PRIETO Alvaro</b><br/>           Research Field : <b>SI BASED NANOSTRUCTURES. HIGH PRESSURE PHYSICS</b><br/>           Research Topic : <b>DB WIRES, BI NL ON SI(001) HIGH PRESSURE PHYSICS</b></p> <p>Permanent Institute:<br/>           University College London<br/>           London Centre for Nanotechnology<br/>           17-19 Gordon Street<br/>           London WC1H 0AH<br/>           UNITED KINGDOM<br/>           Permanent Institute e mail      alvaro.prieto@ucl.ac.uk</p> | SPAIN       | <b>PARTICIPANT</b> |



| No.  | NAME and INSTITUTE   | Nationality | Function           |
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| 172. | <p><b>ROHLFING Michael</b><br/>           Research Field : <b>THEORETICAL PHYSICS</b><br/><br/>           Research Topic : <b>ELECTRONIC STRUCTURE</b></p> <p>Permanent Institute:<br/>           Universitat Osnabrueck<br/>           Fachbereich Physik<br/>           Barbarastrasse 7<br/>           D-49069 Osnabrueck<br/>           GERMANY<br/>           Permanent Institute e mail      mrohlfin@uos.de</p>   | GERMANY     | <b>PARTICIPANT</b> |
| 173. | <p><b>ROMA Guido</b><br/>           Research Field : <b>DEFECTS, DIFFUSION</b><br/><br/>           Research Topic : <b>SEMICONDUCTORS, INSULATORS, NUCLEAR APPLICATIONS</b></p> <p>Permanent Institute:<br/>           CEA Commissariat a l'Energie Atomique<br/>           Centre d'Etudes Saclay<br/>           DMN/SRMP<br/>           F-91191 Gif sur Yvette<br/>           FRANCE<br/>           Permanent Institute e mail      roma@cea.fr</p>                                    | ITALY       | <b>PARTICIPANT</b> |
| 174. | <p><b>ROSINI Marcello</b><br/>           Research Field : <b>SURFACE, INTERFACE, SEMICONDUCTORS, TRANSPORT</b><br/>           Research Topic : <b>ADSORPTION, NUCLEATION, GROWTH, NANOSTRUCTURES</b></p> <p>Permanent Institute:<br/>           Dipartimento di Fisica<br/>           Universita di Modena e Reggio Emilia<br/>           Via Campi 213/A<br/>           41100 Modena<br/>           ITALY<br/>           Permanent Institute e mail      marcello.rosini@unimore.it</p> | ITALY       | <b>PARTICIPANT</b> |

| No.  | NAME and INSTITUTE  | Nationality | Function           |
|------|---|-------------|--------------------|
| 175. | <b>RUIZ-SALVADOR Angel Rabdel</b><br>Research Field : <b>MATERIALS PHYSICAL CHEMISTRY, COMPUTER MODELING</b><br>Research Topic : <b>NANOPOROUS SOLIDS: MODELING, CHARACTERIZATION</b><br><br>Permanent Institute:<br>University of Havana<br>Institute of Materials and Reagents (IMRE)<br>Faculty of Physics<br>10600 Havana<br>CUBA<br>Permanent Institute e mail      rabdel@imre.oc.uh.cu | CUBA        | <b>PARTICIPANT</b> |
| 176. | <b>SAIB Salima</b><br>Research Field : <b>ELECTRONIC STRUCTURE THEORY</b><br>Research Topic : <b>ELECTRONS, PHONONS IN SOLIDS</b><br><br>Permanent Institute:<br>University of M'Sila<br>Physics Department<br>28000 M'Sila<br>ALGERIA<br>Permanent Institute e mail      SAIBSALIMA@YAHOO.FR   | ALGERIA     | <b>PARTICIPANT</b> |
| 177. | <b>SAITO Shoichiro</b><br>Research Field : <b>FIRST PRINCIPLE STUDY</b><br>Research Topic : <b>EXACT EXCHANGE, DFT</b><br><br>Permanent Institute:<br>Graduate School of Engineering<br>Prec. Sci. Tech. Department<br>Osaka University<br>2-1, Yamada-oka, Suita<br>Osaka 565-0871<br>JAPAN<br>Permanent Institute e mail      saito@cp.prec.eng.osaka-u.ac.jp                               | JAPAN       | <b>PARTICIPANT</b> |

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|------|--|-------------------|--------------------|
| 178. | <b>SAKONG Sung</b><br>Research Field : <b>SURFACE, ADSORBATE AND CATALYTIC REACTIONS</b><br>Research Topic : <b>ENERGY DISSIPATION AT SURFACES</b>   | REPUBLIC OF KOREA | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Universitat Duisburg Essen<br>Department of Physics<br>Campus Duisburg<br>Lotharstrasse 1<br>47048 Duisburg<br>GERMANY<br>Permanent Institute e mail      sung.sakong@uni-due.de   |                   |                    |
| 179. | <b>SANAVIO Barbara</b><br>Research Field : <b>BIOPHYSICS</b><br>Research Topic : <b>PROTEINS</b>   | ITALY             | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>S.I.S.S.A.<br>Nanostructure Lab<br>via Beirut 2-4<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      bsanavio@sissa.it   |                   |                    |
| 180. | <b>SANCHEZ GONZALEZ Nadiezhda</b><br>Research Field : <b>MATERIALS SCIENCE, THEORY AND SIMULATIONS</b><br>Research Topic : <b>MAGNETISM AND SPINTRONICS, SURFACES, INTERFACES</b>  | SPAIN             | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Instituto de Ciencias de Materiales de Madrid<br>Consejo Superior de Investigaciones Cientificas-CSIC<br>Sor Juana Ines de la Cruz 3<br>Cantoblanco<br>28049 Madrid<br>SPAIN<br>Permanent Institute e mail      nadia@icmm.csic.es |                   |                    |

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| 181. | <b>SANCHEZ-PORTAL Daniel</b><br>Research Field : <b>ELECTRONIC STRUCTURE CALCULATIONS, SURFACE PHYSICS</b><br>Research Topic : <b>SURFACE PHYSICS, MOLECULAR ELECTRONICS, GRAPHENE</b><br><br>Permanent Institute:<br>Universidad del Pais Vasco<br>Facultad de Quimicas<br>Unidad de Fisica de Materiales<br>Centro Mixto CSIC, UPV, EHU<br>Edificio Korta<br>Avenida de Tolosa 72<br>E-20018 San Sebastian<br>SPAIN<br>Permanent Institute e mail      sqbsapod@sc.ehu.es | SPAIN       | <b>PARTICIPANT</b> |
| 182. | <b>SANFILIPPO Andrea</b><br>Research Field : <b>QUANTUM CHEMISTRY. VAN DER WAALS INTERACTIONS</b><br>Research Topic : <b>VAN DER WAALS INTERACTIONS</b><br><br>Permanent Institute:<br>Fritz-Haber-Institut Der Max-Planck-Gesellschaft<br>Faradayweg 4-6<br>D-14195 Berlin<br>GERMANY<br>Permanent Institute e mail      sanfilip@fhi-berlin.mpg.de  | ITALY       | <b>PARTICIPANT</b> |
| 183. | <b>SANZ-NAVARRO Carlos</b><br>Research Field : <b>COMPUTATIONAL PHYSICS, NANOCCLUSERS</b><br><br>Research Topic : <b>SIMULATION OF ATOMIC CLUSTERS</b><br><br>Permanent Institute:<br>Universidad Autonoma de Barcelona<br>Centro de Investigaciones en Nanociencia y Nanotecnologia<br>Edificio CM7<br>Bellaterra<br>08193 Barcelona<br>SPAIN<br>Permanent Institute e mail      csanz@cin2.es   | SPAIN       | <b>PARTICIPANT</b> |

| No.  | NAME and INSTITUTE   | Nationality   | Function           |
|------|--|---|--------------------|
| 184. | <b>SCHIRO' Marco</b><br>Research Field : <b>STRONGLY CORRELATED MATERIALS</b><br><br>Research Topic : <b>DMFT FOR STRONGLY CORRELATED MATERIALS</b>  | ITALY   | <b>PARTICIPANT</b> |
|      |  | Present institute:<br>S.I.S.S.A.<br>International School for Advanced Studies<br>Via Beirut 2-4<br>34014 Trieste<br>Italy<br>Present Institute e mail      schirom@sissa.it<br>Until when: <b>1 November 2009</b> |                    |
| 185. | <b>SCLAUZERO Gabriele</b><br>Research Field : <b>ELECTRONIC STRUCTURE, BALLISTIC CONDUCTANCE</b><br>Research Topic : <b>NANOWIRES NANOCONTACTS ADSORBATES</b>                                  | ITALY   | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>S.I.S.S.A.<br>International School for Advanced Studies<br>Via Beirut 2-4<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      sclauzer@sissa.it               |   |                    |
| 186. | <b>SENA Alessandro Michael Pasquale</b><br>Research Field : <b>ORDER(N) DFT, SI, BIOMOLECULES, ELECTRON TRANSFER</b><br>Research Topic : <b>ORDER(N) CONSTRAINED DFT FOR ELECTRON TRANSFER</b> | UNITED KINGDOM  | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>University College London<br>Dept.Physics & Astronomy<br>Gower Street<br>WC1E 6BT London<br>UNITED KINGDOM<br>Permanent Institute e mail      a.sena@ucl.ac.uk         |   |                    |

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|------|--|----------------|--------------------|
| 187. | <b>SENATORE Gaetano</b><br>Research Field : <b>ELECTRON SYSTEMS IN LOW DIMENSION</b><br><br>Research Topic : <b>ELECTRON SYSTEMS IN LOW DIMENSION</b><br><br><br>Permanent Institute:<br>Universita' degli Studi di Trieste<br>Dipartimento di Fisica Teorica<br>Strada Costiera 11<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail      SENATORE@TS.INFN.IT   | ITALY          | <b>PARTICIPANT</b> |
| 188. | <b>SERIANI Nicola</b><br>Research Field : <b>DFT, CATALYSIS, NANOSTRUCTURES, OPTIMIZATION</b><br>Research Topic : <b>HETEROGENEOUS CATALYSIS, GENETIC ALGORITHMS</b><br><br><br>Permanent Institute:<br>University of Vienna<br>Institute For Material Physics<br>Sensengasse 8/12<br>1090 Vienna<br>AUSTRIA<br>Permanent Institute e mail      nicola.seriani@univie.ac.at                                    | ITALY          | <b>PARTICIPANT</b> |
| 189. | <b>SHELLEY Matt</b><br>Research Field : <b>DFT, MAXIMALLY LOCALISED WANNIER FUNCTIONS</b><br>Research Topic : <b>THERMOELECTRIC NANOWIRES</b><br><br><br>Permanent Institute:<br>Imperial College London<br>Theoretical Physics Group<br>Department of Physics<br>South Kensington Campus<br>Huxley Building<br>London SW7 2AZ<br>UNITED KINGDOM<br>Permanent Institute e mail      m.shelley07@imperial.ac.uk | UNITED KINGDOM | <b>PARTICIPANT</b> |

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| 190. | <b>SJAKSTE Jelena</b><br>Research Field : <b>MATERIAL SCIENCE, DENSITY FUNCTIONAL THEORY</b><br>Research Topic : <b>ELECTRON-PHONON INTERACTION IN SEMICONDUCTORS</b><br><br>Permanent Institute:<br>Ecole Polytechnique<br>Laboratoire des Solides Irradies<br>Route de Saclay<br>F-91128 Palaiseau Cedex<br>FRANCE<br>Permanent Institute e mail : jelena.sjakste@polytechnique.edu,<br>jelena.sjakste@polytechnique.fr | LATVIA   | <b>PARTICIPANT</b>       |
| 191. | <b>SMOGUNOV Alexander</b><br>Research Field :<br><br>Research Topic :<br><br>Permanent Institute:<br>S.I.S.S.A. - International School for Advanced Studies<br>Via Beirut 2-4<br>34014 Trieste<br>ITALY<br>Permanent Institute e mail : smogunov@sissa.it   | RUSSIAN FEDERATION   | <b>PARTICIPANT</b>       |
|      |   | Present institute:<br>The Abdus Salam International Centre for Theoretical Physics<br>Condensed Matter Section<br>Strada Costiera 11<br>34014 Trieste<br>Italy |                          |
|      |   | Until when:  | <b>24 September 2009</b> |
| 192. | <b>SOKCEVIC Damir</b><br>Research Field : <b>SURFACE AND THIN FILMS PHYSICS</b><br>Research Topic : <b>DFT CALCULATION OF PROPERTIES OF METAL SURFACES</b><br><br>Permanent Institute:<br>Rudjer Boskovic Institute<br>Division of Theoretical Physics<br>Bijenicka Cesta 54<br>P.O. Box 180<br>10002 Zagreb<br>CROATIA<br>Permanent Institute e mail : sokcevic@thphys.irb.hr  | CROATIA  | <b>PARTICIPANT</b>       |

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| 193. | <p><b>SOLA Ester</b></p> <p>Research Field : <b>NEW STRUCTURES,HIGH PRESSURE,QMC AND DFT,FE, TA</b></p> <p>Research Topic : <b>HIGH PRESSURE EFFECTS USING QMC AND DFT</b></p> <p>Permanent Institute:<br/>           University College London<br/>           Department of Earth Sciences<br/>           Gower Street<br/>           London WC1E CBT<br/>           UNITED KINGDOM<br/>           Permanent Institute e mail      e.sola@ucl.ac.uk</p>   | SPAIN       | <b>PARTICIPANT</b> |
| 194. | <p><b>SORELLA Sandro</b></p> <p>Research Field :</p> <p>Research Topic :</p> <p>Permanent Institute:<br/>           SISSA &amp; DEMOCRITOS National Simulation Center<br/>           Via Beirut 6<br/>           34014 Trieste<br/>           ITALY<br/>           Permanent Institute e mail      sorella@sissa.it</p>  | ITALY       | <b>PARTICIPANT</b> |
| 195. | <p><b>SOUZA Ivo Nuno</b></p> <p>Research Field : <b>ELECTRONIC STRUCTURE OF SOLIDS</b></p> <p>Research Topic : <b>ANOMALOUS HALL EFFECT IN FERROMAGNETS</b></p> <p>Permanent Institute:<br/>           University of California<br/>           Department of Physics<br/>           366 Le Conte Hall<br/>           Berkeley CA 94720-7300<br/>           UNITED STATES OF AMERICA<br/>           Permanent Institute e mail      isouza@berkeley.edu</p> | PORTUGAL    | <b>PARTICIPANT</b> |



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| 196. | <b>SPALLANZANI Nicola</b><br>Research Field : <b>COMPUTATIONAL PHYSICS/CHEMISTRY</b><br>Research Topic : <b>TDDFT STUDY OF SMALL BIO-SYSTEMS</b><br><br>Permanent Institute:<br>Dipartimento di Fisica<br>Universita di Modena e Reggio Emilia<br>Via Campi 213/A<br>41100 Modena<br>ITALY<br>Permanent Institute e mail      nicola.spallanzani@unimore.it  | ITALY  | <b>PARTICIPANT</b>                 |
| 197. | <b>SREPUSHARAWOOT Pornjuk</b><br>Research Field : <b>HYDROGEN STORAGE, DFT</b><br>Research Topic : <b>HYDROGEN STORAGE IN MOF-5</b><br><br>Permanent Institute:<br>Khon Kaen University<br>Faculty of Science<br>Department of Physics<br>123/189 Mitra Parp Road<br>40002 Khon Kaen<br>THAILAND   | THAILAND   | <b>PARTICIPANT</b>                 |
|      |  | Present institute:<br>University of Uppsala<br>Condensed Matter Theory Group<br>Department of Physics<br>P.O. Box 530<br>S-75121 Uppsala<br>Sweden |                                    |
|      |  | Present Institute e mail   | pornjuk.srepusharawoot@fysik.uu.se |
|      |  | Until when:  | <b>25 September 2010</b>           |
| 198. | <b>STEVANOVIC Vladan</b><br>Research Field : <b>DENSITY-FUNCTIONAL THEORY AND ITS APPLICATIONS</b><br>Research Topic : <b>NANOSCIENCE, SURFACES, CATALYSIS</b><br><br>Permanent Institute:<br>Ecole Polytechnique Federale de Lausanne<br>Institut de Recherche Numerique en Physique Des Materiaux (I.R.R.M.A.)<br>Bat. PPH, Station 13<br>CH-1015 Lausanne<br>SWITZERLAND<br>Permanent Institute e mail      vladan.stevanovic@epfl.ch | REPUBLIC OF SERBIA   | <b>PARTICIPANT</b>                 |

| <b>No.</b> | <b>NAME and INSTITUTE</b>   | <b>Nationality</b>            | <b>Function</b>    |
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| 199.       | <b>SUN Jian</b><br>Research Field : <b>AB INITIO CALCULATIONS, MOLECULAR DYNAMICS</b><br>Research Topic : <b>METADYNAMICS, PHASE TRANSITIONS</b><br><br>Permanent Institute:<br>Ruhr Universitat Bochum<br>Fakultat Fur Chemie<br>44780 Bochum<br>GERMANY<br>Permanent Institute e mail     jian.sun@theodrem.rub.de,<br>jasonsun98@hotmail.com   | PEOPLE'S REPUBLIC OF<br>CHINA | <b>PARTICIPANT</b> |
| 200.       | <b>TABARES MENDOZA Carolina</b><br>Research Field : <b>ELECTRONIC TRANSPORT, MOLECULAR JUNCTIONS</b><br>Research Topic : <b>NONLINEAR CONDUCTANCE THROUGH MOLECULAR JUNCTIONS</b><br><br>Permanent Institute:<br>Centro de Investigacion en Nanociencia y Nanotecnologia<br>CIN2 ICN CSIC<br>ETSE - 2 planta<br>Campus de la Universitat Autonoma de Barcelona<br>08193 Bellaterra<br>SPAIN<br>Permanent Institute e mail     ctabares@icmab.es | MEXICO                        | <b>PARTICIPANT</b> |
| 201.       | <b>TAIOLI Simone Alessandro</b><br>Research Field : <b>COMPUTATIONAL PHYSICS AND MATERIAL SCIENCE</b><br>Research Topic : <b>AUGER EFFECT AND ELECTRONIC STRUCTURE CALCULATIONS</b><br><br>Permanent Institute:<br>ITC-IRST Istituto Trentino di Cultura<br>Istituto per la Ricerca Scientifica e Tecnologica<br>Divisione SSi - Gruppo MPBA<br>Via Sommarive, 18<br>38050 POVO<br>ITALY<br>Permanent Institute e mail     taioli@fbk.eu        | ITALY                         | <b>PARTICIPANT</b> |

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| 202. | <b>TALEATU Bidini Alade</b><br>Research Field : <b>CONDENSED MATTER PHYSICS</b><br><br>Research Topic : <b>NANOMATERIALS FOR OPTOELECTRONIC APPLICATIONS</b><br><br>Permanent Institute:<br>Obafemi Awolowo University<br>Centre For Energy Research and Development<br>Material Science and Electronics Division<br>220005 Ile Ife<br>Osun State<br>NIGERIA<br>Permanent Institute e mail      bdntaleatu@yahoo.com | NIGERIA     | <b>PARTICIPANT</b><br><br><br><br><br><br><br><br><br><br><br>Present institute:<br>Laboratorio Sincrotrone Elettra<br>Strada Statale 14 - Km. 163.5<br>Basovizza<br>34102 Trieste<br>Italy<br><br>Until when: <b>2 March 2009</b> |
| 203. | <b>TANGNEY Paul Thomas</b><br>Research Field : <b>COMPUTATIONAL PHYSICS AND MATERIALS SCIENCE</b><br>Research Topic :<br><br>Permanent Institute:<br>Imperial College London<br>Department of Materials<br>Exhibition Road<br>London SW7 2AZ<br>UNITED KINGDOM<br>Permanent Institute e mail      p.tangney@imperial.ac.uk   | IRELAND     | <b>PARTICIPANT</b>   |
| 204. | <b>TARAFDER Kartick</b><br>Research Field : <b>ALLOYS, BIO-MOLECULES, MULTIFERROIC MATERIALS</b><br>Research Topic : <b>ELECTRONIC STRUCTURE, TRANSPORT PROPERTIES</b><br><br>Permanent Institute:<br>Uppsala University<br>the Angstrom Laboratory<br>Department of Physics<br>Box 518<br>Se<br>75120 Uppsala<br>SWEDEN<br>Permanent Institute e mail      kartick.tarafder@fysik.uu.se                             | INDIA       | <b>PARTICIPANT</b>   |

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| 205. | <b>TATEYAMA Yoshitaka</b><br>Research Field : <b>AB INITIO FREE ENERGY CALCULATION</b><br><br>Research Topic : <b>FREE ENERGY CALCULATION, TDDFT CALCULATIONS</b><br><br>Permanent Institute:<br>International Center for Materials Nanoarchitectonics<br>National Institute for Materials Science<br>1-1 Namiki, Tsukuba<br>Ibaraki 305-0044<br>JAPAN<br>Permanent Institute e mail      TATEYAMA.Yoshitaka@nims.go.jp | JAPAN       | <b>PARTICIPANT</b> |
| 206. | <b>TEWELDEBERHAN Amanuel Matewos</b><br>Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b><br>Research Topic : <b>ELECTRONIC,STRUCTURAL, &amp; VIBRATIONAL PROPERTIES</b><br><br>Permanent Institute:<br>Dalhousie University<br>Department of Physics<br>B3H 3J5<br>Halifax<br>CANADA<br>Permanent Institute e mail      a.m.teweldeberhan@dal.ca  | ERITREA     | <b>PARTICIPANT</b> |
| 207. | <b>THAKORE Brijmohan Yeshwantsingh</b><br>Research Field : <b>CONDENSED MATTER THEORY</b><br><br>Research Topic : <b>PSEUDOPOTENTIAL THEORY</b><br><br>Permanent Institute:<br>Sardar Patel University<br>Department of Physics<br>P.B. No 10<br>Dist. Anand<br>Vallabh Vidyanagar 388 120<br>Gujarat State<br>INDIA<br>Permanent Institute e mail      brijmohanthakore@rediffmail.com                                 | INDIA       | <b>PARTICIPANT</b> |

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| 208. | <b>TILOCCA Antonio</b><br>Research Field : <b>OXIDE MATERIALS, AMORPHOUS MATERIALS, SURFACES</b><br>Research Topic : <b>BIOACTIVE GLASSES</b>  | ITALY       | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>University College London<br>Department of Chemistry<br>20 Gordon Street<br>WC1H 0AJ London<br>UNITED KINGDOM<br>Permanent Institute e mail      a.tilocca@ucl.ac.uk |             |                    |
| 209. | <b>TORRENT Marc</b><br>Research Field : <b>COND. MATTER, NUM. METHODS FOR ELEC. STRUCTURE</b><br>Research Topic : <b>PAW METHOD, DFPT, ACTINIDS</b>  | FRANCE      | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Commissariat a l'Energie Atomique<br>Bruyeres Le Chatel<br>B.P. 12<br>F-91297 Arpajon Cedex<br>FRANCE<br>Permanent Institute e mail      marc.torrent@cea.fr         |             |                    |
| 210. | <b>TOYODA Masayuki</b><br>Research Field : <b>ELECTRONIC STRUCTURE CALCULATIONS</b><br>Research Topic : <b>MAGNETIC SEMICONDUCTORS</b>   | JAPAN       | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Japan Advanced Institute of Science and Technology<br>1-1 Asahidai, Nomi<br>Ishikawa 923-1292<br>JAPAN<br>Permanent Institute e mail      m-toyoda@jaist.ac.jp       |             |                    |

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| 211. | <b>UMARI Paolo</b><br>Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b><br>Research Topic : <b>MANY-BODY PERTURBATION THEORY</b>   | ITALY       | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>CNR INFM Democritos<br>c/o Sincrotrone Trieste<br>AREA Science Park<br>Strada Statale 14, Km. 163,5 Basovizza<br>34012 Trieste<br>ITALY<br>Permanent Institute e mail      umari@democritos.it  |             |                    |
| 212. | <b>VANDECASTEELE Niels</b><br>Research Field : <b>ELECTRONIC TRANSPORT, EPC, PHONON LIFETIME</b><br>Research Topic : <b>CARBON NANOTUBES, GRAPHENE</b>  | FRANCE      | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>IMPMC Institut de Mineralogie et de Physique des Milieux Condenses<br>Universite' Pierre et Marie Curie<br>140 Rue de Lourmel<br>Campus Boucicaut<br>75015 Paris<br>FRANCE<br>Permanent Institute e mail      vandecas@impmc.jussieu.fr |             |                    |
| 213. | <b>VANIN Marco</b><br>Research Field : <b>THEORETICAL NANOPHYSICS, TRANSPORT</b><br>Research Topic : <b>GRAPHENE, TRANSPORT IN GRAPHENE, NEGF, DFT</b>  | ITALY       | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Technical University of Denmark<br>Center For Atomic Scale Materials Physics<br>Department of Physics<br>Anker Engelundsveg, 1<br>2800 Lyngby<br>DENMARK<br>Permanent Institute e mail      mvanin@fysik.dtu.dk                         |             |                    |

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| 214. | <b>VANPOUCKE Danny Eric Paul</b><br>Research Field : <b>DFT, TOTAL ENERGY CALCULATIONS, SIMULATION OF STM</b><br>Research Topic : <b>STRUCTURAL OPTIMIZATION NANOWIRES SEMICONDUCTORS</b>                                   | BELGIUM   | <b>PARTICIPANT</b> |
|      |   | Present institute:<br>University of Twente<br>Computational Materials Science<br>Faculty of Science and Technology<br>P.O. Box 217<br>7500 AE Enschede<br>Netherlands<br>Present Institute e mail      d.e.p.vanpoucke@tnw.utwente.nl<br>Until when: <b>31 May 2009</b> |                    |
| 215. | <b>VARSAÑO Daniele</b><br>Research Field : <b>CONDENSED MATTER</b><br><br>Research Topic : <b>NANO-BIO SYSTEMS, EXCITED STATES, TDDFT, MBPT</b>   | ITALY   | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>National Research Center on nanoStructures and bioSystems at Surfaces, S3, of CNR INFM<br>via G. Campi 213/a<br>41100 Modena<br>ITALY<br>Permanent Institute e mail      daniele.varsano@unimore.it |   |                    |
| 216. | <b>VAST Nathalie</b><br>Research Field : <b>THEORY FOR COND. MAT. DFT. ELEC-PHONON INTERACTION</b><br>Research Topic : <b>ELEC. LIFETIME. SUPERCONDUCTIVITY. SPECTROSCOPY</b>   | FRANCE  | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Ecole Polytechnique<br>Laboratoire des Solides Irradies<br>Route de Saclay<br>F-91128 Palaiseau Cedex<br>FRANCE<br>Permanent Institute e mail      nathalie.vast@polytechnique.edu                  |   |                    |

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| 217. | <b>VERISSIMO ALVES Marcos</b><br>Research Field : <b>DENSITY FUNCTIONAL THEORY, ELECTRONIC STRUCTURE</b><br>Research Topic : <b>CARBON-BASED SYSTEMS</b>   | BRAZIL      | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Universite Catholique de Louvain<br>Unite de Physico-Chimie et Physique des Materiaux<br>Batiment Boltzmann<br>Place Croix Du Sud 1<br>B-1348 Louvain La Neuve<br>BELGIUM<br>Permanent Institute e mail      marcos.verissimo@uclouvain.be |             |                    |
| 218. | <b>VOLNIANSKA Oksana</b><br>Research Field : <b>MATERIAL SCIENCE, AB INITIO METHODS</b><br>Research Topic : <b>AB INITIO METHODS</b>   | UKRAINE     | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Polish Academy of Sciences<br>Institute of Physics<br>Al. Lotnikow 32/46<br>02-668 Warsaw<br>POLAND<br>Permanent Institute e mail      volnian@ifpan.edu.pl  |             |                    |
| 219. | <b>VON FERBER Christian</b><br>Research Field : <b>STATISTICAL MECHANICS, COMPLEX SYSTEMS,SOFT MATTER</b><br>Research Topic : <b>POLYMER DYNAMICS, SCALING PROPERTIES,SELF ASSEMBLY</b>  | GERMANY     | <b>PARTICIPANT</b> |
|      | Permanent Institute:<br>Coventry University<br>Applied Mathematics Research Centre<br>Priory Street<br>Coventry CV1 5FB<br>UNITED KINGDOM<br>Permanent Institute e mail      c.vonferber@coventry.ac.uk  |             |                    |



| No.  | NAME and INSTITUTE   | Nationality                | Function           |
|------|--|----------------------------|--------------------|
| 220. | <b>WALKER Brent Graham</b><br>Research Field : <b>CONDENSED MATTER PHYSICS</b><br><br>Research Topic : <b>TIME-DEPENDENT DENSITY FUNCTIONAL THEORY</b><br><br>Permanent Institute:<br>Industrial Research Limited<br>P.O. Box 31-310<br>69 Gracefield Road<br>Lower Hutt 5040<br>NEW ZEALAND<br>Permanent Institute e mail      b.walker@irl.cri.nz  | NEW ZEALAND                | <b>PARTICIPANT</b> |
| 221. | <b>WASSMANN Tobias</b><br>Research Field : <b>AB-INITIO CALCULATIONS ON GRAPHENE MATERIALS</b><br>Research Topic : <b>GRAPHENE NANORIBBONS</b><br><br>Permanent Institute:<br>IMPMC Institut de Mineralogie et de Physique des Milieux Condenses<br>Universite' Pierre et Marie Curie<br>140 Rue de Lourmel<br>Campus Boucicaut<br>75015 Paris<br>FRANCE<br>Permanent Institute e mail      tobias.wassmann@impmc.jussieu.fr | SWITZERLAND                | <b>PARTICIPANT</b> |
| 222. | <b>WENG Hongming</b><br>Research Field : <b>DFT CALCULATION, MAGNETISM IN CONDENSED MATTER</b><br>Research Topic : <b>MAGNETIC PROPERTIES OF TMO, MULTIFERROICS</b><br><br>Permanent Institute:<br>Japan Advanced Institute of Science and Technology<br>1-1 Asahidai, Nomi<br>Ishikawa 923-1292<br>JAPAN<br>Permanent Institute e mail      hmweng@jaist.ac.jp  | PEOPLE'S REPUBLIC OF CHINA | <b>PARTICIPANT</b> |

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| 223. | <p><b>WIRTZ Ludger</b></p> <p>Research Field : <b>ELECTRONIC STRUCTURE (DFT AND MBPT)</b></p> <p>Research Topic : <b>OPTICAL PROPERTIES OF NANOTUBES AND GRAPHENE</b></p> <p>Permanent Institute:</p> <p>IEMN Institute for Electronics, Microelectronics and Nanotechnology<br/>           Dept. ISEN<br/>           CNRS<br/>           UMR 8520<br/>           P.P. 60069<br/>           F-59652 Villeneuve d'Ascq Cedex<br/>           FRANCE</p> <p>Permanent Institute e mail      ludger.wirtz@isen.iemn.univ-lille1.fr</p> | GERMANY        | <b>PARTICIPANT</b> |
| 224. | <p><b>YATES Jonathan</b></p> <p>Research Field : <b>COMPUTATIONAL ELECTRONIC STRUCTURE</b></p> <p>Research Topic : <b>COMPUTATIONAL ELECTRONIC STRUCTURE</b></p> <p>Permanent Institute:</p> <p>University of Oxford<br/>           Department of Materials<br/>           Parks Road<br/>           OX1 3PH Oxford<br/>           UNITED KINGDOM</p> <p>Permanent Institute e mail      jonathan.yates@materials.ox.ac.uk</p>   | UNITED KINGDOM | <b>PARTICIPANT</b> |
| 225. | <p><b>YOON Tiem Leong</b></p> <p>Research Field : <b>COMPUTATIONAL CONDENSED MATTER PHYSICS</b></p> <p>Research Topic : <b>AB INITIO COMPUTATION OF CRYSTALLINE SYSTEM</b></p> <p>Permanent Institute:</p> <p>Universiti Sains Malaysia<br/>           School of Physics<br/>           Minden<br/>           11800 USM Penang<br/>           MALAYSIA</p> <p>Permanent Institute e mail      tlyoon@usm.my</p>  | MALAYSIA       | <b>PARTICIPANT</b> |

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| 226. | <b>ZHANG Wenqing</b><br><br>Research Field : <b>AB-INITIO CALCULATION, ENERGY MATERIALS</b><br><br>Research Topic : <b>THERMOELECTRIC, INTERFACE, ELECTRICAL TRANSPORT</b><br><br>Permanent Institute:<br>Chinese Academy of Sciences<br>Shanghai Institute of Ceramics<br>1295 Dingxi Road<br>Shanghai 200050<br>PEOPLE'S REPUBLIC OF CHINA<br>Permanent Institute e mail      wqzhang@mail.sic.ac.cn | PEOPLE'S REPUBLIC OF CHINA | <b>PARTICIPANT</b>  |
| 227. | <b>ZHENG Bing</b><br><br>Research Field :<br><br>Research Topic :<br><br>Permanent Institute:<br>Jilin University<br>Department of Materials Science and Engineering<br>Qianwei Road 2699<br>130012 Changchun<br>PEOPLE'S REPUBLIC OF CHINA<br>Permanent Institute e mail      zhengbing@jlu.edu.cn  | PEOPLE'S REPUBLIC OF CHINA | <b>PARTICIPANT</b><br><br><br><br><br><br><br><br><br><br>zhengb@ictp.it<br><b>14 January 2009</b>  |
| 228. | <b>ZHONG Zhicheng</b><br><br>Research Field : <b>DENSITY FUNCTIONAL CALCULATION ABOUT OXIDES</b><br><br>Research Topic :   | PEOPLE'S REPUBLIC OF CHINA | <b>PARTICIPANT</b><br><br><br><br><br><br><br><br><br><br>Present institute:<br>University of Twente<br>Computational Materials Science<br>Faculty of Science and Technology<br>P.O. Box 217<br>7500 AE Enschede<br>Netherlands<br>Present Institute e mail      z.c.zhong@utwente.nl<br>Until when: <b>14 October 2009</b> |

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| 229. | <p><b>ZOPPI Laura</b><br/>           Research Field : <b>CONDENSED MATTER PHYSICS</b><br/><br/>           Research Topic : <b>ORGANIC MOLECULES ON METALLIC SURFACES</b><br/><br/>           Permanent Institute:<br/>           University of Zurich<br/>           Institute of Organic Chemistry<br/>           Winterthurerstrasse 190<br/>           8057 Zurich<br/>           SWITZERLAND<br/>           Permanent Institute e mail      zoppi@oci.uzh.ch</p> | ITALY       | <b>PARTICIPANT</b> |
| 230. | <p><b>ZYKOVA-TIMAN Tatyana</b><br/>           Research Field : <b>COLLOIDS AND SOFT MATTER</b><br/><br/>           Research Topic : <b>PHASE TRANSITION, CSP, ORGANIC CRYSTALS</b><br/><br/>           Permanent Institute:<br/>           Universitat Mainz<br/>           Institut Fuer Physik<br/>           Staudinger Weg 7<br/>           55099 Mainz<br/>           GERMANY<br/>           Permanent Institute e mail      zykova@uni-mainz.de</p>            | UKRAINE     | <b>PARTICIPANT</b> |