



The Abdus Salam  
International Centre for Theoretical Physics



## Spring College on Computational Nanoscience

Cosponsor(s): Psi-k Network, CECAM and DEMOCRITOS CNR-IOM  
Organizer(s): Directors: A. Foster, N. Marzari, S. Scandolo.  
Trieste - Italy, 17 - 28 May 2010

**Venue: Leonardo da Vinci Building Main Lecture Hall**

### Programme

**Monday, 17 May 2010 ELECTRONIC (I)**  
**Chairperson: S. SCANDOLO**

**17 May 2010**

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|----------------------|--|
| <b>08:30 - 09:45</b> | <b>Registration and Administrative Matters - Leonardo Building, main entrance level, ground floor</b>  |
| <b>09:45 - 10:00</b> | <b>Professor Fernando QUEVEDO / ICTP Director</b><br><b>Opening Remarks</b>  |
| <b>10:00 - 11:00</b> | <b>R.M. MARTIN / Univ. of Illinois at Urbana Champaign, USA</b><br><b>Electronic structure: Yesterday, Today and Tomorrow</b>                      |
| <b>11:00 - 11:30</b> | --- Coffee/tea break ---   |
| <b>11:30 - 12:30</b> | <b>R. NIEMINEN / Helsinki Univ. of Technology, Espoo, Finland</b><br><b>Computational science as nanotechnology pillar</b>                         |
| <b>12:30 - 14:00</b> | --- Lunch break ---  |
| <b>14:00 - 15:00</b> | <b>S. BLUEGEL / Quantum Theory of Materials, IFF, Juelich, Germany</b><br><b>Magnetism at the nanoscale - Part I</b>                               |
| <b>15:00 - 16:00</b> | <b>R.M. MARTIN / Univ. of Illinois at Urbana Champaign, USA</b><br><b>Calculation of mechanical and electro-mechanical properties of materials</b> |

16:00 - 16:30 --- Coffee/tea break ---

16:30 - 17:30 **S. BARONI** / *SISSA & DEMOCRITOS, Trieste, Italy*  
**Variational principles, the Hellmann-Feynman theorem, density functional theory**

**Tuesday, 18 May 2010 CHEMISTRY (I)**

**Chairperson: Morning: S. FABRIS Afternoon: A. MORGANTE**

**18 May 2010**

09:00 - 10:00 **H. HAKKINEN** / *Nanoscience Center, Univ. Jyvaskyla, Finland*  
**Stability of metal nanoclusters - shells of atoms and electrons**

10:00 - 11:00 **G. PACCHIONI** / *Material Sciences, Univ. Milano-Bicocca, Italy*  
**From supported clusters to nanocatalysis - Part I**

11:00 - 11:30 --- Coffee/tea break ---

11:30 - 12:30 **F. BESENBACHER** / *iNANO, Univ. Aarhus, Denmark*  
**Dynamics of nanoclusters on surfaces studied by fast scanning STM**

12:30 - 14:00 --- Lunch break ---

14:00 - 15:00 **H. HAKKINEN** / *Nanoscience Center, Univ. Jyvaskyla, Finland*  
**Chemically passivated gold nanoclusters - building blocks of nano-matter?**

15:00 - 16:00 **G. PACCHIONI** / *Material Sciences, Univ. Milano-Bicocca, Italy*  
**From supported clusters to nanocatalysis - Part II**

16:00 - 16:30 --- Coffee/tea break ---

16:30 - 17:30 **R.M. MARTIN** / *Univ. of Illinois at Urbana Champaign, USA*  
**To be announced**

19:00 - 20:30 **Welcome Reception Cafeteria Terrace Leonardo Building**

**Wednesday, 19 May 2010 MECHANICAL/ASSEMBLY**

**Chairperson: Morning: N. MARZARI Afternoon: H. AKBARZADEH**

**19 May 2010**

09:00 - 10:00 **E. TOSATTI** / *SISSA, Trieste, Italy*  
**Metal nanocontacts: Physics, theory, simulation**

10:00 - 11:00 **D. TOMANEK** / *Physics & Astronomy, Michigan State Univ., East Lansing, MI, USA*  
**Control and assembly of nanoscale structures**

11:00 - 11:30 --- Coffee/tea break ---

11:30 - 12:30 **E. TOSATTI** / *SISSA, Trieste, Italy*  
**Nanofriction: Physics, theory, simulation**

12:30 - 14:00 --- Lunch break ---

**14:00 - 15:00**     **D. TOMANEK** / *Physics & Astronomy, Michigan State Univ., East Lansing, MI, USA*  
**Control and assembly of nanoscale structures - Part II**

**15:30 - 16:30**     (Room: Adriatico Guest House Informatics Laboratories)  
**P. ORDEJON and J.A. TORRES** / *CIN2 Barcelona / Univ. Madrid, Spain*  
**SIESTA TUTORIAL**

**16:30 - 16:45**     --- Coffee break ---

**16:45 - 18:30**     (Room: Adriatico Guest House Informatics Laboratories)  
**P. ORDEJON and J.A. TORRES** / *CIN2 Barcelona / Univ. Madrid, Spain*  
**continuation of SIESTA TUTORIAL**

#### Thursday, 20 May 2010 ELECTRONIC (2)

Chairperson: Morning: **M. PERESSI** Afternoon: **R. RESTA**

20 May 2010

**09:00 - 10:00**     **G. GALLI** / *Univ. of California at Davis, Chemistry, CA, USA*  
**Dielectric properties of materials, solids and nanostructures from first principles - Part I**

**10:00 - 11:00**     **R. NIEMINEN** / *Helsinki Univ. of Technology, Espoo, Finland*  
**Nanostructured carbon and complex oxides**

**11:00 - 11:30**     --- Coffee/tea break ---

**11:30 - 12:30**     **M. STRANO** / *MIT, Chemical Engg., Cambridge, MA, USA*  
**New concepts in molecular and energy transport within carbon nanotubes: thermopower waves, stochastically resonant ion channels, and single molecule biosensors**

**12:30 - 14:00**     --- Lunch break ---

**14:00 - 15:00**     **S. BLUEGEL** / *Quantum Theory of Materials, IFF, Juelich, Germany*  
**Magnetism at the nanoscale - Part II**

**15:00 - 16:00**     **G. GALLI** / *Univ. California at Davis, Chemistry, Davis, CA, USA*  
**Dielectric properties of materials, solids and nanostructures from first principles - Part II**

**16:00 - 16:30**     --- Coffee/tea break ---

**16:30 - 17:30**     **S. BARONI** / *SISSA & DEMOCRITOS, Trieste, Italy*  
**Response functions and lattice vibrations from density-functional perturbation theory**

**17:30 - 18:30**     **POSTER SESSION**

#### Friday, 21 May 2010 CHEMISTRY (2)

Chairperson: Morning: **G. SCOLES**

21 May 2010

**09:00 - 10:00**     **M. SCHEFFLER** / *Theory Department, FHI, Berlin, Germany*  
**Get Real! Multi-scale modeling from first principles of materials properties and function**

**10:00 - 11:00**     **G. PACCHIONI** / *Material Sciences, Univ. Milano-Bicocca, Italy*  
**From supported clusters to nanocatalysis - Part III**

- 11:00 - 11:30 --- Coffee/tea break ---
- 11:30 - 12:30 **H. HAKKINEN** / *Nanoscience Center, Univ. Jyvaskyla, Finland*  
**Catalytic properties of nanoscale gold**
- 12:30 - 14:00 --- Lunch break ---
- 14:00 - 15:30 **Roberto CAR** / *Princeton Univ., Princeton, U.S.A.*  
 DIRAC MEDAL CEREMONY  
**Quantum mechanics in a glass of water**
- 15:30 - 17:00 **Michele PARRINELLO** / *ETH, Zurich, Switzerland*  
 DIRAC MEDAL CEREMONY  
**Coloring the noise or cheating one's way to quantum effects**

**Monday, 24 May 2010 OPTICAL (I)**

24 May 2010

- 09:00 - 10:00 **E. MOLINARI** / *Fisica, Univ. di Modena e Reggio Emilia, Modena, Italy*  
**To be announced**
- 10:00 - 11:00 **S. JOHNSON** / *MIT, Applied Mathematics, Cambridge, MA, USA*  
**Computational Photonics: Band structures and dispersion relations**
- 11:00 - 11:30 --- Coffee/tea break ---
- 11:30 - 12:30 **R. GEBAUER** / *ICTP, Trieste, and Democritos, Trieste, Italy*  
**Time-dependent density functional theory and its applications to linear and non-linear optical properties**
- 12:30 - 14:00 --- Lunch break ---
- 14:00 - 15:00 **E. MOLINARI** / *Fisica, Univ. di Modena e Reggio Emilia, Modena, Italy*  
**To be announced**
- 15:00 - 16:00 **S. JOHNSON** / *MIT, Applied Mathematics, Cambridge, MA, USA*  
**Computational Photonics: Cavities and resonant devices**
- 16:00 - 16:30 --- Coffee/tea break ---
- 16:30 - 17:30 **M. SCHEFFLER** / *Theory Department, FHI, Berlin, Germany*  
**At the fifth rung of Jacob's ladder: A discussion of exact exchange plus local- and nonlocal-density approximations to the correlation functional**

**Tuesday, 25 May 2010 OPTICAL (II)**

25 May 2010

- 09:00 - 10:00 **E. MOLINARI** / *Fisica, Univ. di Modena e Reggio Emilia, Modena, Italy*  
**To be announced**
- 10:00 - 11:00 **S. JOHNSON** / *MIT, Applied Mathematics, Cambridge, MA, USA*  
**Computational Photonics: Forces and quantum fluctuations**

- 11:00 - 11:30 --- Coffee/tea break ---
- 11:30 - 12:30 **Ph. KIM** / *Physics, Columbia Univ., New York, USA*  
**Electric transport in carbon nanotubes and graphene**
- 12:30 - 14:00 --- Lunch break ---
- 14:00 - 15:00 **R. GEBAUER** / *ICTP, Trieste and Democritos, Trieste, Italy*  
**A computationally efficient approach to the computation of TDDFT spectra in complex systems**
- 15:30 - 16:30 (Room: Adriatico Guest House Informatics Laboratories)  
**R. GEBAUER and P. UMARI** / *ICTP, Trieste and Democritos, Trieste, Italy*  
**QE TUTORIAL**
- 16:30 - 16:45 --- Coffee/tea break ---
- 16:45 - 17:45 (Room: Adriatico Guest House Informatics Laboratories)  
**R. GEBAUER and P. UMARI** / *ICTP, Trieste and Democritos, Trieste, Italy*  
**continuation of QE TUTORIAL**

**Wednesday, 26 May 2010 TRANSPORT**  
**Chairperson: A. GOLDONI**

26 May 2010

- 09:00 - 10:00 **A.-P. JAUHO** / *DTU Nanotech, Micro-and Nanotechnology, Lyngby, Denmark*  
**Nanowires and nanopatterned graphene - Computational methods and physical phenomena - Part I**
- 10:00 - 11:00 **F. MAURI** / *IMPMC, Univ. Pierre et Marie Curie, Paris, France*  
**Electric transport in carbon nanotubes and graphene at high field - Part I**
- 11:00 - 11:30 --- Coffee/tea break ---
- 11:30 - 12:30 **L. VENKATARAMAN** / *Applied Physics & Mathematics, Columbia Univ., New York, USA*  
**Electronics and mechanics of single molecule circuits**
- 12:30 - 14:00 --- Lunch break ---
- 14:00 - 15:00 **A.-P. JAUHO** / *DTU Nanotech, Micro-and Nanotechnology, Lyngby, Denmark*  
**Nanowires and nanopatterned graphene - Computational methods and physical phenomena - Part II**
- 15:00 - 16:00 **F. MAURI** / *IMPMC, Univ. Pierre et Marie Curie, Paris, France*  
**Electric transport in carbon nanotubes and graphene at high field - Part II**
- 16:00 - 16:30 --- Coffee/tea break ---
- 16:30 - 17:30 **A.-P. JAUHO** / *DTU Nanotech, Micro-and Nanotechnology, Lyngby, Denmark*  
**Nanowires and nanopatterned graphene - Computational methods and physical phenomena - Part I**
- 17:30 - 18:30 **Poster Session**

**Thursday, 27 May 2010 MECHANICAL / ASSEMBLY**

27 May 2010

- 09:00 - 10:00**     **P. GUMBSCH** / *Fraunhofer-Institut fuer Werkstoffmechanik IWM, Freiburg, Germany*  
**Mechanical properties at the nanoscale - Part I (tentative)**
- 10:00 - 11:00**     **D. FRENKEL** / *Univ. Cambridge, Chemistry, U.K.*  
**Self-assembly at the nanoscale - Part I (tentative)**
- 11:00 - 11:30**     --- Coffee/tea break ---
- 11:30 - 12:30**     **F. STELLACCI** / *MIT, Materials Science & Engg., Cambridge, MA, USA*  
**Self-assembly on flat and curved surfaces**
- 12:30 - 14:00**     --- Lunch break ---
- 14:00 - 15:00**     **D. FRENKEL** / *Univ. Cambridge, Chemistry, U.K.*  
**Self-assembly at the nanoscale - Part II (tentative)**
- 15:00 - 16:00**     **P. GUMBSCH** / *Fraunhofer-Institut fuer Werkstoffmechanik IWM, Freiburg, Germany*  
**Mechanical properties at the nanoscale - Part II (tentative)**
- 16:00 - 16:30**     --- Coffee/tea break ---
- 16:30 - 17:30**     **D. FRENKEL** / *Univ. Cambridge, Chemistry, U.K.*  
**Self-assembly at the nanoscale - Part III (tentative)**
- 19:00 - 20:15**     --- Performance by the Choir of the Trieste Conservatory "G.Tartini" ---

## Friday, 28 May 2010 BIOLOGY

28 May 2010

- 09:00 - 10:00**     **M. VENDRUSCOLO** / *Univ. Cambridge, Chemistry, U.K.*  
**Computational methods for the determination of protein structure and dynamics - Part I**
- 10:00 - 11:00**     **D. ESTRIN** / *CONICET, INQUIMAE, Buenos Aires, Argentina*  
**QM and hybrid QM-MM simulation of biomolecules - Part I**
- 11:00 - 11:30**     --- Coffee/tea break ---
- 11:30 - 12:30**     **M. VENDRUSCOLO** / *Univ. Cambridge, Chemistry, U.K.*  
**Computational methods for the determination of protein structure and dynamics - Part II**
- 12:30 - 14:00**     --- Lunch break ---
- 14:00 - 15:00**     **D. ESTRIN** / *CONICET, INQUIMAE, Buenos Aires, Argentina*  
**QM and hybrid QM-MM simulation of biomolecules - Part II**
- 15:00 - 16:00**     **M. VENDRUSCOLO** / *Univ. Cambridge, Chemistry, U.K.*  
**Computational methods for the determination of protein structure and dynamics - Part III**
- 16:00 - 16:30**     --- Coffee/tea break ---
- 16:30 - 17:30**     **D. ESTRIN** / *CONICET, INQUIMAE, Buenos Aires, Argentina*  
**QM and hybrid QM-MM simulation of biomolecules - Part III**
- 17:30 - 18:00**     **CLOSING REMARKS**

