Research Networking Programmes

Science Meeting – Scientific Report

Scientific report (one single document in WORD or PDF file) should be submitted online within two months of the event. It should not exceed seven A4 pages.

***Proposal Title**: CPMD 2013: Energy, matter, life from ab initio molecular dynamics simulation*

Application Reference N°: 4563

1) Summary (up to one page)

The development of first principles molecular dynamics (FPMD) simulation methods—as accomplished in the influential work of Car and Parrinello (Car-Parrinello molecular dynamics, CPMD)—represented a major breakthrough in computational chemistry. The ability of FPMD to accurately describe dynamic processes, condensed phases, and chemical reactions combined with the growing computational power of the last decades has made them an indispensable tool in solving, rather than modeling, real-world problems.
The CPMD meeting is an internationally renowned conference held every second year. It provides a platform for the discussion of the latest advancements—both in theory and applications—and defines future trends in the field. This year's meeting (CPMD 2013) was hosted from Monday, September 2nd to Friday, September 6th in Leipzig, Germany, and attended by about 150 participants.
The scene of the five days was set on materials science (Monday), life sciences (Wednesday), and method development (Thursday, Friday). Tuesday was an honored guest day. The actual topics covered in all 44 talks were much broader, including for example energy conversion and storage, green chemistry, nanotechnology, geochemistry, drug discovery, and catalysis. Keynote lectures introducing the topics of the day were given by Wanda Andreoni, Thomas Lippert, Nicola Marzari, Carme Rovira, Matthias Scheffler, Michiel Sprik, Walter Thiel, and Xifan Wu. The conference also featured a poster session with plenty of time for individual discussions and a conference dinner on Wednesday, in Leipzig's famous historical restaurant "Auerbach's Keller".
Funding was received from the European Science Foundation and the Deutsche Forschungsgesellschaft.

2) Description of the scientific content of and discussions at the event (up to four pages)

Day 1: Materials Science

The first day of the conference started with a keynote lecture delivered by Nicola Marzari, who presented recent methodological developments designed to perform FPMD simulations in realistic electrochemical environments that include a liquid solvent, a dissociated electrolyte, an applied electrochemical potential, and a varying pH. Alfredo Pasquarello gave a talk about the importance of defects in all functional materials and theoretical tools to determine defect energy levels in the form of charge transition levels. The third speaker of the day, Mark Tuckerman, showed the results of ab initio molecular dynamics studies of the proton conduction mechanism in phosphate based liquids that are important electrolytes in fuel cells.
The afternoon session started with Stefan Wippermann's talk on density functional and many body perturbation theory calculations of the electronic, optical and transport properties of Si-ZnS nanocomposites which are used experimentally as charge transport layers. Marcella Ianuzzi gave an overview of efficient density functional theory (DFT) based computational methods, that allow the investigation of adsorption processes on metallic surfaces. Afterwards, Mauro Boero presented combined first principles simulations and experimental work on the ferrocene/Cu(111) interface which is an ideal model for metal-molecule junctions for future electronic devices. Carlo Pignedoni demonstrated how atomistic simulations can help in the synthesis and characterization of atomically precise, graphene based heterostructures.
In the last session of the day, Bernd Meyer demonstrated that reaction networks in heterogeneous catalysis can be generated from ab initio metadynamics simulations using methanol synthesis as an example. Rochus Schmid delivered a talk on a systematic force field generation strategy for metal organic frameworks based on first principles calculations and finally, Ding Pan explored the dielectric properties of water under extreme conditions as are present in the deep earth and are thus of fundamental interest in geochemistry.

Day 2: Honored Guest Day

Tuesday was an honored guest day with several keynote lectures on various topics. The day started with Teodoro Laino, who reviewed the status and computational materials challenges of Lithium-air batteries, which promise to outperform all known existing battery solutions. Afterwards, Matthias Scheffler presented a keynote lecture on ab initio thermodynamics and statistical mechanics of interfaces. Once more, the importance of defects was highlighted, and strategies to calculate Gibbs free energies were presented. He also explained the deficiencies of the widely-used exchange correlation functions and showed recent advances in these functionals beyond the random-phase approximation, which many of the subsequent speakers planned to use in the future. In last talk of the morning session, Evert Jan Meijer demonstrated how free energy methods and transition path sampling can be used in FPMD simulations to obtain a quantitative picture of reactions involving proton transport in solutions of water and methanol. Finally, Marialore Sulpizi explained the extraction of sum frequency generation infrared spectra (SFG-IR)—which is a popular experimental technique to investigate interfacial water properties—from FPMD simulations.
The afternoon session was introduced by a keynote lecture of Thomas Lippert, who presented the computational resources at the Jülich Supercomputing Center and future efforts to improve computational power and to integrate the CPMD community into Jülich's infrastructure. He also explained resource allocations obtained via international, national, and regional programs, in particular the PRACE project, which was the basis of

most of the large-scale simulations presented on this conference. A second keynote lecture on Car-Parrinello computational electrochemistry delivered by Michiel Sprik followed. With the aid of a Car-Parrinello standard hydrogen electrode, he and his group can compare electrode potentials directly to experiments and assess the effect of the delocalization error in common density functionals, which is the major source of error in these calculations. Results of oxidation potentials of some model aqua-cations (Cu^{+}, Ag^{+}, and Fe^{2+}) and the alignment of energy levels at the rutile MnO_2-water interface were also given. The second day concluded with a poster session and many individual discussions among the scientists.

Day 3: Life Sciences

The morning session on Wednesday was opened by Carme Rovira with a keynote lecture on the prediction of sugar binding and catalytic mechanisms of carbohydrate-active enzymes using classical/first principles MD and metadynamics methods. These enzymes are of fundamental interest in life sciences because of their role in health and diseases, as well as in enzymatic biomass conversion. Following this, Frank Uhlig delivered a talk on the structure and dynamics of the hydrated electron, a subject which has been controversially discussed in recent literature. Later on, Xifan Wu explained the computation of ionization potentials of hydrated hydroxide and hydronium ions with a many-body approach in the second keynote lecture of the day. Patricia Hunt presented FPMD simulations of aqueous chloride solutions, linking electronic and molecular structure of these ubiquitous solutions.

In the afternoon session, Carlo Camilloni talked about a combined study of NMR measurements, molecular dynamics simulations, and density functional theory on the enzymatic proline isomerization by Cyclophilin A. The group found that Cyclophilin A provides an electrostatic environment that acts on the substrate through electrostatically levering the dipole associated with the carboxylic group of the glycine. Jens Dreyer presented results of FPMD and metadynamics simulations of the proton transport in the cation-selective membrane channel Gramicidin A, elucidating the role of the membrane dipole potential for the free energy barrier of proton permeation.

The last session commenced with Jorge Kohanoff's talk on DNA damage by low-energy electrons investigated by FPMD simulations. Low-energy electrons play an important role in irradiation-caused DNA damage and a thorough understanding of this process is of utmost importance in combating cancer. Giulia Rosetti presented computational techniques to investigate the Cu(II) binding to intrinsically disordered proteins which play a key role in several neurodegenerative diseases, such as Parkinson. The last speak of the day, Francesco Luigi Gervasio, presented a combined computational and experimental study on the role of conformational changes and allosteric regulation in protein kinases. Conformational shifts in kinases lead to several diseases, such as cancer, thus understanding how allosteric signals control the conformational equilibrium is believed to lead to a new rational drug design.

Day 4, 5: FPMD-based Methods

In the first talk on Thursday morning, Simone Raugei demonstrated how FPMD simulations and metadynamics can be used in the rational design of molecular electrocatalysts based on inexpensive and abundant metals such as Ni, Mn, and Fe for oxidation and production of H_2. Afterwards, Davide Branduardi combined the string method—which is a technique aimed at calculating a free energy in high dimensionality on a limited portion of phase space—with metadynamics to achieve a broad an accurate description of the conformational transitions of ATP-Mg^{2+} in water. Wanda Andreoni delivered a keynote lecture on techniques to disclose reaction pathways with CPMD

simulations and their application in processes such as CO_2 capture and sequestration or structural transformations in nanocarbons.

The afternoon session started Giovanni Bussi, who explored the mechanism and dynamics of RNA folding and conformational transitions and of RNA/protein interactions using FPMD simulations and state-of-the-art free energy methods. Walther Thiel presented a keynote lecture about the use of semiempirical quantum-chemical methods for the investigation of fast nonradiative relaxation processes after photoexcitation. These simulations were used, e.g., to unveil the photostabilitiy of DNA bases in different environments, the mechanism of photoinduced molecular rotors, or the complete photochemical cycle of a GFP chromophore with ultrafast excited-state proton transfer. Following this, Vittorio Limongelli reported recent work the accurate estimation of free energy landscapes in biological systems. In particular, he discussed cyclooxygenases, adenosine deaminase and thrombin binding aptamer.

Gareth Tribello introduced the final session of the day with a talk on dimensionality reduction to generate simplified representations of the high-dimensional data obtainable from atomistic simulations, which is of high interest with the progressively increasing complexity of this data. Furthermore, he explained how these techniques can be used to map complex free energy surfaces. Jeremy Palmer talked about liquid-liquid phase transitions in some classical water potentials and presented an exhaustive study of the free energy surface of those liquids using umbrella sampling and well-tempered metadynamics. This sparked a particularly heated discussion, as other groups show different results using the same water model and umbrella sampling. The last speaker of the day, Fabio Pietrucci, showed how graph theory can be used in molecular dynamics simulations to greatly extend the accessible timescales, allowing to discover complex multi-step reaction pathways and leading to an efficient characterization of high-dimensional free energy landscapes.

The last day of the CPMD meeting was opened by Ralph Gebauer who presented a new approach to finding accurate, parameter-free approximations to the exchange-correlation energy functional which avoid self-interaction and capture strong electron correlations. This approach is particularly powerful in the high correlation limit, i.e. at intermediate and large interatomic separations, and even beats coupled cluster calculations with single, double and perturbative triple electron-hole excitation, which is often considered the "gold-standard" of quantum chemistry. Rodolphe Vuilleumier demonstrated how maximally localized Wannier orbitals can be used to derive classical force fields from FPMD simulations. Focus was not only on the electrostatic interactions between fragments, but on all terms of the interaction, including repulsion and long-range dispersion. Jürg Hutter followed and presented a novel algorithm , based on a hybrid Gaussian and Plane Waves (GPW) approach with the resolution-of-identity (RI) approximation, developed for MP2, scaled opposite-spin MP2 (SOS-MP2) and direct-RPA (dRPA) correlation energies of finite and extended systems. The algorithm is implemented in the popular CP2K code.

In the last session of the conference, Brandon Wood showed results on CPMD simulations of III-V-semiconductor-water interfaces that are the most important photocathodes in solar hydrogen production. The results point to the importance of key dynamical processes in determining the electrochemical properties of the semiconductor-water interface. The conference was closed after Jun Cheng’s talk on proton coupled electron transfer in water photooxidation at the TiO_2 water interface. By combining FPMD simulations with free energy perturbation theory the group was able to compute the thermochemistry of proton coupled electron transfer, to understand the delocalization error in standard GGA density functionals, and to propose a simple model to understand how the band structures of materials modulate the electronic energy levels (redox potentials) of intermediates.

3) Assessment of the results and impact of the event on the future directions of the field (up to two pages)

Demographic Reasons

A total of 125 scientists from 18 different countries ranging from Australia to the United States came together to discuss and present their recent progress on all the topics related to FPMD, to share their ideas and to gain insight into the latest developments in the field. Apart from academia, several industrial companies sent representatives, as well, which highlights the importance of the CPMD meeting for theoretical chemistry. With hosting and organizing this meeting, Leipzig as well as Bonn were established as important scientific locations in the FPMD community, and the Mulliken Center for Theoretical Chemistry (Bonn) has fortified its position as an important center for theoretical chemistry.

Scientific Reasons

The unique feature of the CPMD meeting is the wide range of topics that are connected to it. FPMD is a combination of molecular dynamics (MD) simulations and quantum chemistry (QC) theory. Its ability to accurately describe covalent, electrostatic, and van-der-Waals bonds, allows the accurate description of characteristic properties of condensed matter. New approaches in method development even aim to challenge sophisticated methods considered nowadays as the “gold-standard”. The sheer number of different problems which were solved by FPMD with less effort than with conventional methods shows the importance of this accuracy, both from a fundamental research and an industrial point of view. Examples of problems tackled are understanding diseases such as cancer or Parkinson, rational drug design, as well as fuel cells, batteries and catalysts.

It is needless to say, that working groups are unable to be exerts in all of these fields. However, each pioneering new idea at one side of the methodological spectrum helps to bring the whole field forward. One particular example is the evaluation of free energies from FPMD simulations, which starts with the development of methods to obtain these energies, covers visualization and characterization of free energy landscapes, until both can finally be applied to solve real-world problems. Intensifying interaction between groups is therefore of utmost importance, and was realized by a range of new collaborative ideas developed during the meeting, such as working groups joining their forces on common research projects, proposals and workshops.

Knowledge Transfer

During the meeting, the necessary exchange between developers and users of the FPMD software took place. Thereby, ongoing software development could be directed and researchers using the software were informed about new and existing features. The conference, in particular the poster session, also provided a great opportunity for PhD students to present their work, and to receive input and feedback from the experts.

A plethora of discussions were carried out within the scientific community, initializing new national and international cooperations. Especially, the reliability of recent methodological developments was discussed and highlighted necessary steps to improve accuracy and efficiency of computational methods. The latter is especially important for industrial companies because FPMD methods are still time consuming and are usually avoided unless reliable data is needed. Connecting with industrial companies is important to understand their exigencies and to allow FPMD to be not just an academic matter.

4) Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants

Annex 4a: Programme of the meeting

	Monday	Tuesday	Wednesday	Thursday	Friday
	09.02.2013	09.03.2013	09.04.2013	09.05.2013	09.06.2013
	Material Science	Honored Guest Day	Life Science	AIMD-based Methods I	AIMD-based Methods II
08:00					
08:15					
08:30	Registration				
08:45					
09:00					Ralph Gebauer
09:15					
09:30		Teodoro Laino	Carme Rovira		Rodolphe Vuilleumier
09:45					
10:00	Opening Ceremony of CPMD 2013	Matthias Scheffler		Simone Raugei	Juerg Hutter
10:15					
10:30	Nicola Marzari		Frank Uhlig	Alessandro Curioni	coffee break
10:45					
11:00		Evert Jan Meijer	coffee break	coffee break	Brandon Wood
11:15					
11:30	coffee break	coffee break	Xifan Wu	Davide Branduardi	Jun Cheng
11:45					
12:00	Alfredo Pasquarello	Jochen Blumberger		Wanda Andreoni	Closing remarks
12:15					
12:30	Mark Tuckerman	Marialore Sulpizi	Patricia Hunt		
12:45					
13:00	lunch break	lunch break	lunch break	lunch break	
13:15					
13:30					
13:45					
14:00					
14:15					
14:30	Stefan Wippermann	Thomas Lippert	Carlo Camilloni	Giovanni Bussi	
14:45					
15:00	Marcella Iannuzzi		Ursula Roethlisberger	Walter Thiel	
15:15					
15:30	Mauro Boero	Michiel Sprik	Jens Dreyer		
15:45					
16:00	Carlo Pignedoli		coffee break	Vittorio Limongelli	
16:15					
16:30	coffee break	Poster Session	Jorge Kohanoff	coffee break	
16:45					
17:00	Bernd Meyer		Giulia Rossetti	Gareth Tribello	
17:15					

17:30	Rochus Schmid		Francesco Luigi Gervasio	Jeremy Palmer	
17:45					
18:00	Ding Pan			Fabio Pietrucci	
18:15					
18:30					
18:45					
19:00			Conference Dinner		
19:15					
19:30					
19:45			(till midnight)		
20:00					

Annex 4b: Full list of speakers and participants

Full list of speakers

Prof. Dr.	Wanda	Andreoni	École Polytechnique Fédérale de Lausanne (EPFL)
Dr.	Jochen	Blumberger	University College London
Prof. Dr.	Mauro	Boero	University of Strasbourg -CNRS
Dr.	Davide	Branduardi	Max Planck Institute of Biophysics
Dr.	Giovanni	Bussi	Scuola Internazionale Superiore di Studi Avanzati - SISSA
Dr.	Carlo	Camilloni	University of Cambridge
Dr.	Jun	Cheng	University of Cambridge
Prof. Dr.	Alessandro	Curioni	IBM Research Zurich
Dr.	Jens	Dreyer	German Research School for Simulation Sciences GmbH
Dr.	Ralph	Gebauer	International Center for Theoretical Physics (ICTP)
Prof. Dr.	Francesco Luigi	Gervasio	University College London
Dr.	Patricia	Hunt	Imperial College London
Prof. Dr.	Juerg	Hutter	University of Zurich
Dr.	Marcella	Iannuzzi	University of Zurich
Prof. Dr.	Jorge	Kohanoff	Queen's University Belfast
Dr.	Teodoro	Laino	IBM Research Zurich
Dr.	Vittorio	Limongelli	University of Naples "Federico II"
Prof. Dr.	Thomas	Lippert	Jülich Supercomuting Centre (JSC)
Prof. Dr.	Nicola	Marzari	École Polytechnique Fédérale de Lausanne (EPFL)
Prof. Dr.	Evert Jan	Meijer	University of Amsterdam
Prof. Dr.	Bernd	Meyer	University of Erlangen-Nürnberg
Dr.	Jeremy	Palmer	Princeton University
Dr.	Ding	Pan	University of California, Davis
Prof. Dr.	Alfredo	Pasquarello	EPFL SB ITP CSEA
Dr.	Fabio	Pietrucci	Ecole Polytechnique Fédérale Lausanne
Dr.	Carlo	Pignedoli	EMPA
Dr.	Simone	Raugei	Pacific Northwest National Laboratory
Prof. Dr.	Ursula	Roethlisberger	Ecole Polytechnique Fédérale Lausanne
Dr.	Giulia	Rossetti	German Research School for Simulation Sciences GmbH
Prof. Dr.	Carme	Rovira	University of Barcelona
Prof. Dr.	Matthias	Scheffler	Fritz Haber Institute of the Max Planck Society
Dr.	Rochus	Schmid	Ruhr-University Bochum
Prof. Dr.	Michiel	Sprik	University of Cambridge
Prof. Dr.	Marialore	Sulpizi	Johannes Gutenberg Universität Mainz
Prof. Dr.	Walter	Thiel	Max-Planck-Institut für Kohlenforschung
Dr.	Gareth	Tribello	Queen's University Belfast
Prof. Dr.	Mark	Tuckerman	New York University
	Frank	Uhlig	Academy of Sciences of the Czech Republic
Prof. Dr.	Rodolphe	Vuilleumier	Departement de chimie de l'ENS
Dr.	Stefan	Wippermann	Max-Planck-Institute for Iron Research

Dr.	Brandon	Wood	Lawrence Livermore National Laboratory
Prof. Dr.	Xifan	Wu	Temple University

Full list of participants

Sacha	Abadie	Evry Val d'Essonne
Hans Tobias	Alznauer	Leibniz Universitaet Hannover
Christoph	Allolio	MLU Halle-Wittenberg
Padmanabhan	Anbazhagan	University of Oulu
Takeshi	Baba	Osaka University
Gül	Bekcioglu	Martin-Luther-Universität Halle-Wittenberg
Andrzej	Bil	University of Zurich
Mauro	Boero	University of Strasbourg -CNRS
Marie-Laure	Bonnet	Evry Val d'Essonne
Daniele	Bovi	University of Rome - La Sapienza -
Martin	Brehm	University of Leipzig
Vania	Calandrini	German Research School for Simulation Sciences GmbH
Enrico	Caldarulo	ETH - Zurich
Roberto	Car	Princeton University
Paolo	Carloni	German Research School for Simulation Sciences GmbH
Ashu	Choudhary	Indian Institute of Technology Kanpur
Jérôme	Cuny	Université Paul Sabatier
János	Daru	Eotvos University, Budapest
Polydefkis	Diamantis	Ecole Polytechnique Fédérale Lausanne
Przemyslaw	Dopieralski	University of Wrocław
Martin	Dracinsky	Durham University
Christof	Drechsel-Grau	Ruhr-University Bochum
Melanie	Eggers	University of Bonn
Johannes	Frenzel	Ruhr-University Bochum
Marie-Pierre	Gaigeot	Université d'Evry val d'Essonne
Federico	Giberti	ETH - Zurich
Dorothea	Golze	University of Zurich
Oldamur	Hollóczki	University of Bonn
Frank	von Horsten	Atotech Deutschland GmbH
Javier	Iglesias-Fernández	Universitat de Barcelona
Venkataramana	Imandi	Indian Institute of Technology Kanpur
Bakó	Imre	Institute of Organic Chemistry
Aneta	Jezierska-Mazzarello	University of Wrocław
Andreas	John	Leibniz-Institut für Polymerforschung
John	Kattirtzi	University of Cambridge, Chemistry Department
Barbara	Kirchner	University of Bonn
Miriam	Kohagen	Academy of Sciences of the Czech Republic

Katarzyna	Kulczycka-Mierzejewska	University of Warsaw
Stanislav	Kozmon	Masaryk University, CEITEC MU
Manju	Kumari	Masaryk University, CEITEC MU
Thomas	Kühne	Johannes Gutenberg-University Mainz
Kari	Laasonen	Aalto University
Sebastian	Lehmann	University of Leipzig
Xiandong	Liu	University of Campridge
Jan	Los	Johannes Gutenberg University Mainz
Changru	Ma	École Polytechnique Fédérale de Lausanne
Friedrich	Malberg	University of Bonn
Rosa	Marta	Università di Modena e Reggio Emilia
Katharina	Meier	IBM Research Zurich
Federica	Moraca	"Magna Graecia" of Catazaro
Marco	Nava	Department of Chemistry and Applied Biosciences, ETH Zurich,
Nikita	Orekhov	Joint Institute for High Temperatures, Russian Academy of Sciences
Jaroslaw	Panek	University of Wrocław
Michele	Parinello	Department of Chemistry and Applied Biosciences, ETH Zurich
Jung Mee	Park	Korea Institute for Advanced Study
Leila Salimi	Parvaneh	Johannes Gutenberg University
Sanita	Pavlovica	University of Latvia
Eva	Perlt	University of Leipzig
Morgane	Pfeiffer-Laplaud	Evry Val d'Essonne
Fabio	Pitari	University of L'Aquila
Eva	Pluhařová	Insitut of organic chemictry and biochemistry, AS CR
Victor	Rojas-Cervellera	Universitat de Barcelona
Matti	Ropo	Tampere University of Technology
Jyoti	Roy Choudhuri	Indian Institute of Technology Kanpur
Hiroko	Satoh	National Institute of Informatics
Arne	Scherrer	Martin-Luther-Universität Halle-Wittenberg
Matthias	Schöppke	University of Leipzig
Daniel	Sebastiani	MLU Halle-Wittenberg
Ari Paavo	Seitsonen	University of Zurich
Nicolas	Sieffert	Université Joseph Fourier Grenoble I
Amninder	Singh Virk	University of Western Sydney, Australia
Gabriele Cesare	Sosso	Eidgenössische Technische Hochschule Zürich
Riccardo	Spezia	CNRS / Université d'Evry Val d'Essonne
Grigory	Smirnov	Joint Institute for High Temperatures of the RAS
Christian	Spickermann	Atotech Deutschland GmbH
Vladimir	Stegailov	Joint Institute for High Temperatures, Russian Academy of Sciences
Andras	Stirling	Research Centre for Natural Sciences
Yoshitaka	Tateyama	National Institute for Materials Science
Parul	Tewatia	Amity University

Omar	Valsson	Universita della Svizzera italiana and ETH Zurich
Vincenzo	Verdolino	Universita' della Svizzera Italiana USI-ETH
Vanessa	Werth	Leibniz Universitaet Hannover
Brandon	Wood	Lawrence Livermore National Laboratory
Xifan	Wu	Temple University
Mei	Yuan	The University of Adelaide
Stefan	Zahn	University of Leipzig