0.1 Report on Workshop CPMD2011: Extending the limits of ab initio molecular dynamics for Chemistry, Materials Science and Biophysics

Barcelona

September 5-9 2011

CECAM, ESF and Psi-k

Roberto Car, Michele Parrinello, Paolo Carloni and Carme Rovira

http://www.pcb.ub.es/cpmd2011

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 facilitated interactions between the most prominent researchers working in this area and emerging young scientists in an informal environment. The lectures included new AIMD developments, metadynamics, QM/MM methods, CP2K, AIMD applications in materials science, chemistry and biochemistry, water and aqueous solutions and large scale simulations.

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, heme proteins, hydrogen oxidation and hydrogen production, anticancer prodrugs, photoactive proteins.

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.

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").

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 (Tuesday morning) covered recent advances such as well tempered MTD, bias exchange MTD and parallel tempering MTD, as well as the development of related tools (Plumed). Examples of application in materials science, physics, chemistry and biochemistry were presented during the rest of the meeting. The new methods being developed to enhance the sampling of the phase space generated a lively discussion on how to obtain quantitative energy data.

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").

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.

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. Irmgard Frank presented simulations of photoreactions and mechanically induced chemical reactions.

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).
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 phase 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 were mainly centralized by 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.

Suggestions for new workshops/tutorials/conferences on the topic

Because of the high number of registrations (more than the size of the conference room can afford) we closed 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 (specially the last). 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, parallel sessions should 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 grownon 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 TiO2(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

12:00 – 12:30 Michele Cascella (University of Bern, Switzerland) Understanding and engineering functionality of vitamin transporters of the CRAL-TRIO family by computer simulations
12:30 – 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 PRESENTED POSTERS

P1. Computer modelling of quantum effects by using classical mechanics. H. Dammak, M. Laroche, M. Hayoun, J. J. Greffet and Y. Chalopin.
P2. Amorphous TeGeI: Structure and Comparison with Similar Systems. Iva Voleska, Jaakko Akola and Tomas Wagner.
P3. Rationalizing the stereoselectivity of proline-catalyzed asymmetric aldol reactions in water. J. Ribas-Ariño, M.A. Carvajal, A. Chaumont and M. Masia.
P4. The conformational free energy landscape of 2-deoxy--D-glucopyranose by ab initio metadynamics. Implications for catalysis of -glycosidases. Javier Iglesias-Fernández, Albert Ardèvo1, Xevi Biarnés, Antoni Planas and Carme Rovira.
P5. Density Functional Surface Stability Study of Oxidized Cu(110) & AFM Tip identification. J. Bamidele, Y. Kinoshita, T. Satoh, S. H. Lee, Y. Naitoh, Y. J. Li et al.
P6. Molecular Modeling of Interfacial Proton Transport in Polymer Electrolyte Membranes. Swati Vartak, Ata Roudgar and Michael Eikerling.
P7. Force-transformed free energy surfaces. Przemyslaw Dopieralski, Jordi Ribas-Arino and D. Marx.
P8. Protonation states of active site of class C -lactamase. Ravi Tripathi and Nisanth N. Nair.
P9. AIMD study of the mechanism of Wacker reaction. Janos Daru and Andras Stirling.
P10. Oxidative addition of water and spontaneous formation of H2 at rhodium/alumina interface. Tushar K Ghosh and Nisanth N. Nair.
P11. The role of water in metal catalyzed transfer hydrogenation. Anna Pavlova and Evert J. Meijer.
P12. Solvent reorganization effect on electron transfer to a flavin molecule. Murat Kilic and B. Ensing.
P13. Superhalogen molecules as strong electron acceptors. Celina Sikorska and Piotr Skurski.

P14. First principles study of LiNH2/Li2NH hydrogen storage system. Giacomo Miceli, M. Ceriotti, C. Cucinotta, M. Bernasconi, M. Parrinello.
P15. Frequency modulation of vibrational N-H modes by collective molecular motions in porphycene from ab initio calculations and IR spectroscopy. Łukasz Walewski, Sylwester Gawinkowski, Jacek Waluk and Bogdan Lesyng.
P16. Ethylene polymerization processes catalyzed by half-metallocene titanium(IV) complexes – molecular dynamics approach. Łukasz Piękoś, Artur Michalak.
P17. Ab initio molecular dynamics study of finite temperature and pressure effects on the structural and electronic properties of the SiC/double layer graphite interface. A. M. Ukpong and Nitthaya Chetty.
P18. Atomic level characterisation of the binding and secretion of FHA by the TpsB transporter FhaC. Harish Kumar Ravi, Francesca Collu and Michele Cascella.
P19. Ab initio molecular dynamics simulation and free energy exploration of copper (I) complexation by chloride and bisulphide in hydrothermal fluids. Yuan Mei, D. M Sherman, J. Brugger and W. Liu.
P20. Ab Initio Molecular Dynamics Simulations for Endocyclic Cleavage-Induced Anomerization Reactions of Glycosides. Hiroko Satoh, Teodoro Laino, and Jürg Hutter.
P21. Activation parameters and their variation from molecular simulation. Christof Drechsel-Grau and Michiel Sprik.
P22. Vibrational Spectroscopy of Biomolecules by mixed Quantum/Classical Molecular Dynamics. Daniele Bovi, R. Spezia, A. Mezzetti, R. Vuilleumier, M.-P. Gaigeot, L. Guidoni.
P23. In Silico Prescreening of Computanionally Designed Enzymes. Bernardo Sosa Padilla Araujo, Thomas F. Miller III and Stephen L. Mayo
P24. Ab initio molecular dynamics study of AunTi clusters. J. Beloševic-Cavor, V. Koteski and J. Radaković.
P25. Computation of equilibrium isotope fractionation between minerals and aqueous solutions. Piotr M. Kowalski and Sandro Jahn.
P26. Spectroscopic fingerprint of water around small hydrophobic solutes. Maria Montagna, Fabio Sterpone, and Leonardo Guidoni.
P27. Quantum Monte Carlo methods for molecular polarizabilities within a hybrid QMC/MM scheme. Emanuele Coccia and Leonardo Guidoni
P28. Modelling solute-solvent interactions in molecular liquids. Ling Ge
P29. Ab Initio Molecular Dynamics Simulations of Aqueous Glycine Solutions: Solvation Structure and Vibrational Spectra. Jian Sun, Harald Forbert, and Dominik Marx.
P30. Computational studies on the selectivity of -tocopherol transfer protein. R. Helbling, W. Aeschimann, F. Simona, A. Stocker and M. Cascella.
P31. Deamidation of Peptides: Succinimide Hydrolysis Pathways. Saron Catak, Bart De Sterck, Rosa E. Bulo, Michel Waroquier and Veronique Van Speybroeck.
P32. Solvation properties of alkai and halide ions in water from Car-Parrinello molecular dynamics simulations. Ausias-March Calvo, M. Masia, I. Skarmoutos, and E. Guàrdia.
P33. Structure, Dynamics and Computational Vibrational Spectroscopy for Ac-Ala-LysH+ Peptides (n = 5, 10, 15). Mariana Rossi, V. Blum, A. Tkatchenko, and M. Scheffler.

P34. Modeling of non-adiabatic transitions in energetic materials. Andrey Mukhanov and V. Stegailov

P35. Density Functional Evaluation of the Composition, Charge, and Magnetic Structure of Nitrogenase FeMo-Cofactor. Travis V. Harris and Robert K. Szilagyi

P36. Adsorption of hydrazine (N2H4) and fluoroform (F3CH) on hexagonal ice(0001): first principles investigations on blue-shifted hydrogen bonds and the mechanism of chirality changes. Paweł Rodziewicz and Bernd Meyer.

P37. The role of d-shell polarization in the dynamics of nanocluster collisions. Ricardo Ramírez, F. Muñoz, M. Kiwi, G. García, J. Rogan and J. A. Valdivia

P38. DFT and Molecular Dynamic study of metal ions in different solvents. N. Sadanandam, Srinivas Tulishetti, and Jayant K. Singh.

P39. Magnetostructural Dynamics of a Rieske-type [2Fe-2S] Protein. Md. Ehesan Ali, Nisanth N. Nair, Volker Staemmler, and Dominik Marx.

P40. Stochastic Optimization of Capping Potentials for Hybrid QM/MM Calculations. Christoph Schiffmann, Daniel Sebastiani.

P41. Scaling and convergence of all-atom DFT calculations by order-N density-matrix-based methods. Antonio S. Torralba, Tsuyoshi Miyazaki and David R. Bowler.

P42. The nature of [PdCl2(C2H4)(H2O)] as active species in the wacker process. New insights from ab initio molecular dynamics simulations. Gábor Kovács, András Stirling, Agustí Lledós and Gregori Ujaque.

P43. Ab initio molecular dynamics simulation of proton transport in a biological ion channel. Jens Dreyer, Chao Zhang, Emiliano Ippoliti, Paolo Carloni.

P44. The mechanism of ozonolysis on C70 fullerene surface. The influence of endohedral noble gas substituent. Andrzej Bil, Zdzisław Latajka, Carole A. Morrison.

P45. Electronic and optical properties of carotenoids: The case of Peridnin. Daniele Varsano and Leonardo Guidoni.

P46. Predicting color tuning in opsin proteins: A difficult case for first-principle methods? Omar Valsson

P47. EPR spectral lineshapes via ab initio MD simulations. Hossam Elgabarty and Daniel Sebastiani

P48. Physisorption and diffusion pathways of H2 molecule on graphene by first principle calculations. Francesca Costanzo, Francesco Ancilotto and Pier Luigi Silvestrelli

P49. First principles molecular dynamics simulation of liquid cyclopentasilane. Pham Tien Lam, Tatsuya Shimoda, Nobuo Otsuka and Dam Hieu Chi

P50 Proton transport mechanisms in phosphorus oxoacids. L. Vilciauskas, M. E. Tuckerman, G. Bester, S. J. Paddison, K.-D. Kreuer

P51. An Efficient Novel Method for Smooth and Adaptive MM→QM Switching. M. Böckmann, N.L. Doltsinis and D. Marx

P52. Study of cisplatin and transplatin binding to the copper transporter Ctr1 from QM/MM and classical MD simulations. T. H. Nguyen, E. Ippoliti, F. Arnesano, G. Natile and P. Carloni

P53. Structure and solvation effects on ionic liquids. Alfonso S. Pensado, Martin Brehm, Barbara Kirchner

P54. Protonation of a hydroxide anion bridging two divalent magnesium cations in water. Jung Mee Park and Mauro Boero

P55. Excited state solvation dynamics of a molecular THz probe. Christoph Allolio and Daniel Sebastiani
P56. Investigation of the CO2 reaction mechanisms on Ni-clusters deposited on a CeO2(111) surface using CP2K. K. Hahn, A. Seitsonen and J. Hutter
P57. Density Functional Theory study on the Molecular Structure and Reactivity of 5-fluorouracil. Iskra Koleva, Paulina Gorolomova and Galina Gencheva
P58. Infrared gas phase spectra of strongly hydrogen bonded ammonia hydrogen halides complexes obtained from CPMD simulations. Paweł Panek and Zdzisław Latajka
P59. Determination of the potential energy surface of small molecules via Quantum Monte Carlo for the calculation of equilibrium structures and harmonic frequencies. A. Zen, M. Barborini, D. Zhelyazov, S. Sorella and L. Guidoni
P60. Theoretical study on coordination ability of the ligands 2,2‘-Dipyridylamine and 2,2‘-Dipyridylketone. Paulina Gorolomova and Galina Gencheva
P61. Spectral tuning by protein field on peridinin molecules in two different forms of Peridinin - Chlorophyll a – Protein. Gaia Di Paolo and Leonardo Guidoni
P62. Hydrophobicity and hydrophilicity in ionic liquids: Car-Parrinello and classical molecular dynamics simulation. Mohammad H. Ghatee, Amin Reza Zolghadr and F. Moosavi
P63. Reconstruction of the Free Energy Surface of a Transition metal Catalyzed Reaction. Eva Perlt, M. Brüssel, P. di Dio and B. Kirchner
P64. Calculation of the electronic structure of graphdiyne. Željko Crljen and G. Baranovic
P65. Cyclization reaction of trimeric aluminium complexes studied by ab initio metadynamics. G. Lanzani, A. P. Seitsonen, M. Iannuzzi, J. Hutter and S. O. Pehkonen
P66. Model systems approach to the study of UV light stimulated DNA-proteins crosslink reaction. Marco Micciarelli, C. Altucci, R. Velotta, B. Curchod, I.Tavernelli, U. Roethlisberger.
P67. A concerted triple-jump in the recombination of hydronium and hydroxide Ions. Ali Hassanali, Meher Prakash, Hagai Eshet and Michele Parrinello
P68. Atomistic simulation of the interaction of an electrolyte with graphite nanostructures. A. V. Lankin, G. E. Norman and V. V. Stegailov
P69. N···CO weak bond as a solvation probe. D. Kozlowski, J. Ilmé and P. Fleurat-Lessard
P70. Charge localization dynamics induced by oxygen Vacancies on the TIO2(110) Surface and titania and gold-promoted titania surfaces interaction with small molecules. Matteo Farnesi Camellone and D. Marx
P71. Combining ab-initio molecular dynamics with a dipole-field model to study acid dissociation reactions. Patrick Maurer, Vibin Thomas and Radu Iftimie
P72. Theoretical investigation of the amino acid – titania interaction. S. Köppen, J. Bartels, W. Friedrichs, L. Colombi Ciacchi and W. Langel
P73. Catalytic synthesis of methanol over cu/zno: exploration of energy surfaces for determining adsorption sites for CO2. L. Martínez-Suárez, J. Frenzel, B Meyer and D. Marx
P74. Massively parallel applications in biophysics by using CPMD. Emiliano Ippoliti, Chao Zhang, Jens Dreyer and Paolo Carloni

P75. Predicting new crystal structures from first-principles. D. Schärf and T. Kühne
P76. Reaction pathways for the pyrolysis of glycerol, propylene glycol and triacetin in the gas phase and at solid surfaces. C. Tuma, T. Laino, A. Curioni, E. Jochnowitz and S. Stolz
P77. Tully's surface hopping method in practice: FIREBALL calculations of photoactive organic materials. Enrique Abad, James P. Lewis , Pavel Jelínek and José Ortega
P78. The interactions of nitrogen dioxide with graphene and with Rh clusters stabilized by graphene. Sara Furlan and Paolo Giannozzi
P79. Acidity constants of the -MnO2 (110) surface from Density Functional Theory based molecular dynamics. J. A. Kattirtzi, J. Cheng, M. Sulpizi and M. Sprik
P80. Synthesis, characterization and modeling of ruthenium catalysts for water oxidation. José Luis Vallés Pardo, M. C. Guijt, Khurram S. Joya, Francesco Buda and Huub J.M. de Groot
P81. A novel grand-canonical approach towards linear scaling: Application to liquid methane under extreme conditions. Dorothee Richters, M. Ceriotti and T. D. Kühne
P82. Supramolecular packing and hydrogen bonding in organic functionalized materials from first principles. Dmytro Dudenko, D. Sebastiani, M. Ryan Hansen and H. W. Spiess
P83. New insights into polonium solution chemistry. R. Ayala, J. M. Martínez, R. R. Pappalardo and E. Sánchez-Marcos
P84. IR spectra of some model complexes of biological importance from Born-Oppenheimer molecular dynamics calculations. Artur Smaga, Joanna Sadlej, Łukasz Walewski and Bogdan Lesyng
P85. Study of the structure of chalcogenide glasses by ab initio molecular dynamics and 77Se NMR simulation. Kateryna Sykina, C. Roiland, L. Le Pollès, B. Bureau and Eric Furet
P86. Improving the convergence of estimators in path integral molecular dynamics via higher order Trotter factorization schemes. Alejandro Pérez and Mark E. Tuckerman
P87. Thermodynamics of electron flow in the bacterial decaheme cytochrome MtrF. Marian Breuer, P. P. Zarzycki, K. M. Rosso and J. Blumberger
P88. Catalytic itinerary in 1,3-1,4--glucanase unraveled by QM/MM metadynamics. X. Biarnés, A. Ardèvo1, A. Planas, C. Rovira.
P89. Locality and fluctuations: trends in imidazolium-based ionic liquids and beyond. Katharina Wendler, S. Zahn, F. Dommert, R. Berger, C. Holm, B. Kirchner and L. Delle Site
P90. The role of hydrogen bond in water diffusion. Qu Chen, Yingchun Liu, Qi Wang and K. E. Gubbins
P91. Understanding the instability of IRMOF-1 in humid environments. Luca Bellarosa and N. López
P92. On binding and reactivity of potent covalent inhibitors of fatty acide amide hydrolase. G. Palermo, M. Neri, P. Campomanes, I. Tavernelli, A. Cavalli, U. Rothlisberger and M. De Vivo
P93. First step in the charge separation process in the reaction center of photosynthetic bacteria. Thomas Eisenmayer

ABSTRACTS OF PRESENTED PAPERS: The book of abstracts (7MB) is available at the conference web page (http: //www.pcb.ub.es/cpmd2011/)

LIST OF PARTICIPANTS

ORGANIZERS

1. Roberto Car (Princeton University, USA)
2. Michele Parrinello (ETH Zurich, Switzerland)
3. Paolo Carloni (German Research School, Germany)
4. Carme Rovira (ICREA - Parc Científic de Barcelona, PCB, Spain)

PLENARY SPEAKERS

5. Giulia Galli (University of California, Davis, USA)
6. Ursula Röthlisberger (EPFL Lausanne, Switzerland)
7. Michael L. Klein (Temple University, USA)
8. Erio Tosatti (SISSA, Trieste, Italy)
9. Annabella Selloni (University of Princeton, Princeton, USA)
10. Marco Bernasconi (University of Milano, Italy)
11. Juerg Hutter (University of Zurich, Switzerland)
12. Alessandro Curioni (IBM Research, Zurich, Switzerland)

INVITED SPEAKERS

13. Roman Martoñak (Comenius University, Bratislava, Slovakia)
14. Carla Molteni (Kings College, London, UK)
15. Marialore Sulpizi (University of Mainz, Germany)
16. Jochen Blumberger (University College London, UK)
17. Irmgard Frank (University of Hannover, Germany)
18. Mauro Boero (CNRS, Strasbourg, France)
19. Ali Alavi (University of Cambridge, Cambridge, UK)
20. Marcella Iannuzzi (PSI Villingen, Switzerland)
21. Chris Mundy (PNNL Richland, Washington, USA)
22. Alessandra Magistrato (SISSA, Trieste, Italy)
23. Simone Raugei (PNNL, Richland, Washington, USA)
24. Barbara Kirchner (University of Leipzig, Germany)
25. Pier Luigi Silvestrelli (University of Padova)
26. Jörg Behler (Ruhr-Universität, Bochum, Germany)
27. Eduardo Hernández (CSIC, Madrid, Spain)
28. Teodoro Laino (IBM Research, Zurich)
29. Bern Ensing (University of Amsterdam)
30. Francesco Luigi Gervasio (CNIO, Madrid, Spain)
31. Michele Cascella (Universität Bern, Switzerland)
32. Joost Vandevondele (University of Zurich, Switzerland)
33. Marie-Pierre Gaigeot (Université d'Evry val d'Essonne, France)

34. Ivano Tavernelli (EPFL Lausanne)
35. Leonardo Guidoni (University of Rome, Italy)
36. Jim Pfaendtner (University of Washington, USA)
37. Giovanni Bussi (SISSA, Trieste, Italy)
38. Mateo Dal Peraro (EPFL Lausanne, Switzerland)
39. Michele Ceriotti (University of Oxford, UK)
40. Rustam Khaliullin (University of Zurich, Switzerland)
41. Gareth Tribello (ETH Zurich, Switzerland)
42. Massimiliano Bonomi (University of California, USA)
43. M. Alfonso-Prieto (Temple University, USA)
44. Pietro Vidossich (Universitat Autònoma de Barcelona, Spain)
45. Xevi Biarnés (Universitat Ramon Llull, Barcelona)
46. Pablo Campomanes (EPFL Lausanne)
47. Chao Zhang (German Research School, Jülich, Germany)
48. Antonio Rodríguez-Fortea (University Rovira i Virgili, Tarragona, Spain)
49. Robert DiStasio (Princeton University, USA)
50. Jun Cheng (Emmanuelle College, London)
51. Albert Ardèvol (Parc Científic de Barcelona, Spain)
52. Alessandro Barducci (ETH Zurich, Switzerland)
53. Davide Donadio (Max Plank Institute for Polymer Science, Mainz, Germany)
54. Matthias Krack (Paul SCherrer Institute, Switzerland)
55. Modesto Orozco (IRB Barcelona, Spain)

REST OF PARTICIPANTS

56. Enrique Abad. Universidad Autónoma de Madrid, Spain
57. Md. Ehesan Ali. Ruhr-Universitaet Bochum, Germany
58. Christoph Allolio. FU Berlin, Germany
59. Regla Ayala. Universidad de Sevilla, Spain
60. David Balcells. Universitat Autònoma de Barcelona, Spain.
61. Samuel Baltazar. Universidad de Santiago de Chile, CHile
62. Radhakrishnan Balu. US Army Research Lab, USA
63. Joseph Bamidele. King's College London, UK
64. Albert Bartok-Partay. University of Cambridge, UK
65. Luca Bellarosa. Institut Català d'Investigació Química (ICIQ), Spain
66. Jelena Belosevic Cavor. Institute of Nuclear Sciences Vinca, Serbia
67. Andrzej Bil. University of Wroclaw, Poland
68. Marcus Böckmann. Ruhr-Universitaet Bochum, Germany
69. Josep Maria Bofill. Universitat de Barcelona, Spain
70. Monika Borkowska-Panek. University of Wroclaw, Poland
71. Daniele Bovi. University of Rome, Italy
72. Marian Breuer. University College London, UK
73. Ausias March Calvo. Universitat Politècnica de Catalunya, Spain
74. Alejandro Torres. Parc Científic de Barcelona, Spain
75. David Cantu. Iowa State University, USA
76. Rodrigo Casasnovas. Universitat de les Illes Balears, Spain

77. Saron Catak. Ghent University, Belgium
78. Qu Chen. Zhejiang University, China
79. Jun Cheng. University of Cambridge, UK
80. Nithaya Chetty. University of Pretoria, South Africa
81. Emanuele Coccia. University of Rome, Italy
82. Francesca Costanzo. University of Padova, Italy
83. Zeljko Crljen. Rudjer Boskovic Institute, Croatia
84. Hichem Dammak. Ecole Centrale Paris, France
85. Janos Daru. HAS Chemical Research Center, Hungary
86. Gaia Di Paolo. CNISM, Italy
87. Przemyslaw Dopieralski. Ruhr-Universitaet Bochum, Germany
88. Christof Drechsel-Grau. Ruhr-Universitaet Bochum, Germany
89. Jens Dreyer. German Research School for Simulation Sciences, Germany
90. Dmytro Dudenko. Max Planck Institute for Polymer Research, Germany
91. Thomas Eisenmayer. University of Leiden, Netherlands
92. Hossam Elgabarty. FU Berlin, Germany
93. Matteo Farnesi Camellone. Ruhr-Universitaet Bochum, Germany
94. Sara Furlan. University of Trieste, Italy
95. Alberto Garcia. Institut de Ciència de Materials de Barcelona-CSIC, Spain
96. Ling Ge. Imperial College, UK
97. Paulina Gorolomova. Sofia University, Bulgaria
98. Elvira Guardia. Universitat Politècnica de Catalunya, Spain
99. Konstanze Hahn. University of Zurich, Switzerland
100. Travis Harris. University of Montana, USA
101. Ali Hassanali. ETH Zurich, Switzerlñand
102. Marc Hayoun. CEA-Ecole Polytechnique, France
103. Rachel Helbling. Universität Bern, Switzerland
104. Javier Iglesias-Fernández. Parc Científic de Barcelona, Spain
105. Mehmet Ali. Ilhan Universität Duisburg-Essen, Germany
106. Ivan Infante. Universidad Pais Vasco, Spain
107. Emiliano Ippoliti. German Res. Sch. Simul. Sci., Germany
108. Tushar Kanti Ghosh. Indian Institute of Technology Kanpur, India
109. John Kattirtzi. University of Cambridge, UK
110. Murat Kilic. University of Amsterdam, Netherlands
111. Iskra Koleva. Sofia University, Bulgaria
112. Susan Köppen. University of Bremen, Germany
113. Gábor Kovács. Universitat Autònoma de Barcelona, Spain
114. Piotr Kowalski. GFZ German Research Centre for Geosciences, Germany
115. David Kozlowski. CEA, DAM, DIF, France
116. Katarzyna Kulczycka- Mierzejewska. University of Warsaw, Poland
117. Giorgio Lanzani. University of Oulu, Finland
118. Agusti Lledos. Universitat Autònoma de Barcelona, Spain
119. Luis Martinez Suarez. Universitat Autònoma de Barcelona, Spain
120. Gerald Mathias. LMU Munich, Germany
121. Patrick Maurer. Private, Switzerland
122. Eloi Marín. Parc Científic de Barcelona

123. Yuan Mei. The University of Adelaide, Australia
124. Marco Micciarelli. EPFL Lausanne, Switzerland
125. Giacomo Miceli. Università Milano-Bicocca, Italy
126. Letif Mones. University of Cambridge, UK
127. Alessandro Monesi. University of Bolonia, Italy
128. Maria Montagna. University of L'Aquila, Italy
129. M. Merced Montero-Campillo. Universidade do Porto, Portugal
130. Andrey Mukhanov. Joint Institute for High Temperature of RAS, Rusia
131. Víctor Muñoz. Universitat Autònoma de Barcelona, Spain
132. Sadanandam Namsani. Indian Institute of Technology Kanpur, India
133. Trung Hai. Nguyen German Res. School for Sim. Sciences, Germany
134. Elisabeth Ortega. Universitat Autònoma de Barcelona, Spain
135. Manuel Angel Ortuno. Universitat Autònoma de Barcelona, Spain
136. Giulia Palermo. EPFL Lausanne, Switzerland
137. Pawel Panek. University of Wroclaw, Poland
138. Jung Mee Park. Korea Institute for Advanced Study, Korea
139. Anna Pavlova. University of Amsterdam, Netherlands
140. Alejandro Perez Paz. University of the Basque Country, UPV/EHU, Spain
141. Eva Perlt. University of Leipzig, Germany
142. Tien Lam Pham Japan Advanced Institute of Science and Technology, Japan
143. Lukasz Piekos. Jagiellonian University, Poland
144. Ricardo Ramirez. Universidad Catolica, Chile
145. Harish Ravi. Universität Bern, Switzerland
146. Jordi Ribas. Universitat de Barcelona, Spain
147. Dorothee Richters. Universität Mainz, Germany
148. Luis Rodriguez. Universitat Autònoma de Barcelona, Spain
149. Pawel Rodziewicz. University of Bialystok, Poland
150. Ute Roehrig. Swiss Institute of Bioinformatics, Switzerland
151. Víctor Rojas. Parc Científic de Barcelona, Spain
152. Mariana Rossi. Fritz-Haber-Institut der MPG, Berlin, Germany
153. Antonio Sánchez Torralba. Spanish Nat. Cancer Res. Center (CNIO), Spain
154. Alfonso Sanmartin Pensado. University of Leipzig, Germany
155. Hiroko Satoh. National Institute of Informatics, Japan
156. Daniel Schärf. Uni Mainz, Germany
157. Christoph Schiffmann. FU Berlin, Germany
158. Celina Sikorska. University of Gdansk, Poland
159. Artur Smaga. University of Warsaw, Poland
160. Xavier Solans-Monfort. Universitat Autònoma de Barcelona, Spain
161. Holger Somnitz. University of Duisburg-Essen, Germany
162. Bernardo Sosa Padilla Araujo. California Institute of Technology, USA
163. Vladimir Stegailov. Russian Academy of Sciences, Russia
164. Jian Sun. Ruhr-Universität Bochum, Germany
165. Kateryna Sykina. CNRS, France
166. Ravi Tripathi. Indian Institute of Technology Kanpur, India
167. Christian Tuma. IBM Zurich, Switzerland
168. Gregori Ujaque. Universitat Autònoma de Barcelona, Spain

169. Atsushi Urakawa. Institut Català d'Investigació Química (ICIQ), Spain
170. José Luis Vallés Pardo. Universiteit Leiden, Netherlands
171. Omar Valsson. University of Twente, Netherlands
172. Daniele Varsano. University of Rome, Italy
173. Swati Vartak. Simon Fraser University, Canada
174. Linas Vilciauskas. Max-Planck-Institut für Festkörperforschung, Germany
175. Iva Voleská. University of Pardubice, Czech Republic
176. Lukasz Walewski. University of Warsaw, Poland
177. Katharina Wendler. Max Planck Institute for Polymer Research, Poland
178. Andrea Zen. University of Rome, Italy
179. Changjun Zhang. UCL, London, UK
180. Amin Reza Zolghadr. Shiraz University, Iran