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PROJECT
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Location : E-MRS Meeting, Warsaw, Poland
Date of Science Meeting : 13/09/2010 - 17/09/2010
Convenor Name : Professor Fabrizio CLERI, Villeneuve d'Ascq, France

SUMMARY

The Symposium "Computer modelling in nanoscience and nanotechnology", organized by C. Massobrio (Strasbourg), F. Cleri (Lille), R. Kozubski (Krakow) and C. Dellago (Vienna) in the framework of the 2010 Fall Meeting of the European Materials Research Society in Warsaw, Poland, has been an active forum of interaction and exchanges among scientists involved in the atomic-scale, computer based modeling of nanostructures.

The themes included large molecules of technological interest, supramolecular structures in interaction, or adsorbed at surfaces, and bulk systems for which nanostructural units could be clearly identified. Organic structures relevant for life science applications were also considered. Modern approaches of atomic-scale computer modeling were shown to be equally applied to these systems, providing an accurate characterization of their structures and interaction mechanisms. A special focus of this symposium has been also on the self-assembly and self-recognition of nanoscale objects (clusters, macromolecules, micelles, proteins, etc) by long-range forces.

To ensure adequate exposure and interaction with the experimental counterpart, two leading scientists (out of a total of 12 invited speakers) reporting on experimental open issues and recent achievements in these areas were invited.

It is worth noting that such an event, still of moderate impact as far as the number of participants (around 50 registered participants), is somewhat unique in its kind in Europe, being the only "theory" symposiums usually organized within both the Spring and Fall Meetings of the E-MRS. We hope that it will grow in the coming years.

SCIENTIFIC CONTENT AND DISCUSSION

The Symposium, which followed a similar event organized by the same team (without C. Dellago) during the E-MRS Fall Meeting 2008, was a considerable success. With a total of more than 40 registered participants, 12 invited talks, 21 contributed talks,

and 38 posters, the attendance in the various session was never below 25 people, which, on the scale of the typical E-MRS Meeting Symposia in Warsaw, is quite a respectable number. (Also considering that – due to an unfortunate coincidence – in the same days it was held the “Psi-K Conference” in Berlin, a vast event which takes place every 5 years, and gathered more than 1200 participants in the field of electronic structure and atomistic computer simulations.)

The 33 talks were arranged in a number of sessions, notably:

1) Monday afternoon: Self-Assembly and Colloids
2) Tuesday morning: Biosystems and water
3) Tuesday afternoon: Solid-phase materials, metals
4) Wednesday morning: Methodological developments
5) Thursday morning: Applications in nanomaterials 1
6) Thursday afternoon: Applications in nanomaterials 2

The two poster session, on the other hand, were unstructured, since the contributed papers were somewhat scattered on several different topics. We assigned the Prize for the Best Poster to the work “Simulation of diamond nanocluster formation in the interstellar medium”, presented by a young Russian scientist from St. Petersburg, A. Siklitskaya.

The contribution and sporsorship of the European Science Foundation has been constantly acknowledged, both in the opening and closing speech, and by displaying the ESF logo in several occasions, including the access door, the poster sessions, etc.

Session 1: *Self assembly and colloids*

This session was opened by two invited talks, by T. Vlugt (Delft) and J. Doye (Oxford). The two invited talks discussed in full details simulation methods and results of studies in the area of self-assembly, the first talk being dedicated to the physisorption of nanocrystals, while the second being centered about biological systems such as viral capsids and DNA nanostructures. The other invited talk by D. Vuillaume (Lille), was an invited experimental contribution, dealing with the self-assembly of molecular monolayers on semiconductor surfaces, in the context of nanoscale molecular electronics. Together with the three contributed talks, the session provided a stimulating discussion with many questions from the attendants, about the methods and peculiarities of coarse graining methods to attack the problems connected with self assembly. The latter are notoriously difficult to tackle, because of the dominant role of weak forces (Van der Waals, hydrogen bonding, long range electrostatics), and of the entropic effective interactions brought about by the conforational degrees of freedom.

Session 2: *Biosystems and water*

The first invited talk in this session was given by M. Boero (Tsukuba, now in Strasbourg), who demonstrated the capabilities offered and the challenges posed by the use of coupled quantum-classical molecular dynamics methods (the so-called QM/MM), however necessary in the case of complex biological interactions involving

enzymes and nucleic acids. It was highlighted the prominent role of water molecules in catalytic reactions. Water was the protagonist also of the contributed talks by Iannuzzi et al. (Zurich), by Scipioni (Mainz) and by Menzl (Vienna). The other invited talk was given by C. Molteni (London), which showed the capability of the "metadynamics" method for searching transition paths and finding switching between different isomers, in a variety of biological systems all involving the amino acid proline.

Session 3 : *Solid-phase materials, metals*

This section grouped a number of contributions concerning the computer simulation of metallic and semiconductor nanosystems. The invited talk by T. Oda (Kanazawa, Japan) opened exciting perspectives in the simulation of magnetic anisotropy in bimetallic systems, such as FePt, with great relevance to advanced spintronics. The other invited talk, by Elena Levchenko (Newcastle, Australia) dealt with classical MD simulations of surface segregation in the Ni-Al systems, focusing on the cases of nanoparticle surfaces, and thin films surfaces and interfaces. The contributed talks concerned the simulation of GaN/AlN junctions; the study of recrystallization fronts in amorphous-crystalline Si interfaces; the study of hydrogen diffusion at the Mg/MgH2 interface by ab initio molecular dynamics; the classical molecular dynamics simulation of liquid NiAl.

Session 4: *Methodological developments*

This session was one of the most interesting of the whole Symposium, since it provided a sort of common denominator to several subjects, which had been touched upon in the previous sessions, and which would have become the subject of forthcoming talks as well. A substantial part of the session was dedicated to the accurate calculation of Van der Waals interaction, both by first principles via the extension of Wannier functions (invited talk by P. L. Silvestrelli, University of Padova), or by semi-empirical methods based on a combination of DFT and LCAO theory (contributed talk by Y. Dappe, Stransbourg and Paris). T. Wesolowski from Geneva gave a brilliant and interesting talk on the large field of orbital-free DFT functionals, highlighting the numerous connections with existing, more simplified methods, and showing the exceptional level of precision that can be attained by such methods in calculating spectroscopic properties. Spectroscopy and the calculation of ELNES spectra was also the subject of a contributed talk by the Kohyama group (Nagoya, Japan). A contribution from the Dellago's group in Vienna presented recent developments in transition path sampling and search for rare event in molecular dynamics simulations.

Session 5: *Applications in nanomaterials*

This session was split into two parts, due to the large number of contributions it gathered. In the first part, the invited talk by T. Mallah (Paris 11) set the scene, with a second experimental contribution which presented the opportunities offered by the field of functional nanocrystals, especially relative to magnetic and switching behavior. Elaborate core-multishell nano objects of several different kinds, grown in Mallah's labs, were presented, which clearly may pose significant challenges to the

computer simulation community. Contributed talks dealt with magnetism in bimetallic alloys (Goyhenex, Strasbourg), ceramic nanocomposites (K. Nalepka, from Krakow), carbohydrate-mediated adhesion (Zucca, from Lille).
The other invited talks were given by Ari Seitsonen (now in Zurich), regarding a careful comparison of the ability of different DFT exchange-correlation functionals in the description of hydrogen bonding and solvation in water; and by F. Della Sala (Lecce) about advanced DFT simulation methods for hybrid nanosystems, such as self-assembled monolayers of organic molecules adsorbed on metallic surfaces.

In conclusion of the Meeting, K. J. Kurzydlowski, Former Deputy Minister of Science and Higher Education of the Polish Republic, gave a conclusive invited talk, covering the perspectives of multi-scale modelling and its applications, in several domains of materials nanotechnology.

RESULTS AND IMPACT ON FUTURE DIRECTIONS

Overall, the Symposium fulfilled its goals. It was demonstrated that the knowledge of structural conformation and evolution of atomic-scale objects with temperature and external constraints (such as pressure, stress, external fields, etc.) is a necessary prerequisite to understand and characterize the behavior of nanostructures. These have to be intended as systems bearing peculiar properties at the nanometer scale compared to their bulk counterparts. With the advent of nanoscience and nanotechnology, the need for a detailed, atomic-level understanding of the interactions governing the synthesis, aggregation, self-assembly, surface deposition, recognition of nanoscale objects, becomes crucial.

In 2008, we had organized a first E-MRS Fall Meeting Symposium, again In Warsaw, on the subject of “Morphology and dynamics of nanostructures and disordered materials via atomic-scale modelling “. As a natural extension of the ideas developed and exploited in 2008, we had this time reoriented our goals, by concentrating on the characterization of nanosystems at the atomic scale by computer simulation.

An important outcome was to put in evidence that in the most recent applications of atomic-scale simulations of the dynamics and structure of nano objects, an increasingly relevant role is played by the weak interactions, such as Van der Waals forces. The great successes of the DFT theory, and its numerical implementations into commercial and shareware computer codes, have traditionally concentrated on covalently bonded systems, and more recently also on metallic-bonded systems, while bonding in organic molecules have been always at the focus of such methods. However, the challenges posed by the aggregation, self-assembly, and self-organization of complex nanostructures, quantum dot systems, core-shell and multifunctional nanoparticles, self-assembled monolayers, molecule-sheated nanocrystals, biological ligand-receptor couples, biological membranes, viral capsids and nucleic acids, and so on, heavily rely on the capability of the simulation methods to incorporate the long-ranged, weak forces that are usually neglected, or treated more empirically, when dealing with the covalent or metallic interactions of condensed or liquid-phase systems.
In this respect, the Symposium has given a real contribution to the title theme, “Computer simulations for nanoscience and nanotechnology”, avoiding to give just a

mere list of, yet important, but often too focused contributions on traditional methods. Rather, it was possible to explore several original applications to systems, which, just a few years ago, would have been discarded as “not interesting” or “too complex”. It can only be hoped that such an increased understanding can spread across the computational materials science community at large, in Europe and elsewhere, while pushing for the development and improvement of new and more advanced simulation methods.

In fact, such a Meeting is on the point of becoming a kind of biennial periodic event, where to discuss the progress and applications of advanced computational methods of the structure and dynamics of molecular and nanoscale systems; Such an opportunity is rather unique, since the theme it is usually diluted in other, larger meetings, or rather completely ignored.

It should be noted that this Symposium is the only one computational meeting organized in the framework of the European Materials Research Society, both for the Spring Meeting (usually held in Strasbourg) and the Fall Meeting (usually held in Warsaw). We hope that the group of organizers, which is every year extended to a fourth, different person, could remain stable in time. **The continued support of an organization like the European Science Foundation has been and will be essential.** Even with a small contribution, it will allow us to pursue in this effort, and to foster the fall-outs of advanced computational methods towards the materials science community. This larger impact should not be underestimated, since this Symposium typically is held together with a series of many other parallel Symposia, attended mostly by experimentalists, experts in various sectors of the materials sciences, which can in this way have the unique occasion to witness the progresses and potential applications of the computational methods to their own problems.

FINAL PROGRAMME OF THE MEETING

Monday 13/09

Understanding interactions between capped nanocrystals (**invited**)
Thijs J.H. Vlugt P.Z. Schapotschnikow Process and Energy Laboratory, Delft University of Technology, Leeghwaterstraat 44, 2628 CA Delft, The Netherlands

Coarse-grained simulations of self-assembling systems: Patchy colloids, protein complexes and DNA nanostructures (**invited**)
Jonathan Doye, Physical & Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford

Simulation of single-chain polymer nanoparticles exhibiting supramolecular collapse
P. Englebienne, A. J. Markvoort, P. Hilbers, E. W. Meijer Department of Biomedical Engineering, Department of Chemical Engineering and Chemistry, and Institute for Complex Molecular Systems, Eindhoven University of Technology, Eindhoven, The Netherlands

Control of the molecule-electrode contact at the atomic level and conductance of molecular junctions: an experimental point of view. (**invited**)
D. Vuillaume. IEMN-CNRS, univ. of Lille. France.

Atomic scale simulations of plasma etching processes
Antonino La Magna, Loredana Chiaramonte CNR–IMM, Z.I. VIII Strada 5, 95121 Catania, Italy. G.Garozzo, R. Colombo, G. Fazio Numonyx Via Olivetti 5 Agrate Brianza

Equilibrium shape of Au nanoparticles from first-principles calculations
Georgios D. Barmparis and Ioannis N. Remediakis, Department of Materials Science and Technology, University of Crete, 71003 Heraklion, Crete, Greece

Monday's poster session with 19 contributed papers.

Tuesday 14/09
Leucyl-tRNA Synthetase Water-Mediated Editing Reaction (**invited**)
Mauro BOERO, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504 CNRS-UdS, 23 rue du Loess, BP 43, F-67034 Strasbourg, France, JAIST, 1-1 Asahidai, Nomi-shi, Ishikawa 923-1292, Japan, and CREST, Japan Science and Technology Agency, Sanban-cho, 102-0075 Tokyo, Japan

Boron Nitride Nanomesh interacting with water and atomic hydrogen
Marcella Iannuzzi, Yun Ding, Juerg Hutter, Physikalisch Chemisches Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

Water solvation: Infrared response of diluite salt solutions experiments vs theory
Roberto Scipioni, Max Planck Institute for Polymer Research, 10 Ackermannweg, 55124 Mainz Germany

Molecular switches by trans-cis isomerization: the case of proline (**invited**)
Carla Molteni, King's College London, Physics Department (UK)

Collective behavior of single-file water chains in nanopore membranes
Georg Menzl (University of Vienna), Jürgen Köfinger (NIH, Bethesda), Christoph Dellago (University of Vienna)

Toward a computer modelling in magnetic anisotropy and its electric-field-control for nano-structures (**invited**)
Tatsuki Oda, Institute of Science and Engineering, Kanazawa University, Japan

Density functional study of GaN/AlN junctions
Jakub Sołtys 1, Michał Łopuszyński 1, Jacek Piechota 1 and Stanisław Krukowski 1,2 1Interdisciplinary Centre for Materials Modelling, University of Warsaw, ul. Pawinskiego 5a, 02-106 Warsaw, Poland 2 Institute of High Pressure Physics, Polish Academy of Sciences, ul. Sokołowska 29/37, Warsaw, Poland

Classical molecular dynamics for diffusion mechanisms and interface migration in nanodevices
E. Lampin, C. Krzeminski, IEMN - BP 60069 - 59652 Villeneuve d\'Ascq Cedex - France

Molecular Dynamics Study of Diffusion and Surface Segregation in Ni-Al Nanoparticles and Thin Films (**invited**)
Elena V. Levchenko, Alexander V. Evteev, Irina V. Belova and Graeme E. Murch The University Centre for Mass and Thermal Transport in Engineering Materials Priority Research Centre for Geotechnical and Materials Modelling School of Engineering The University of Newcastle Callaghan, NSW 2308 Australia

Molecular Dynamics Simulation of Liquid Ni50Al50 Alloy
Alexander V. Evteev1, Elena V. Levchenko1, Daniel R. Beck1,2, Irina V. Belova1 and Graeme E. Murch1 1The University Centre for Mass and Thermal Transport in Engineering Materials Priority Research Centre for Geotechnical and Materials Modelling School of Engineering The University of Newcastle Callaghan, NSW 2308 Australia 2University of Aalen, Faculty of Industrial Engineering/Surface Engineering, Beethovenstr. 1, 73430 Aalen, Germany

Numerical simulation of hydrogen dynamics at a Mg-MgH2 interface
S. Giusepponi and M. Celino, ENEA, C.R. Casaccia, Via Anguillarese 301, 00123 Rome, Italy

Tuesday's poster session with 19 contributed papers.

Wednesday 15/09

Van der Waals interactions in Density Functional Theory using Wannier functions (**invited**)
Pier Luigi Silvestrelli, Dipartimento di Fisica "G. Galilei", Università di Padova, via Marzolo 8, I-35131 Padova, Italy, and DEMOCRITOS National Simulation Center, Trieste, Italy.

An accurate formalism to describe weak interactions : the LCAO-S^2 + vdW approach
Y. J. Dappe IPCMS Strasbourg France

Optimizing transition interface sampling: general algorithm and application to dielectric relaxation of water-filled carbon nanotubes
Ernesto E. Borrero and Christoph Dellago Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090, Vienna, Austria

Orbital-free embeding strategy for modelling electronic structure of molecules in condensed phase: exact theory and practical applications (**invited**)
Tomasz WESOLOWSKI, Department of Physical Chemistry, University of Geneva, 30, quai Ernest Ansermet, CH-1211 Genève, Switzerland

ELNES of Ti-doped SiO2 glass using first-principles calculations
Tomoyuki TAMURA (A), Shingo TANAKA (B), Masanori KOHYAMA (B) A Nagoya Institute of Technology, Japan B National Institute of Advanced Industrial Science and Technology, Japan

Thursday 16/09

Controlled growth at the molecular level of functional coordination nanocrystals: magnetic and switching behavior (**invited**)
Talal Mallah (a), Laure Catala(a), Yoann Prado (a), FIorence Volatron(a), Corinne Mathonière (b), Alexandre Gloter (c), Odile Stéphan (c) (a) Université Paris Sud 11, Institut de Chimie Moléculaire et des Matériaux d\'Orsay, ICMMO-CNRS, 91405 Orsay, France. (b) Institut de Chimie de la Matière Condensée de Bordeaux, ICMCB-CNRS, 87, Avenue du Docteur Albert Schweitzer, 33608 Pessac, France. (c) Université paris Sud 11, Laboratoire de Physique des Solides, LPS-CNRS, 91405 Orsay, France.

Link between structural and electronic/magnetic properties in bimetallic compounds and overlayers
A. Jaafar, C. Goyhenex, Institut de Physique et Chimie des Materiaux de Strasbourg,CNRS-UDS, UMR 7504, 23, rue du Lœss, BP 43, Strasbourg Cedex2, F- 67034, France. G. Treglia, Centre Interdisciplinaire de Nanoscience de Marseille, UPR 3118 CNRS, Campus de Luminy Case 913, F-13288 Marseille Cedex 9, France. L. Zosiak, R. Kozubski, M.Smoluchowski Institute of Physics Jagellonian University, Reymonta 4, 30-059 Krakow, Poland.

Atomistic model of the interface of the ceramic matrix nano-composite Al2O3-Ni
Kinga Nalepka1), 2) 1) Department of Strength and Fatique of Materials and Structures, Faculty of Mechanical Engineering and Robotics, AGH University of Science and Technology, Al. Mickiewicza 30, 30-059 Krakow, 2) Institute of Fundamental Technological Research, Polish Academy of Sciences, Pawińskiego 5B, 02-106 Warszawa

Solvation of ions in ambient and super-critical water from ab initio molecular dynamics (**invited**)
Ari P Seitsonen, IMPMC, CNRS & Université Pierre et Marie Curie, 4 place Jussieu, case 115, F-75252 Paris Cedex 05, and Physikalisch-Chemisches Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich , Guillaume Ferlat, IMPMC, Université Pierre et Marie Curie, 4 place Jussieu, case 115, F-75252 Paris Cedex 05, Rodolphe Vuilleumier, Département de Chimie de l'École Normale Supérieure, 24 rue Lhomond, F-75231 Paris Cedex 05

Molecular dynamics simulation of carbohydrate-mediated adhesion
Rinaldo Zucca and Fabrizio Cleri, Universite de Lille I, Institute d\'Electronique MIcroelectronique et Nanotechnologie (IEMN Cnrs UMR 8520), F59652 Villeneuve d\'Ascq, France

Electronic properties of hybrid nanosystems with orbital-dependent density-functional methods (**invited**)
Fabio Della Sala, Institute of Nanoscience (CNR) and Center for Biomolecular Nanotechnologies (IIT) Lecce, Italy

Ring statistics analysis of topological networks: New approach and application to amorphous GeS2 and SiO2
Sébastien Le Roux and Philippe Jund* Central Michigan University Michigan U.S.A. *Institut Charles Gerhardt, Université Montpellier 2

Global optimisation studies of silica clusters and hydroxylated silica clusters.
Edwin Flikkema, Institute of Mathematics and Physics, Aberystwyth University, Penglais, Aberystwyth SY23 3BZ, United Kingdom; Stefan Bromley, Computational Materials Science Laboratory, Universitat de Barcelona, Marti i Franques 1, E-08028 Barcelona, Spain

Hydrogen Stability and Aggregation in Dislocation in Silicon
Masahiko Matsubara, Julien Godet and Laurent Pizzagalli Institut PPRIME, Departement de Physique et de Mecanique des Materiaux, CNRS UPR 3346, Universite de Poitiers, SP2MI, BP30179, 86962 Futuroscope Chasseneuil Cedex, France

DFT modeling of the interaction of small analyte molecules with an acridine dye adsorbed on the surface of amorphous silica
Alexander Bagaturyants, Elena Rykova, Vladimir Chashchikhin, Ruslan Minibaev, Vyacheslav Sazhnikov, Andrei Scherbinin, Michael Alfimov Photochemistry Center, Russian Academy of Sciences, Moscow, Russian Federation

Closing talk (invited)

Design of novel engineering materials via atomic-scale modelling
J. WRÓBEL, M. MUZYK, P. ŚPIEWAK, T. WEJRZANOWSKI, K.J. KURZYDŁOWSKI Warsaw University of Technology, Faculty of Materials Science and Engineering, 141 Woloska St., 02-507 Warsaw, Poland