

ESF Science Meeting

Reference Number: 3994

Acceptance submitted: 17/1/2012

ESF Activity

Unit(s): PESC

Activity Title: Advanced Concepts in Ab Initio Simulations of Materials

Activity Acronym: Psi-K2

PROJECT

Science Meeting: Conference

Title of Science Meeting: 2012 EMRS Fall Meeting Symposium I: "Computer modelling in nanoscience and nanotechnology: an atomic-scale perspective II"

Location: Warsaw University of Technology, Poland

Date of Science Meeting: 17/09/2012 - 20/09/2012

Convenor Name: Dr Carla Molteni, King's College London (UK)

SUMMARY

The Symposium "*Computer modelling in nanoscience and nanotechnology II*", organized by C. Massobrio (Strasbourg), F. Cleri (Lille), R. Kozubski (Krakow) and C. Molteni (London) in the framework of the 2012 Fall Meeting of the European Materials Research Society (EMRS) in Warsaw, Poland, was an active forum of interaction and exchanges among scientists involved in computational modeling, based on first principles and/or empirical methods, of nanostructures at the atomic scale.

Topics of the invited and contributed talks included systems of technological interest, such as SiC and carbon-based materials including graphene, nanostructures in interaction or adsorbed at surfaces, nanocrystals and nanowires, and systems of biological interest. The application of state-of-the-art atomistic simulation techniques to these materials was shown to provide an accurate characterization of their structures and interaction mechanisms. Particular attention was also given to the latest method developments (e.g. linear scaling methods and neural network potentials); this was achieved with a good fraction of invited and contributed talks dealing with the most recent methodological advances.

The Symposium consisted of 12 invited and 18 contributed talks, plus two poster sessions, for a total of 64 high quality abstracts. It was the only theory and modeling symposium within the 13 Symposia of the EMRS Fall meeting and we hope it will grow in the coming years.

SCIENTIFIC CONTENTS AND DISCUSSION

The Symposium, which followed two similar events organized by part of the same team during the EMRS Fall Meetings of 2008 and 2010, was a considerable success. With 12 invited talks, 18 contributed talks, and 34 posters, the attendance to the various sessions was never below 30 people, with peaks of 45, which, on the scale of the typical EMRS Meeting parallel Symposia held in Warsaw, is a very respectable number.

The 30 talks were arranged in nine sessions, dedicated to simulations of various materials and properties, and to method developments. The sessions are listed below.

- 1) 17/9/12 - Monday afternoon: *Complex materials*
- 2) 18/9/12 - Tuesday morning: *Computational methods I*
- 3) 18/9/12 - Tuesday afternoon: *Computational methods II*
Nanocarbon
- 4) 19/9/12 - Wednesday morning: *Nanostructures*
- 5) 20/9/12 - Thursday morning: *Biomaterials*
Adsorption phenomena
- 6) 20/9/12 - Thursday afternoon: *Heat transport properties*
Electronics and optical properties

The speakers were a balanced mixture of experienced scientists and early stage researchers including postdoctoral and PhD students; 1/3 of the talks were given by women. 8/30 talks were given by scientists from East European countries.

The two poster sessions, held on Monday 17/9/12 and Tuesday 18/9/12 late afternoons, were practically unstructured, since the contributed papers were scattered on several different topics. We assigned the Prize for the Best Poster to the work "*Growth of Ni and Cu nanostructures on Cu(111)*", presented by Berk Onat, a young scientist from Istanbul Technical University (Turkey).

The contribution and sponsorship of the European Science Foundation have been constantly acknowledged, both in the opening and closing speech, and by displaying the *Psi-K* logo in several occasions.

Highlights from the Sessions:

Session 1, Complex Materials:

The two invited talks of this section focused on pressure induced amorphization in sulfur (Martonak) and on structural transformations following nanoindentation in silicon and gallium arsenide (Chrobak). Both studies made use of density functional theory simulations that are particularly suitable to describe the complex mechanisms of breaking and remaking of bonds occurring in these processes.

Session 2/3, Computational Methods I/II:

The two sessions focused on methodological developments and novel techniques. In particular, Behler presented a method for constructing interatomic potentials, based on techniques inspired by neuronal network research, convincingly demonstrating that the existence of an ab-initio data set can be exploited to devise interatomic potentials with no obligation of going through the predefinition of an analytical form. Examples were provided clearly showing the efficiency and predictive power of this technique, provided that reliable ab-initio data sets are available. Michaelides discussed the importance of quantum nuclear effects and van der Waals interactions for water structures at surfaces and how these can be practically included in calculations.

Session 4, Nanocarbon:

Colombo illustrated how to evaluate the Young modulus of non-stoichiometric graphene conformers. The session was complemented by talks on carbon onions with twisted geometries and on transport through carbon-based materials.

Session 5, Nanostructures:

Skylaris showed the power of linear scaling density functional theory method for modeling large nanostructures. Metallic nanowires and nanoparticles were the topics of other talks of this session, including that of Mottet on the phase diagram of nanoalloys.

Session 6, Biomaterials:

Harris gave an introductory overview, suited for non experts in biophysics, of the increasing use and usefulness of atomistic simulation techniques to understand complex systems of biological interests. She illustrated how simulations can complement experimental data with two examples on the effects of superhelical stress on DNA and on the formation of amyloid fibers. Koeppen focused on the challenges for modelling the interaction of proteins with oxide surfaces.

Session 7, Adsorption phenomena:

Density functional theory with suitable functionals was the method of choice in all the talks of this session, focused on adsorption phenomena of metal-organic complexes at insulating surfaces (Shluger), oxygen on rhenium (Hernandez) and carbon monoxide on gold nanoparticles (Barmaris).

Session 8, Heat transport properties:

The contributions of Donadio and Lampin showed that modern atomic –scale techniques can meet the challenge of mimicking effectively heat flows in materials of increasing sizes. In particular, Lampin made explicit a new methodology that allows the assessment of the thermal flow by exciting the conjugated thermal current and observing its decay in a totally unbiased manner.

Session 9, *Electronics and optical properties*:

Ruini presented a study of optical excitations of elongated graphene nanoflakes and ribbons, which have potential applications as nanoantennae and in other plasmonic devices. Govoni studied carrier multiplication events in isolated and interacting silicon nanocrystals, relevant for photovoltaic applications.

RESULTS AND IMPACT ON FUTURE DIRECTIONS

Overall, the Symposium fulfilled its goal to provide the European materials science community with a broad overview of advances, challenges and accomplishments in the area of computational materials science, with a focus on atomic-scale studies. It was demonstrated that the knowledge of the structural evolution at the atomistic scale with temperature and external constraints (such as pressure, stress, external fields, etc.) is necessary to understand and characterize the behavior of nanostructures, which show peculiar properties compared to their bulk counterparts. With the advent of nanoscience and nanotechnology, a detailed, atomic-level understanding of the interactions governing the synthesis, aggregation, self-assembly, surface deposition and recognition of nanoscale objects becomes crucial and can be achieved with the help of state-of-the-art simulation methods, as demonstrated by many contributions in the Symposium.

We had organized other two EMRS Fall Meeting Symposia, also in Warsaw, in 2008 and 2010, the first one on the subject of “*Morphology and dynamics of nanostructures and disordered materials via atomic-scale modelling*”, while the second evolved into “*Computer simulations for nanoscience and nanotechnology*”, of which the present Symposium represents the two-years update.

This year Symposium has given a real contribution to its title theme, by exploring several original and innovative investigations of a range of challenging and often technologically relevant systems in nanoscience and nanotechnology (from graphene to nanoclusters, from DNA to water on surfaces). Moreover state-of-the-art methods, which can effectively push the boundaries of computer simulations towards more complex nanostructures by increasing the affordable size, time scale and accuracy, have been discussed and critically assessed.

This Symposium is becoming a biennial periodic event, where to discuss the progress and applications of advanced computational methods of the structure and dynamics of molecular and nanoscale systems, within a large European materials science conference. It should be noted that it is the only computational Symposium organized in the framework of EMRS, both for the Spring Meeting (usually held in Strasbourg) and the Fall Meeting (usually held in Warsaw). The Symposium is typically held together with a series of many other parallel Symposia, attended mostly by experimentalists with expertise in various sectors of materials science. For them this is a unique opportunity to witness the progress and potential applications of computational methods to their own problems. Hence the broad impact of this Symposium should not be underestimated.

The support of the European Science Foundation has been and will be essential to publicize the power of advanced computational methods within the European materials science community through the organization of similar Symposia.

FINAL PROGRAMME OF THE SYMPOSIUM

Abstracts and poster details available at

http://www.emrs-strasbourg.com/index.php?option=com_abstract&task=view&id=190&year=2012&Itemid=&id_season=8

17/9/12 - Monday afternoon: COMPLEX MATERIALS (Chair: C. Goyhenex)

Pressure-induced amorphization in sulfur: an ab initio molecular dynamics study (invited)

Authors: Dušan Plašienka, Roman Martoňák

Affiliations: Department of Experimental Physics, Comenius University, Mlynská Dolina F2, 842 48 Bratislava, Slovakia

Atomistic modelling of Si and C migration at (0001) surface of SiC crystal.

Authors: M. Kozłowski, A. Biborski, R. Kozubski,

Affiliations: Jagiellonian University Institute of Physics ul. Reymonta 4 30-059 Kraków Poland

Structural and electronic properties of the silicon carbide allotropes as predicted by exact exchange calculations

Authors: Nevill Gonzalez Szwacki, Jacek A. Majewski

Affiliations: Faculty of Physics, University of Warsaw, PL-00-681 Warszawa, Poland

Electronic properties of the interphase boundaries involving high-pressure phases of silicon and gallium arsenide. (invited)

Authors: Dariusz Chrobak

Affiliations: University of Silesia, Institute of Materials Science, Bankowa 12, 40-007 Katowice, Poland

Confinement effects for point defects in perovskite ultrathin films

Authors: E. Blokhin, E. A. Kotomin, D. Gryaznov, R. A. Evarestov, J. Maier

Affiliations: Max Planck Institute for Solid State Research, Stuttgart, Germany; Institute for Solid State Physics, University of Latvia, Riga, Latvia; Department of Quantum Chemistry, St. Petersburg State University, Stary Peterhof, Russia

Poster session I (9 contributed papers)

19/9/12 - Tuesday morning: COMPUTATIONAL METHODS I (Chair: C. Massobrio)

Ab initio simulations of wet and dry interfaces (invited)

Author: Angelos Michaelides

Affiliations : Thomas Young Centre, London Centre for Nanotechnology, Department of Chemistry, University College London, UK

Prediction of Thermodynamic Properties of Materials: The Impact of DFT Exchange-Correlation Functionals

Authors: J. Wróbel, P. Śpiewak, L.G. Hector Jr., J. Yang, W. Wolf, K. J. Kurzydłowski

Affiliations: Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland; GM R&D Center, 30500 Mound Road, Warren, MI, 48090-9055, USA; Materials Science and Engineering, University of Washington, Seattle, WA, 98195-2120, USA; Materials Design S.a.r.l., 18, rue de Saisset, 92120 Montrouge, France

Quantum coloured noise thermostat for heat transfer

Authors: Natalia Bedoya, Jean-Louis Barrat, David Rodney

Affiliations : Université de Grenoble 1/CNRS, LIPhy, Fondation Nanosciences, SIMAP, Saint Martin d'HF-38402

General-Purpose Interatomic Potentials for Materials Science Based on Neural Networks (invited)

Author : Jörg Behler

Affiliations : Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

A variational theory for the computation of non-equilibrium stationary electron dynamics

Authors: A. La Magna, I. Deretzis

Affiliations : Consiglio Nazionale delle Ricerche Istituto per la Microelettronica e i Microsistemi Z.I VIII Strada 5, I 95121 Catania, Italy

18/9/12 - Tuesday afternoon: COMPUTATIONAL METHODS II (Chair: J. Behler)

Electronic structure of transition metal nanoalloys (invited)

Authors : L. Zosiak, C. Goyhenex, R. Kozubski and G. Trégli

Affiliations : IPCMS, UMR7504 CNRS- Université de Strasbourg, 23 rue du Loess F-67034 Strasbourg Cedex 2 (France); Institute of Physics, Jagellonian University, Reymonta 4, 30-059 Krakow, Poland; CINaM-CNRS, Campus de Luminy, Case 913, 13288 Marseille Cedex 9

Optimized energy landscape exploration using the ab initio based activation-relaxation technique nouveau: A tool for growth study in nanosciences

Authors : Eduardo Machado-Charry, Laurent Karim Béland, Damien Caliste, Luigi Genovese, Thierry Deutsch, Normand Mousseau and Pascal Pochet

Affiliations : Nanosciences Foundation, 23 rue des Martyrs, 38000 Grenoble, France; L_Sim, SP2M, UMR-E CEA/UJF-Grenoble 1, INAC, Grenoble, F-38054, France http://inac.cea.fr/L_Sim; Département de Physique and Regroupement Québécois sur les Matériaux de Pointe (RQMP), Université de Montréal, C.P. 6128, Succursale Centre-Ville, Montréal, Québec, H3C 3J7, Canada

18/9/12 - Tuesday afternoon: NANOCARBON (Chair: E. Lampin)

From nanodiamonds to twisted onions.

Authors : Alexandra Siklitskaya, Serge Yastrebov, Roger Smith

Affiliations : A.F. Ioffe Physical Technical Institute, 26 Polytechnicheskaya St. , St. Petersburg, 194021 Russia ; Loughborough University, Leicestershire, UK LE11 3TU

Young modulus of non-stoichiometric graphene (invited)

Author : Luciano Colombo

Affiliations : Department of Physics, University of Cagliari, and CNR-IOM, Unita' Cagliari (I)

Charge injection through single and double Carbon bonds

Authors : Yannick J. Dappe, Guillaume Schull, Cesar González, Hervé Bulou, Richard Berndt

Affiliations : Service de Physique de l'Etat Condensé, DSM/IRAMIS/SPEC, CEA Saclay URA CNRS 2464, Batiment 462, F-91191 Gif-Sur-Yvette Cedex, France; CEA Saclay, DSM/DRECAM/SPCSI, Batiment 462, F-91191 Gif sur Yvette, France; Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504 (CNRS – Université de Strasbourg), 67034 Strasbourg, France; Instituto de Ciencia de Materiales de Madrid (CSIC) 28049-Madrid, Spain; Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Poster session II (25 contributed papers)

19/9/12 - Wednesday morning: NANOSTRUCTURES (Chair: A. Michaelides)

Nanostructure simulations from large-scale density functional theory calculations with thousands of atoms (invited)

Author : Chris-Kriton Skylaris

Affiliations : School of Chemistry, University of Southampton, Highfield, Southampton SO17 1BJ, UK

Structural Phase Transition of Ag Nanowire to A Nanotube

Authors : Mine Konuk Onat, Sondan Durukanoglu

Affiliations : Department of Physics, Istanbul Technical University, Maslak, 34469 Istanbul, Turkey; Faculty of Engineering and Natural Sciences, Sabanci University, Orhanli, Tuzla 34950 Istanbul, Turkey

Core-shell Fe@Au nanoparticles: A DFT study

Authors : Magali Benoit, Cyril Langlois, Nicolas Combe, Marie-Josée Casanove

Affiliations : CEMES-CNRS, 29 rue Jeanne Marvig, 31055 Toulouse Cedex, France; MATEIS, INSA Lyon, 7, Avenue Jean Capelle, 69621 Villeurbanne Cedex, France; CEMES-CNRS, 29 rue Jeanne Marvig, 31055 Toulouse Cedex, France; CEMES-CNRS, 29 rue Jeanne Marvig, 31055 Toulouse Cedex, France

Nanocalloys structure modelling: phase transitions and phase diagrams (invited)

Authors : C. Mottet, A. Lopés, J. Los, G. Trégli

Affiliations : CINaM -CNRS/AMU

Insight into nanoparticulate magnesium hydride dehydrogenation and doping thermodynamics: A Density Functional Theory study

Authors : S. A. Shevlin, Z. X. Guo

Affiliations : University College London

20/9/12 - Thursday morning: BIOMATERIALS (Chair: C. Molteni)

Atomistic Molecular Dynamics Simulations of Biological Macromolecules (invited)

Author : Sarah Harris

Affiliations : School of Physics and Astronomy, University of Leeds, UK

Comparative analysis of the adsorption of chymotrypsin on two oxide materials surfaces with opposite charge

Authors : S. Koeppen, K. Li, L. Colombi Ciacchi

Affiliations : Faculty of Production Engineering and Bremen Centre of Computational Materials Science, University of Bremen, Bremen 28359, Germany

20/9/12 Thursday morning: ADSORPTION PHENOMENA (Chair: R. Kozubski)

Computational treatment of large molecules on insulators: Co-Salen on NiO <100>

Authors : David Z. Gao, Matthew B. Watkins, Alexander L. Shluger

Affiliations : Department of Physics and Astronomy and London Centre for Nanotechnology, University College London, London WC1E 6BT, UK; WPI-AIMR, Tohoku University, Sendai, Japan

Combined experimental/theoretical study of oxygen adsorption on Re (0001) (invited)

Authors : Eduardo R. Hernandez

Affiliations : Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Campus de Cantoblanco, Madrid, Spain

First-principles study of adsorption on Au(hkl) and the shape of gold nanoparticles

Authors : G. D. Barmparis, I. N. Remediakis

Affiliations : Department of Materials Science and Technology, University of Crete, 71003 Heraclion, Crete, Greece

20/9/12 - Thursday afternoon: HEAT TRANSPORT PROPERTIES (Chair: F. Cleri)

Atomistic modeling of heat transport: from nanostructured materials to devices (invited)

Authors : Davide Donadio

Affiliations : MPI for Polymer Research, Mainz, Germany

Calculation of thermal resistances by approach-to-equilibrium molecular dynamics

Authors : E. Lampin , P. A. Francioso, P. L. Palla and F. Cleri

Affiliations : Institut d'Electronique, de Microélectronique et de Nanotechnologies (IEMN);

Université de Lille I - BP 60069 - 59652 Villeneuve d'Ascq Cedex – France

20/9/12 - Thursday afternoon: ELECTRONICS AND OPTICAL PROPERTIES (Chair: L. Colombo)

Carrier Multiplication in isolated and interacting silicon nanocrystals for photovoltaic applications by ab initio calculations

Authors : M. Govoni , I. Marri and S. Ossicini

Affiliations : Dept. of Science and Methods for Engineering, University of Modena and Reggio Emilia, Via Amendola 2 Pad. Morselli, Reggio Emilia, Italy

Illuminating Graphene Nanostructures (invited)

Authors : Alice Ruini , Caterina Cocchi, Deborah Prezzi, S. Corni, Marilia J. Caldas and Elisa Molinari

Affiliations : Physics Dept., University of Modena and Reggio Emilia, Modena, Italy; S3 Center - CNR Nanoscience Institute, Modena, Italy; Instituto de Fisica, Universidade de São Paulo, SP, Brazil

Ab initio calculations for the H centers in SrF₂ as well as surface H centers and F centers aggregation in BaF₂ and CaF₂

Authors : R. I. Eglitis , H. Shi, R. Jia, L. Yue and X. He

Affiliations : Institute of Solid State Physics, University of Latvia, 8 Kengaraga Str., Riga LV1063, Latvia; School of Science, Beijing Institute of Technology, 100081, Beijing, PR China; Department of Mathematics and Natural Sciences, Bergische Universität Wuppertal, D-42097, Wuppertal, Germany; Fachbereich Physik, Universität Osnabrueck, Osnabrueck, Germany