**CPMD2011: Extending the limits of ab initio molecular dynamics for Chemistry, Materials Science and Biophysics**

Barcelona, 5-9 September 2011, http://www.pcb.ub.es/cpmd2011

**Organizers: Roberto Car** (Princeton University, USA)**, Michele Parrinello** (ETH Zurich, Switzerland)**, Paolo Carloni** (German Research School, Germany)**, Carme Rovira** (ICREA **-** Parc Científic de Barcelona, PCB, Spain)

**Summary**

Density functional theory based molecular dynamics simulation (ab initio or Car-Parrinello MD) represented a milestone in computational physics and has dramatically influenced the methodology behind electronic structure calculations for solids, liquids and molecules. *Ab initio* MD is becoming a standard tool in molecular simulations of physical, chemical and biological processes. The CPMD2011 workshop aimed to be a platform for discussion of the latest progress in theory and applications, as well as defining the dominant trends in the field for the next years. The conference should facilitate interactions between the most prominent researchers working in this area and emerging young scientists in an informal environment.

The conference covered the following topics: Latest AIMD developments, Metadynamics, QM/MM methods, CP2K, AIMD applications in materials science, Chemistry and Biochemistry, Water and aqueous solutions, Large scale simulations.

**Scientific content**

The conference lasted five days and it was organized as follows. The first half was oriented towards methods and AIMD applications in solid state physics and materials science, whereas the second half was devoted to chemistry and biochemistry. Due to the high number of posters received (93) we decided to make two poster sessions. The full list of posters and abstracts are available at the conference web page.

There were several sessions dedicated to methods (especially metadynamics and QM/MM) and codes/tools (CPMD, CP2K and Plumed). One morning session was devoted to ***metadynamics***, which enables the simulation of rare events and, as a consequence, the search for transition states and the exploration of reaction mechanisms of increasing complexity. The metadynamics session was on Tuesday morning and covered the recent advances (well tempered MTD, bias exchange MTD, parallel tempering MTD, etc.) as well as the development of related tools (e.g. Plumed). Examples of application in materials science, physics, chemistry and biochemistry were presented during the rest of the meeting. Starting with a plenary by Ursula Röthlisberger, the state of the art of ***hybrid methods*** (mainly QM/MM) was presented, following by a discussion on how to improve the computational overload and accuracy of such calculations. Other methods presented were those specifically devoted to calculation of acidity constants at interfaces (talk by Marialore Sulpizi), nuclear quantum effects (talk by Michele Ceriotti), neural network potential energy surfaces (talk by Jorg Behler), Montecarlo methods (talks by Ali Alavi and Leonardo Guidoni) and charge constrained density functional theory (talk by Jochen Blumberger). Three talks were focused on how to account for van der Waals interactions in DFT calculations. Concerning codes, Alessandro Curioni delivered a plenary on the state of CPMD code and new scalability frontiers in ab-initio *MD*. Starting with a plenary by Jürg Hutter, one afternoon session was devoted to CP2K, a very efficient AIMD code that is growing in importance as new capabilities are implemented.

Because of the importance of classical simulations in many of the topics covered by the meeting (in the study of enzymatic reactions, for instance, classical simulations are the starting point of the QM/MM simulations, and metadynamics was initially formulated in the context of classical MD), we decided to open the meeting also to applications of classical approaches to favor constructive discussions on how to address realistic problems. (lectures by Jim Pfaendner, Modesto Orozco on biochemistry simulations, Davide Donadio and Jorg Behler on applications to materials science, for instance).

Clearly, the improvements of algorithms and increase in computer power have stimulated the field of AIMD in recent years. It is today possible to study problems of a level of complexity that was inconceivable ten years ago. The selected applications were intended not only to survey some of these problems, but also to highlight current limitations and future challenges. The topics of interest were the following: phase

transformations, phase-change materials, thermoelectric materials, actinide materials, graphene, polyoxometalates, Li-air batteries, photo- and electrocatalysis, water/hydrophobic interfases, ionic liquids, chemical reactions in solution, enzymatic reactions, hydrogen oxidation and hydrogen production, anticancer prodrugs, photoactive proteins.

**Discussion at the event**

Erio Tosatti opened the meeting with a speech on "Open problems problems in solid state physics" such as changes from Mott insulating to metallic and superconducting, friction and nanofriction, phase transitions, stick-slip sliding, etc. Some of these problems cannot be tackled with first-principles approaches yet, thus being future challenges. This was an aspect of discussion that continued specially after the plenary talks of Michael L. Klein ("HPC challenges for the next decade and beyond") and Giulia Galli ("On the search of sustainable energy sources").

The new methods being developed (some of them presented along the metadynamics session on Tuesday morning) to enhance the sampling of the phase space generated a lively discussion on how to obtain quantitative energy data. Several promising approaches have been presented. The description of van der Waals interactions (a well known shortcoming of the common DFT functionals) in AIMD simulations was discussed, specially after the talks of Robert DiStasio Jr. ("An efficient real-space implementation of the van der Waals energy and analytical forces in plane-wave ab initio molecular dynamics") and Pier Luigi Silvestrelli ("van der Waals interactions in DFT using wannier functions").

On the topic of the simulation of chemical reactions, the talk of Pietro Vidossich on explicit solvent modeling in homogeneous cataysis showed that it starts to be feasible to model chemical reactions not only in aqueous environments.

Discussions included the crucial importance of methods development to check the accuracy/predictability of ab initio simulations, thereby helping scientists to understand and even predict structure/function relationships of complex systems. But as important as obtaining accurate results is to advance in the simulation of systems of increasing complexity. Answering relevant questions in Biochemistry and Biophysics requires modeling of large and complex systems. Quite impresive examples were presented such as Ribozyme/Protein systems, carbohydrate-building enzymes, heme proteins and DNA/RNA-processing enzymes. As discussed in the talk of Ursula Röthlisberger, size is not any more a problem (at least not so much as it used to be) but length still is. Therefore the development and continuous test of methods for enhancing the sampling of pahse space becomes crucial.

Michele Parrinello closed the conference highlighting the quality of the research presented, the importance of the new programs and tools being developed (such as CP2K and Plumed). He also stressed the importance of accuracy issues in AIMD simulations.

**To what extent were the objectives of the workshop achieved**

The workshop excellently fulfilled the expectations of very high-level oral presentations and constructive discussions. Most participants were junior researchers, which is definitely a good point, but on the other hand they did not participate actively in the discussions, which instead were mainly centralized by the senior researchers. The conference room was at full occupation during the complete meeting (even the last day), which is something not very common that tells about the high quality of the oral presentations.
The conference logistics went extremely well.

**Suggestions for new workshops/tutorials/conferences on the topic** We early realized that there was a high number of registrations (more than the size of the conference room can afford) therefore we had to close the registration some weeks before the deadline. Clearly, the topic of the conference, the low registration and accommodation fee and Barcelona itself, made the conference very attractive for both senior and young researchers. We suggest that these aspects are taken into account for future CPMD conferences and that they should be planned for a higher number of participants (200-250). Due to the large number of topics presented, a program including parallel could also be considered.

**CONFERENCE PROGRAM**

**Monday, September 5, 2011**

08:00 – 09:30 **Registration**

09:30 – 10:00 **Opening ceremony: Fernando Albericio** (Director of Parc Científic de Barcelona, Spain)
**Michael Klein** (Temple University, USA), **Roberto Car** (Princeton University, USA), **Michele Parrinello** (ETH Zurich), **Carme Rovira** (ICREA – Parc Científic de Barcelona)

10:00 – 10:50 **Opening lecture** (Chair: Michele Parrinello) by **Erio Tosatti** (International School for Advanced Studies, SISSA, Trieste, Italy)**.**
*The most beautiful sea: open problems in solid state physics.*

10:50 – 11:20 **Coffee break**

**Session I: materials science** (Chair: Giovanni Bussi).
11:20 – 11:50 **Roman Martoňák** (Comenius University Bratislava, Slovakia).
*Pressure-induced structural transitions in BN from ab initio metadynamics*

11:50 – 12:20 **Davide Donadio** (Max Planck Institute for Polymer Science, Mainz, Germany).
*Thermal transport in thermoelectric materials*

12:20 – 12:50 **Jörg Behler** (Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Germany)
*Neural network potential energy surfaces for atomistic simulations*

12:50 – 15:00 **Lunch**

15:00 – 15:50 Plenary II (Chair: Roberto Car). **Giulia Galli** (University of California, Davis, USA)
*It's all about energy and clean water*

**Session II: methods** (Chair: Roberto Car)
15:50 – 16:20 **Marialore Sulpizi** (University of Mainz, Germany)
*Calculation of acidity constants at interfaces*

16:20 – 16:40 **Michele Ceriotti** (University of Oxford, UK)
*Nuclear quantum effects in water by colored-noise path integral dynamics*

16:40 – 17:00 **Chao Zhang** (German Research School for Simulation Sciences, Jülich, Germany)
*Excess proton at water/hydrophobic interfaces: an ab initio molecular dynamics study*

17:00 – 18:30 **Coffee break & POSTER SESSION I** (odd numbers)

**Tuesday, September 6, 2011**

09:00 – 09:50 Plenary III (Chair: Ursula Röthlisberger). **Michael L. Klein** (Temple University, Pennsylvania, USA).
*HPC Challenges for the Next Decade and Beyond – From Discovery to Applications at the Nano-Bio-Med Frontier*

**Session III: metadynamics** (Chair: Ursula Röthlisberger)
09:50 – 10:20 **Giovanni Bussi** (International Scho ol for Advanced Studies, SISSA, Trieste, Italy)
*Accelerated sampling of the conformational space in biomolecules: From small proteins to RNAs*

10:20 – 10:40 **Gareth Tribello** (ETH Zurich, Lugano, Switzerland)
*Exploiting machine learning in enhanced sampling calculations*

10:40 – 11:10 **Coffee break**

**Session III: metadynamics** (cont.) (Chair: Michael L. Klein)
11:10 – 11:40 **Francesco Gervasio** (Centro Nacional de Investigaciones Oncológicas, Madrid, Spain)

*Understanding the plasticity of oncogenic tyrosine kinases through experimentally validated ParallelTempering-metadynamics and PathCV calculations*

11:40 – 12:00 **Alessandro Barducci** (ETH Zurich, Lugano, Switzerland)
*Determination of protein multimerization free-energy landscape using explicit-solvent MD simulations*

12:00 – 12:20 **Massimiliano Bonomi** (University of California, San Francisco, USA)
*Enhanced sampling in the well-tempered ensemble*

12:20 – 12:40 **Xevi Biarnés** (IQS-Universitat Ramon Llull, Barcelona, Spain)
*METAGUI – A new VMD extension to analyze and visualize metadynamics simulations*

12:40 – 13:00 **Albert Ardèvol** (Parc Científic de Barcelona, Spain)
*How does nature make glycosidic bonds. A metadynamics investigation*

13:00 – 15:00 **Lunch**

15:00 – 15:50 Plenary IV (Chair: Marialore Sulpizi)
**Jürg Hutter** (University of Zurich, Switzerland)**.** *CP2K: Developments and Applications*

**Session IV: methods/CP2K** (Chair: Marialore Sulpizi)
15:50 – 16:20 **Matthias Krack** (PSI Lugano, Switzerlad). *Simulation of Actinide Materials*

16:20 – 16:50 **Joost Vandevondele** (University of Zurich, Switzerland)
*Simulating large condensed phase systems with GGA and hybrid density functionals*

16:50 – 17:20 **Coffee break**

**Session IV: methods/CP2K** (cont.) (Chair: Leonardo Guidoni)
17:20 – 17:50 **Ivano Tavernelli** (Ecole Federale Polytechnique de Lausanne, EPFL, Switzerland)*Nonadiabatic molecular dynamics with explicit external electrostatic and electromagnetic fields*

17:50 – 18:20 **Ali Alavi** (University of Cambridge, UK). *Quantum Monte Carlo approach to the Full CI problem*

**Wednesday, September 7, 2011**

09:00 – 09:50 Plenary V (Chair: Paolo Carloni). **Alessandro Curioni** (IBM Zurich, Switzerland)
*New scalability frontiers in ab-initio MD*

**Session V: materials science** (Chair: Paolo Carloni)
09:50 – 10:20 **Marcella Iannuzzi** (University of Zurich, Switzerland)
*Moire' structure or nanomesh: the case of graphene and h-BN epitaxially grown on transition metals*

10:20 – 10:40 **Rustam Khaliullin** (University of Zurich, Switzerland)
*Unraveling microscopic origins of complex behavior in carbon and sodium*

10:40 – 11:10 **Coffee break**

**Session V: materials science** (cont.) (Chair: Agustí Lledós)
11:10 – 11:30 **Antonio Rodríguez-Fortea** (Universitat Rovira Virgili, Tarragona, Spain)
*Formation mechanisms of small polyoxometalates: a combined study using computational methods and mass spectrometry*

11:30 – 12:00 **Irmgard Frank** (U. Hannover, Germany). *First-principles simulation of chemical dynamics*

12:00 – 12:30 **Eduardo Hernández** (Instituto de Ciencia de Materiales de Madrid, CSIC, Spain)
*Melting of lithium from first principles simulations*
12:30 – 15:00 **Lunch**

15:00 – 15:50 Plenary VI (Chair: Simone Raugei ). **Annabella Selloni (Princeton University, USA)**

*First principles simulations of materials and processes in photo- and electro-catalysis*

**Session VI: water / aq. solutions** (Chair: Simone Raugei)
15:50 – 16:20 **Chris Mundy** (Pacific Northwest National Laboratory, PNNL, USA)
*A first-principles approach to understanding the specific ion effect*

16:20 – 16:40 **Robert A. DiStasio Jr.** (Princeton University, USA)
*An efficient real-space implementation of the van der Waals energy and analytical forces in plane-wave ab initio molecular dynamics with applications to liquid water*

16:40 – 17:00 **Jun Cheng** (University of Cambridge, UK)
*Oxidative dehydrogenation of water on aqueous rutile $TiO_2$(110) from DFTMD simulations*

17:00 – 18:30 **Coffee break & POSTER SESSION II** (even numbers)

**Thursday, September 8, 2011**

09:00 – 09:50 Plenary VII (Chair: Ute Röhriger). **Ursula Röthlisberger** (Ecole Federale Polytechnique de Lausanne, EPFL, Switzerland)
*About positive and negative catalysis: biochemistry with the Car-Parrinello method*

**Session VII: biochemistry** (Chair: Ute Röhrig)
09:50 – 10:20 **Mauro Boero** (Institut de Physique et Chimie des Matériaux de Strasbourg, France)
*LeuRS Synthetase: A Reactive QM/MM Investigation of Water Mediated Editing Reactions in a Hybrid Ribozyme/Protein System*

10:20 – 10:40 **Mercedes Alfonso-Prieto** (Temple University, Pennsylvania, USA)
*Understanding the redox properties of catalases by means of CPMD QM/MM calculations*

10:40 – 11:10 **Coffee break**

**Session VIII: chemistry** (Chair: Elvira Guardia)
11:10 – 11:40 **Marie-Pierre Gaigeot** (Université d'Evry val d'Essonne, France)
*DFT-based molecular dynamics simulations applied to vibrational spectroscopy. Illustrations on floppy polypeptides in the gas phase and immersed in the liquid phase, and on solid-liquid interfaces*

11:40 – 12:10 **Barbara Kirchner** (University of Leipzig, Germany)
*Ionic liquids from ab initio molecular dynamics simulations*

12:10 – 12:40 **Pier Luigi Silvestrelli** (University of Padova, Italy)
*Van der Waals interactions in DFT using Wannier functions*

12:40 – 13:00 **Pietro Vidossich** (Universitat Autònoma de Barcelona, Spain)
*Explicit solvent modeling in homogeneous catalysis: selected case studies*

13:00 – 15:00 **Lunch**

15:00 – 15:50 Plenary VIII (Chair: Carla Molteni). **Marco Bernasconi** (University of Milano-Bicocca, Milano, Italy)
*Ab-initio simulations of phase change materials for data storage*

**Session IX: materials** (Chair: Carla Molteni)
15:50 – 16:20 **Jochen Blumberger** (University College London, UK)
*Charge constrained density functional theory: implementation, successes and failures*

16:20 – 16:50 **Simone Raugei** (Pacific Northwest National Laboratory, PNNL, USA)
*Ni(II) complexes for hydrogen oxidation and hydrogen production: an ab-initio MD investigation*

16:50 – 17:20 **Leonardo Guidoni** (University of Rome, Italy)
*Geometry relaxation and vibrational spectroscopy by Quantum Monte Carlo*
20:30 **Conference dinner** .

**Friday, September 9, 2011**

**Session XI: biochemistry** (Chair: Emiliano Ippoliti)
09:30 – 10:00 **Jim Pfaendner** (University of Washington, Seattle, USA)
*Adventures in the well-tempered ensemble – getting more by spending less*

10:00 – 10:30 **Modesto Orozco** (University of Barcelona, Spain)
*New aproaches to represent protein dynamics*

10:30 – 11:00 **Coffee break**

**Session XI: biochemistry** (cont.) (Chair: Jochen Blumberger)
11:00 – 11:30 **Alessandra Magistrato** (International School for Advanced Studies, SISSA, Italy)
*Molecular mechanism of cancer disease investigated via molecular dynamics simulations*

11:30 – 12:00 **Mateo Dal Peraro** (Ecole Federale Polytechnique de Lausanne, EPFL, Switzerland)
*Computational characterization of the catalytic two-metal-ion mechanism in DNA/RNA-processing enzymes*

12:10 – 12:40 **Michele Cascella** (University of Bern, Switzerland)
*Understanding and engineering functionality of vitamin transporters of the CRAL-TRIO family by computer simulations*

12:40 – 13:00 **Carla Molteni** (Kings College London, UK)
*Is green tea good for you? Insights from atomistic simulations*

13:00 – 15:00 **Lunch**

**Session XII: biochemistry** (Chair: Mauro Boero)
15:00 – 15:20 **Pablo Campomanes** (Ecole Federale Polytechnique de Lausanne, EPFL, Switzerland)
*Molecular basis of novel anticancer prodrugs activation*

15:20 – 15:50 **Bern Ensing** (University of Amsterdam, Netherlands)
*CPMD simulation of photoactive proteins in action*

**Session XIII: materials science** (Chair: Mauro Boero)
15:50 – 16:20 **Teodoro Laino** (IBM Zurich, Switzerland)
*Toward the understanding of chemical degradation of aprotic solvents for Li-air batteries*

16:20 – 16:40 **Concluding remarks** (Michele Parrinello)
16:40 **Departure**

**LIST OF SPEAKERS** (8 plenary speakers + 43 invited speakers)

1. Giulia Galli (University of California, Davis, USA )
2. Ursula Röthlisberger (EPFL Lausanne, Switzerland)
3. Michael L. Klein (Temple University, USA)
4. Erio Tosatti (SISSA, Trieste, Italy)
5. Annabella Selloni (University of Princeton, Princeton, USA)
6. Marco Bernasconi (University of Milano, Italy)
7. Juerg Hutter (University of Zurich, Switzerland)
8. Alessandro Curioni (IBM Research, Zurich, Switzerland)
9. Roman Martoňak (Physics and Informatics Comenius University, Bratislava, Slovakia)
10. Carla Molteni (Kings College, London, UK)
11. Marialore Sulpizi (University of Mainz, Germany)
12. Jochen Blumberger (University College London, UK)
13. Irmgard Frank (University of Hannover, Germany)
14. Mauro Boero (CNRS, Strasbourg, France)

15. Ali Alavi (University of Cambridge, Cambridge, UK)
16. Marcella Iannuzzi (PSI Villingen, Switzerland)
17. Chris Mundy (PNNL Richland, Washington, USA)
18. Alessandra Magistrato (SISSA, Trieste, Italy)
19. Simone Raugei (PNNL, Richland, Washington, USA)
20. Barbara Kirchner (University of Leipzig, Germany)
21. Pier Luigi Silvestrelli (University of Padova)
22. Jörg Behler (Ruhr-Universität, Bochum, Germany)
23. Eduardo Hernández (CSIC, Madrid, Spain)
24. Teodoro Laino (IBM Research, Zurich)
25. Bern Ensing (University of Amsterdam)
26. Francesco Luigi Gervasio (CNIO, Madrid, Spain)
27. Michele Cascella (Universität Bern, Switzerland)
28. Joost Vandevondele (University of Zurich, Switzerland)
29. Marie-Pierre Gaigeot (Université d'Evry val d'Essonne, France)
30. Ivano Tavernelli (EPFL Lausanne)
31. Leonardo Guidoni (University of Rome, Italy)
32. Jim Pfaendtner (University of Washington, USA)
33. Giovanni Bussi (SISSA, Trieste, Italy)
34. Mateo Dal Peraro (EPFL Lausanne, Switzerland)
35. Michele Ceriotti (University of Oxford, UK)
36. Rustam Khaliullin (University of Zurich, Switzerland)
37. Gareth Tribello (ETH Zurich, Switzerland)
38. Massimiliano Bonomi (University of California, USA)
39. M. Alfonso-Prieto (Temple University, USA)
40. Pietro Vidossich (Universitat Autònoma de Barcelona, Spain)
41. Xevi Biarnés (Universitat Ramon Llull, Barcelona)
42. Pablo Campomanes (EPFL Lausanne)
43. Chao Zhang (German Research School, Jülich, Germany)
44. Antonio Rodríguez-Fortea (University Rovira i Virgili, Tarragona, Spain)
45. Robert DiStasio (Princeton University, USA)
46. Jun Cheng (Emmanuelle College, London)
47. Albert Ardèvol (Parc Científic de Barcelona, Spain)
48. Alessandro Barducci (ETH Zurich, Switzerland)
49. Davide Donadio (Max Plank Institute for Polymer Science, Mainz, Germany)
50. Matthias Krack (Paul SCherrer Institute, Switzerland)
51. Modesto Orozco (IRB Barcelona, Spain)

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