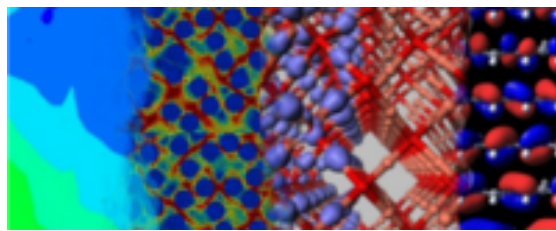


International Workshop on Multiscale Modelling of Materials for Energy Conversion Applications



Report of Contributions

Contribution ID: 1

Type: **Talk**

Challenges for in silico design of organic semiconductors for photovoltaic applications

Thursday, November 8, 2012 3:40 PM (45 minutes)

Interest in the field of organic electronics is largely provoked by the possibility to fine-tune properties of organic semiconductors by varying their chemical structure. Often, compound design is solely guided by chemical intuition, even though material development would benefit from more rigorous structure-property relationships, which link the chemical structure, material morphology and macroscopic properties. To formulate such relationships, an understanding of physical processes occurring on a microscopic level as well as the development of methods capable of scaling these up to macroscopic dimensions are required. The aim of computer simulations is to facilitate this by zooming in on the behaviour of electrons and molecules and by bridging micro- and macroscopic worlds. Here, we describe the current status of methods which allow the linking of molecular electronic structure and material morphology to the mesoscopic/microscopic dynamics of charge carriers and excitons. Special attention is paid to the challenges these methods face when aiming at quantitative predictions.

Author: Dr ANDRIENKO, Denis (Max Planck Institute for Polymer Research)

Co-authors: B., Baumeier; C., Poelking; M., Schrader

Presenter: Dr ANDRIENKO, Denis (Max Planck Institute for Polymer Research)

Session Classification: Session: Organic electronics, photovoltaics (Click for details or select 'Detailed view')

Track Classification: Organic electronics, photovoltaics

Contribution ID: 2

Type: **Talk**

Designing Nanoporous Materials for Hydrogen

Thursday, November 8, 2012 9:55 AM (45 minutes)

A Multi-Scale computational approach, combining both quantum and classical methods, is used for both, evaluating the hydrogen storage capacity of different materials 'in silico', and designing novel materials with enhanced storage capacity. Accurate ab-initio methods employed for investigating the nature of hydrogen interaction with different types of nanoporous materials, while Grand Canonical Monte Carlo simulations show their storage performance under different thermodynamic conditions. Carbon based materials and Metal Organic Frameworks (MOFs) are intensively investigated in different scales of size and theory. The storage capacity of Nanotubes (C-NT, BN-NT, SiC-NT) [1-3], Nanoscrolls [4], MOFs [5] and COFs [9] is evaluated under various conditions of temperature and pressure. Novel materials like pillared graphene [6] were designed and tested. Finally, the improvement of the storage capacity by functionalization [7] and doping [8] is evaluated under various thermodynamic conditions [10].

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- 9."Designing 3-D COFs with enhanced hydrogen storage capacity." E. Klontzas, E. Tylianakis, G.E. Froudakis, Nano Letters, 10 (2010) 452-454.
- 10."Hydrogen storage in nanotubes nanostructures", G.E. Froudakis, Materials Today 14 (2011) 324-328

Author: Prof. FROUDAKIS, George (Department of Chemistry - University of Crete)

Presenter: Prof. FROUDAKIS, George (Department of Chemistry - University of Crete)

Session Classification: Session: Grand challenges in multiscale modelling (Click for details or select 'Detailed view')

Track Classification: Grand challenges in multiscale modelling

Contribution ID: 3

Type: **Talk**

Modeling of Electrochemical Interfaces in Polymer Electrolyte Fuel Cells

Friday, November 9, 2012 9:00 AM (45 minutes)

The deployment of cost-competitive, highly efficient, and environmentally benign energy conversion and storage technologies is a major global challenge. In spite of excellent technological prospects, commercialization of advanced electrochemical energy systems, such as Polymer Electrolyte Fuel Cells (PEFCs) and metal-air batteries in transportation, electronics, and stationary power generation is far from being guaranteed.

For the commercialization of PEFC technology, the concomitant reduction in Pt loading would be the decisive breakthrough, meeting rigorous targets of the DOE (reduce Pt loading by factor > 10 , improve stability by factor > 2.5 by 2010). Critical progress hinges on new concepts in the design of advanced materials as well as fundamental understanding of basic (electro) chemical processes. In particular, material morphologies and processes at the nanoscale are decisive for maximizing the ratio of power density to Pt loading. As pointed out by fuel cell industry leaders, automakers, and experts; fundamental understanding of electrode-electrolyte interfaces is key and of vital importance for lowering the cost and improving fuel cell performance and durability. Current trends in fuel cell research activities indicates that phenomenological concepts are slowly transformed into a discipline that will be able to address many challenges, opportunities and research needs in the areas of basic science of fuel cell materials.

This presentation focuses on multi-scale modeling and molecular-level understanding of interfacial structure and interfacial processes at catalyst-support, catalyst-electrolyte, and support-electrolyte interfaces in catalyst layers (CL) of Polymer Electrolyte Fuel Cells (PEFC). Recent results in experiment and modeling indicate that catalyst activity and utilization could be improved by substantial factors. The fundamental understanding of relevant catalyst systems is, however, inept for guiding the design of electrodes with optimized structures, processes and overall performance. This challenge will be addressed. Initially, we focus on modeling of morphology, electronic structure, and electrochemical processes at various interfaces in supported catalyst nanoclusters. Physical properties will be studied by applying multi-scale molecular simulations. Thereafter, we will utilize this insight in view of developing physical models for microstructure and electrokinetic performance in catalyst layers of PEFC. Anticipated structure vs. property relations will provide enhanced capabilities for the rational design of advanced catalytic nanoarchitectures for PEFC.

Authors: Dr MALEK, Kourosh (National Research Council of Canada (NRC) and Simon Fraser University, Canada); EIKERLING, Michael

Presenter: Dr MALEK, Kourosh (National Research Council of Canada (NRC) and Simon Fraser University, Canada)

Session Classification: Session: Energy storage (Click for details or select 'Detailed view')

Track Classification: Energy storage

Contribution ID: 4

Type: **Talk**

ATK: An open platform for atomic-scale modeling

Thursday, November 8, 2012 9:10 AM (45 minutes)

Atomistix ToolKit (ATK) from QuantumWise is a platform for atomic-scale modeling that provides a user-friendly interface to a wide variety of state-of-the-art simulation codes, including DFT, tight-binding and classical potential methods developed by QuantumWise, as well as external software packages. The platform has a modular structure which allows for development of third-party plugins for extended and customized functionality, a similar concept as the apps known from the iPhone/Android world. This makes the platform extremely versatile and efficient for working on a broad class of nanoscale problems.

ATK is market leader within Quantum Transport simulations. ATK is designed to describe open boundary conditions where the electron density is calculated using NonEquilibrium Green's Function (NEGF) formalism and the electronic structure can be described at the DFT or tight binding level. The electro-statics is described self-consistently through a Poisson multi-grid solver, and allows for electro-static couplings between continuum models and the atomistic models.

For simulation of systems with millions of atoms ATK provides a classical potential package. In the EU project ATOMMODEL with Fraunhofer SCAI, we are developing a new model for on the fly generation of classical potentials from first principles data. The new model will be implemented in the Tremolo-X simulation packages, which will be available from ATK.

QuantumWise profile

QuantumWise specializes in fast and reliable atomic-scale modeling solutions, delivered via an easy-to-use interface. The software package is called Atomistix ToolKit (ATK), and is used by leading academic groups and commercial companies in the areas of materials for electronic devices, catalysis, new emerging electronic devices, graphene materials and other new nanoscale materials.

Author: Dr STOKBRO, Kurt (QuantumWise A/S)

Presenter: Dr STOKBRO, Kurt (QuantumWise A/S)

Session Classification: Session: Grand challenges in multiscale modelling (Click for details or select 'Detailed view')

Track Classification: Grand challenges in multiscale modelling

Contribution ID: 5

Type: **Talk**

A service-oriented approach for multiscale materials modelling and current challenges

Thursday, November 8, 2012 11:35 AM (25 minutes)

Macroscopic effects in complex materials arise from physical phenomena on multiple length (from nano- through micrometer) and time (from femto- through microsecond) scales and therefore properties of such materials can be predicted accurately basing on the properties of the contained building blocks. This makes not only the physical description easier to understand but also computer simulations of whole macroscopic devices feasible due to the effective linear scaling. However the application of multiscale methods in materials research is currently still a challenge. In particular, the diversity of the required fields of expertise limits the feasibility of multiscale techniques, especially for experimental and industrial researchers.

In the MMM@HPC project a significant effort has been done to enable non-expert users to use multiscale models. Using directed acyclic graphs, so-called workflows, and a service-oriented approach we implement sequential multiscale models in computer simulations by integration of existing methods operating on the individual scales. This approach is particularly practical and scales well for loosely hierarchically coupled sub-models. The main advantage is that the complexity of the individual methods is hidden and only parameters and data relevant for the overall workflow are exposed to the modeller and the end user. Also the technical details of the computing infrastructure are effectively hidden making the access to the resources and installed applications transparent.

In this contribution we will provide an overview of our progress in development and deployment of an e-infrastructure for multiscale modelling and discuss current and upcoming challenges such as the data complexity, licensing issues and sustainability, including the uptake of the methodology by the community and ensuring long-term support and operation of the infrastructure.

Author: Dr KONDOV, Ivan (Karlsruhe Institute of Technology)

Co-authors: BOZIC, Stefan (Karlsruhe Institute of Technology); Dr MEDED, Velimir (Karlsruhe Institute of Technology); Prof. WENZEL, Wolfgang (Karlsruhe Institute of Technology)

Presenter: Dr KONDOV, Ivan (Karlsruhe Institute of Technology)

Session Classification: Session: Grand challenges in multiscale modelling (Click for details or select 'Detailed view')

Track Classification: Grand challenges in multiscale modelling

Contribution ID: 6

Type: **Talk**

Top-down and bottom-up modeling paradigms for the simulation of batteries and supercapacitors

Friday, November 9, 2012 11:00 AM (25 minutes)

Electrochemical devices for electric energy storage, such as lithium ion batteries, lithium air batteries and super-capacitors, are expected to play an important role in the future widespread development of a sustainable energy network for a large diversity of applications. However, several technical challenges related to the materials chemical and structural properties as well as operation conditions should be still solved to enhance their specific capacity and durability. The development of physical models and numerical methods to simulate these devices operation by connecting the materials properties with the experimental observables (e.g. charge discharge curves) can reveal helpful tools for achieving this.

In this talk I will review some of the ongoing efforts within the community to develop top-down cell models (connecting detailed macroscopic descriptions of mechanisms with global parameters representing microscopic mechanisms) and bottom-up cell models (scaling up detailed descriptions of microscopic mechanisms onto global parameters to be used in macroscopic models) to simulate electrochemical storage devices. The importance of developing a multiparadigm approach synergistically connecting these two complementary views will be highlighted and some of the remaining methodological and numerical challenges will be discussed on the basis of analogies with past modeling works for fuel cells.

//// References:

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Author: Prof. ALEJANDRO A., Alejandro A. (CEA-LITEN)

Presenter: Prof. FRANCO, Alejandro A. (CEA-LITEN)

Session Classification: Session: Energy storage (Click for details or select 'Detailed view')

Track Classification: Energy storage

Contribution ID: 7

Type: **Talk**

Multiscale Modelling with High Performance Architectures

Thursday, November 8, 2012 2:00 PM (25 minutes)

I will give a brief overview of the goals and present status of the MMM@HPC project and its relation to applications and other activities in multiscale modelling and high-performance computing.

Author: Prof. WENZEL, Wolfgang (Karlsruhe Institute of Technology)

Presenter: Prof. WENZEL, Wolfgang (Karlsruhe Institute of Technology)

Session Classification: Session: Grand challenges in multiscale modelling (Click for details or select 'Detailed view')

Track Classification: Grand challenges in multiscale modelling

Contribution ID: 8

Type: **Talk**

Closing remarks

Track Classification: Energy conversion: photovoltaics, dye-sensitized cells

Contribution ID: 9

Type: **Talk**

Modeling Dye-Sensitized Solar Cells from First Principles: Understanding the mechanism, improving the efficiency

Friday, November 9, 2012 2:00 PM (45 minutes)

We present computer simulations on the fundamental constituents of Dye-sensitized solar cells (DSCs) and their interactions at the respective molecular/solid/liquid interfaces. Predictive dye design and modeling of realistic semiconductor (TiO₂, ZnO) nanostructures enables us to investigate the structural, electronic and optical properties of dyes adsorbed onto semiconductor surfaces by means of DFT and TDDFT calculations. Thus, the alignment of ground and excited state energy levels for the interacting DSC constituents is presented and discussed in relation to experimental photovoltaic performances. Modeling of the combined dye / semiconductor / electrolyte heterointerfaces is then achieved by performing ab initio molecular dynamics simulations of semiconductor adsorbed dyes in the solution and electrolyte environments. In particular, we present the case of Ru(II)-dyes on TiO₂ and their interaction with a Cobalt-based electrolytes. The nature and localization of the electronic states at the dye/semiconductor/electrolyte interface is discussed in relation to the device efficiency parameters. The mechanistic details of dye regeneration and the recombination pathways with the oxidized dye and with TiO₂-injected electrons are presented. A multiscale approach to the simulation of the mesoporous TiO₂ film based on a first-principle description of the individual and aggregated nanocrystals is finally presented.

Author: Dr DE ANGELIS, Filippo (CNR-ISTM)

Presenter: Dr DE ANGELIS, Filippo (CNR-ISTM)

Session Classification: Session: Energy conversion: photovoltaics, dye-sensitized cells (Click for details or select 'Detailed view')

Track Classification: Energy conversion: photovoltaics, dye-sensitized cells

Contribution ID: 10

Type: Talk

Impact of the Interface Electrochemistry on the Li-Battery Performance: A first-step study towards multi-scale modeling

Friday, November 9, 2012 9:45 AM (45 minutes)

Li-Ion batteries have become indispensable in the field of portable electronics and hybrid electric vehicles. If their high energy density is a major asset, their life and reliability are still inadequate to respond favorably to industry specifications to which they are subject. Understanding the degradation modes of the different elements of a Li-Ion battery is now one of the major objectives of the scientific community involved in this field. To achieve this, one possible strategy is to identify the indicators of failure in order to prevent degradation of our batteries and, hopefully, propose alternatives to this degradation. For the most part, the aging/degradation phenomena of a battery arise from the electrochemical reactivity at interfaces and from side reactions occurring between the different elements of the battery (electrode/electrode, electrode/electrolyte). These reactions occur, for example, when the redox mechanisms at the origin of the device performance are modified by a change in texture or morphology of the electrode during the charge/discharge. An essential step in the understanding and treatment of these phenomena is to define, in a systematic way the mechanical, electronic, chemical, electrical and ionic factors that are most relevant to describe the device as a whole. In other words, we need to understand how thermodynamics and kinetics are related in these systems. Understanding these parameters is a challenge for computational chemists, in particular at the atomistic level using first-principles methods. This presupposes to calculate, independently and without prejudging their impact on battery performance, a set of elementary reactions occurring in the bulk, at the surfaces and at the interfaces of the electrode, and to inject the as-obtained *ab initio* parameters in a model of higher scale to determine which of these elementary processes is dominant in the degradation mechanism. With these calculations, it is then possible to translate, at a macroscopic level, all the basic mechanisms occurring at the atomic scale, in order to identify factors causing degradation phenomena of Li-Ion batteries. The methodology we developed to investigate this first-step study towards multi-scale modeling will be presented for a set of Li-based materials, the so-called conversion materials. Our aim is to show how nano-sized effects crucially affect both the thermodynamics and the kinetics of the reactions and more specifically the electrochemical response of the battery.

Authors: DALVERNY, Anne-Laure; FILHOL, Jean-Sébastien; DOUBLET, Marie-Liesse; KHATIB, Rémi

Presenter: Dr DOUBLET, Marie-Liesse (Institut Charles GERHARDT)

Session Classification: Session: Energy storage (Click for details or select 'Detailed view')

Track Classification: Energy storage

Contribution ID: 11

Type: Talk

Three-dimensional modelling of transport, injection and recombination in organic light-emitting diodes

Friday, November 9, 2012 2:45 PM (25 minutes)

Charge transport in organic semiconductors can be described by hopping of charge carriers between localized states. The energetic disorder present in those organic semiconductors leads to the percolation of charge carriers, resulting in an inhomogeneous filamentary three-dimensional current density. We present a complete Monte Carlo modelling study of charge transport, injection and recombination in organic light-emitting diodes. The effects of space charge, image-charge potentials close to the electrodes, finite injection barriers, and the complete dependence of the mobility on the temperature, the carrier density and the electric field are taken into account. While the obtained 3D current density is very inhomogeneous, the total current through the devices agrees quite well with existing analytical models. The inclusion of short-range Coulomb interactions leads to a slight change of the total current due to two effects: blocking of filaments and declothing of charge carriers. The recombination rate in a bulk organic semiconductor can be well described by the Langevin recombination formula when the correct mobility, correcting for the presence of both electrons and holes, is used. All these results were obtained while assuming a cubic lattice of sites, a Miller-Abrahams hopping formalism and a Gaussian site energy distribution. Recently, we started with a multi-scale computational scheme in which we integrate several different simulation methods covering one or more length- and/or time-scales. By means of a coarse-grained Monte Carlo method and well established force field parameterizations, the morphology of the organic semiconductor can be simulated. These morphologies are then used in DFT simulations to calculate the site energies of the hopping sites and the transfer integrals between those sites. The corresponding site energies and transfer integrals are then used in a kinetic Monte Carlo program to simulate the three-dimensional charge carrier current density and recombination profiles.

Authors: BELJONNE, D. (Universite de Mons); VAN OOST, F.W.A. (Universite de Mons); CORNIL, J. (Universite de Mons); VAN DER HOLST, J.J.M. (Universite de Mons); BOBBERT, P.A. (Universite de Mons); COELHOORN, R (Universite de Mons)

Presenter: VAN DER HOLST, J.J.M. (Universite de Mons)

Session Classification: Session: Energy conversion: photovoltaics, dye-sensitized cells (Click for details or select 'Detailed view')

Track Classification: Energy conversion: photovoltaics, dye-sensitized cells

Contribution ID: 12

Type: **Talk**

Modeling of lateral hole diffusion on dye sensitized metal oxide monolayer.

Friday, November 9, 2012 3:10 PM (25 minutes)

In Dye Sensitized Solar Cells (DSSC), photocurrent generation results from electron injection into a nanocrystalline oxide electrode from a photo-oxidized dye molecule adsorbed on to the oxide surface while the dye is normally regenerated by a Hole Transporting Medium (HTM). In an alternative mechanism, the dye may be regenerated through the lateral transport of holes between dye molecules on the oxide surface. Such lateral transport may have application in solid state devices by providing an additional pathway for the holes to reach the solid HTM, especially when the HTM is in poor contact with the dye molecules. Although there is experimental evidence for this 'hole hopping' mechanism, the factors controlling it are not yet understood in detail. In this work we introduce a multi-scale method to model hole diffusion dynamics through a monolayer of dye molecules anchored to a nanocrystalline film. We treat the intermolecular charge transfer step as a non-adiabatic hopping process and calculate the hopping rate as a function of the electronic coupling (J) and the reorganization energy (λ). First we propose a numerical method based on quantum chemical calculations to calculate the inner- and outer-sphere reorganization energies and show that the nature of the surrounding medium dominates λ , consistent with the high values of λ observed experimentally ($\lambda \sim 1$ V). Next, we again use quantum chemical methods to study the influence of the dyes arrangement at the nanoscale on J . Finally we incorporate these parameters into a continuous time random walk (CTRW) to estimate the hole diffusion coefficient at the scale of the dyes monolayer. We randomize the waiting times distribution to treat the configurational disorder. We show how this procedure leads to anomalous diffusion of holes. The results show reasonable agreement with experimental measurements on a range of dye sensitized films. Our method provides a deeper insight on how to control the lateral hole transport between dye molecules and is expected to assist in the design of higher performance devices.

Authors: MOIA, Davide; KIRKPATRICK, James; NELSON, Jenny; BARNES, Piers; VAISSIER, Valerie (Imperial College London)

Presenter: VAISSIER, Valerie (Imperial College London)

Session Classification: Session: Energy conversion: photovoltaics, dye-sensitized cells (Click for details or select 'Detailed view')

Track Classification: Energy conversion: photovoltaics, dye-sensitized cells

Contribution ID: 13

Type: **Talk**

Microstructural Characterisation and Modelling of Organic Photovoltaic Materials

Friday, November 9, 2012 3:35 PM (25 minutes)

Nowadays, the best performing designs of organic solar cell are based on blend films of a conjugated polymer and a fullerene derivative. The best studied example is the blend of poly(3-hexylthiophene-2,5-diyl) (P3HT) as the donor and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) as the acceptor. The performance of such devices is strongly related to the blend microstructure. The best performing systems feature a phase separation of 10 of nanometers. Crystallisation of the polymer donor is known to drive phase separation processes. Therefore, in the selection of new semiconductor materials for improved light harvesting or higher photovoltage, it is essential to understand the effect of the chemical structure on microstructure and to find ways to control it. In this work, we present combined experimental and simulation studies of two groups of conjugated polymers. In the first study, we use grazing incidence X-ray diffraction and molecular dynamics to study the effect of modifying the structure and attachment of side chains in poly[2,1,3-benzothiadiazole-4,7-diyl[4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2,6-diyl]] (PCPDTBT) and related polymers. It has been observed that either replacing the carbon bridging atom between the backbone and the side chains with a silicon atom or shortening the side chains increases the tendency of the polymer to aggregate, resulting in an increased crystallinity and hole mobility. The second study concerns the side chain dynamics of two conjugated poly-alkyl-thiophenes with different side chain length, P3HT and poly(3-octylthiophene) (P3OT). Here we use quasi-elastic neutron scattering and molecular dynamics to study the effect of side chain structure on the polymer dynamics.

Authors: GUILBERT, Anne (Imperial College London); URBINA, Antonio; BRADLEY, Donal D.C.; PIRES, Ellis (Imperial College London); MACDONALD, J. Emyr; FROST, Jarvist M. (Imperial College London); NELSON, Jenny; AGOSTINELLI, Tiziano (Imperial College London)

Presenter: GUILBERT, Anne (Imperial College London)

Session Classification: Session: Energy conversion: photovoltaics, dye-sensitized cells (Click for details or select 'Detailed view')

Track Classification: Energy conversion: photovoltaics, dye-sensitized cells

Contribution ID: 14

Type: **Talk**

Calculations of the free energy of sII clathrate hydrates

Friday, November 9, 2012 11:25 AM (25 minutes)

Clathrate hydrates are of great technological interest because of their capacity to store gas at relatively high density. They are therefore considered as prospective candidates for hydrogen storage materials. Extreme pressures are required to form stable pure hydrogen clathrate hydrates, which makes it impractical to use pure hydrogen clathrates in technological applications. However, the synthesis pressure of hydrogen hydrates can be significantly decreased by accommodating a second guest molecule, referred to as promoter, in the large cavities. Here we study the relationship between potential promoter molecules and the stability of binary sII hydrogen hydrates at a wide range of temperatures (233 K – 293 K) by means of Monte Carlo simulations. Our aim is to predict what would be an efficient promoter molecule using properties such as size, dipole moment, and hydrogen bonding capability. The gas clathrate configurational and free energies are compared and entropy was found to make a considerable contribution to the free energy. Therefore, full free energy calculations are required to assess the stability of clathrate hydrates filled with different promoter molecules. Unfortunately, no predictive property could be distinguished.

Authors: ATAMAS, A. (Radboud University Nijmegen); CUPPEN, Herma M. (Radboud University Nijmegen); DE LEEUW, S. W. (Leiden University)

Presenter: ATAMAS, Alexander (Radboud University Nijmegen)

Session Classification: Session: Energy storage (Click for details or select 'Detailed view')

Track Classification: Energy storage

Contribution ID: 15

Type: **Talk**

A virtual scientific computational environment for mobile devices

Thursday, November 8, 2012 2:50 PM (25 minutes)

Until now all client computers for scientific computation has been limited to windows and Linux powered workstations which are connected High Performance Computers (used as servers). The virtual scientific computational environment will move scientific computation from the desktop clients to mobile clients. Virtual scientific environment and Virtual network communication application (virtual graphic environment and ultra-high speed file transfer, UDT protocol) should be ported to the mobile devices. These mobile clients will be connected to the HPCs via Wi-Fi, LTE, 3G and Virtual Private Networks (VPN). Benchmarking of the Wi-Fi and 3G connectivity of various mobile devices proved that Wi-Fi connectivity has the best and stable connection. The current channel binding technology gives up to 450Mbps, this speed is expected to double with the 1Gbps Wi-Fi routers which will soon be available. Scientists and researchers can now have the flexibility of performing graphical scientific computations on the go. A hybrid cluster (60 Kepler GPUs, 256 cores) which will have up to up to 3x processing performance and efficiency (compared to the Tesla) with the new SMX, Dynamic parallelism and Hyper-Q functionalities is planned to be built in 5 months. Scientists and researchers will be able to experience virtual scientific calculations in mobile environment soon.

Authors: CHO, Haneol (Korea Institute of Science and Technology); LEE, Kyu Hwan; BOATENG, Samuel

Presenter: CHO, Haneol (Korea Institute of Science and Technology)

Session Classification: Session: Grand challenges in multiscale modelling (Click for details or select 'Detailed view')

Track Classification: Grand challenges in multiscale modelling

Contribution ID: 16

Type: **Talk**

Multiscale modelling on petascale supercomputers

Thursday, November 8, 2012 11:10 AM (25 minutes)

The availability of High Performance Computing (HPC) has revolutionized many fields in science and engineering, allowing insights into phenomena which are not obtainable from experiment alone. However, using HPC facilities is daunting for many researchers who find that in order to exploit the resources effectively they must understand concepts of parallel computing and architectures, intricacies of operating systems and working environments unlike those used on common workstations. Further challenges are becoming apparent as Europe, the US, Japan, China and other countries start bringing into production clusters capable of performances extending into the Petaflop range, the so-called "Petascale". For these systems, not only do the application codes have to be parallel but the level of parallelism has to be very high, extending to thousands of cores. Other characteristics of Petascale architectures, such as low core memory and limited I/O bandwidth, are also important and influence the software applications and scientific problems available to researchers. In this study we examine how these factors are affecting users in multiscale modelling where many very different codes are employed. We also discuss the opportunities and implications for application programmers and users as HPC centres move beyond Petascale and in the near future to Exascale systems.

Author: EMERSON, Andrew (CINECA Computer Centre)

Presenter: EMERSON, Andrew (CINECA Computer Centre)

Session Classification: Session: Grand challenges in multiscale modelling (Click for details or select 'Detailed view')

Track Classification: Grand challenges in multiscale modelling

Contribution ID: 17

Type: **Talk**

Divide-and-Conquer Learn-on-the-Fly: A Hybrid Quantum-Classical Approach for Simulating the Nanomechanical Properties of Metallic Systems

Thursday, November 8, 2012 2:25 PM (25 minutes)

Simulations performed with the molecular dynamics (MD) method constitute an important tool in the study of the mechanical properties of nanoscale systems. The MD method is classical in nature and its main limitations stem from the empirical nature of the employed potentials, whose functional form is postulated a priori, and from not taking the electronic effects explicitly into account. In consequence, results obtained in such a strictly classical fashion do not necessarily correctly model physical reality in all cases, particularly for systems that are far from equilibrium, such as nanostructures undergoing plastic deformation; i.e. classical potentials are said to lack transferability. The explicit inclusion of electronic effects offered by quantum-based approaches, which start from first principles (ab initio) does yield a transferable description of the interatomic interactions; this, however, is associated with significant computational complexity, which prevents these approaches from being directly applied to systems involving more than several hundred atoms, and even then in practice the performed simulations are usually not dynamical. Hybrid (quantum-classical) approaches realize a compromise whereby a subset of the system (such as a region where bond-reorganization is taking place) is treated with a first-principles approach whilst the remainder undergoes classical MD. The Learn-on-the-Fly (LOTF) technique (Csanyi et al., PRL 93 (17), 2004) offers a particularly elegant way of embedding the results of quantum-mechanical calculations within an MD simulation, by periodically, locally re-parametrizing the empirical potential so that it reproduces the accurate forces obtained from first principles in the region of interest. In its original formulation it has been successfully applied to the fracture of silicon, where the classical Stillinger-Weber potential is shown to give qualitatively wrong predictions. We present Divide-and-Conquer Learn-on-The-Fly (Dziedzic et al., PRB 83 (22), 2011) – a generalization of LOTF, which is suitable for systems where the interaction range is longer, such as d-shell metals. We show how the force-matching stage can be recast to make the problem of simultaneously optimizing thousands of parameters in situ to match thousands of atomic forces computationally tractable. We demonstrate the feasibility of our approach on several examples: simulating nanoindentation and nanoscratching of Cu monocrystals, calculating the structure and properties of liquid Au and the structure of selected AuCu nanoclusters.

Authors: DZIEDZIC, Jacek; RYBICKI, Jarosław**Presenter:** DZIEDZIC, Jacek**Session Classification:** Session: Grand challenges in multiscale modelling (Click for details or select 'Detailed view')

Contribution ID: 18

Type: Talk

Modelling Charge Transfer States in Organic Photovoltaics

Thursday, November 8, 2012 4:25 PM (25 minutes)

Recently, much attention has been paid to the formation of charge transfer (CT) states at the donor : acceptor interface in organic photovoltaic materials, and to their role in charge pair generation.¹ However, until now few theoretical studies have addressed the electronic properties of CT states in detail. In this work, we use density functional theory (DFT) methods to study the energies and properties of CT states of a complex consisting of an oligomer of a donor polymer (poly-3-hexyl-thiophene (P3HT), Poly((9,9-dioctylfluorenyl-2,7-diyl)-alt-5,5-(40,70-di-2-thienyl-20,10,30-benzothiadiazole)) (PFODTBT), and the thiophene-isoindigo based polymer, P3TI) and an acceptor molecule (fullerene derivatives phenyl C61 butyric acid methyl ester (PCBM), phenyl C71 butyric acid methyl ester (PC71BM), and bis-indenofullerene ICBA). The effects of position, relative orientation, and specific chemical structure of the molecules on charge distribution, absorption and emission spectra, and overlap of electronic states between the molecules are studied. Results are analysed in comparison with electroluminescence data on polymer:fullerene blends containing different fullerene derivatives. We discuss how studies on this model system help to elucidate the role of charge transfer states in charge generation and so help develop design rules for better photovoltaic materials.

Authors: KIRKPATRICK, James; NELSON, Jenny; FEW, Sheridan

Presenter: FEW, Sheridan

Session Classification: Session: Organic electronics, photovoltaics (Click for details or select 'Detailed view')

Track Classification: Organic electronics, photovoltaics

Contribution ID: 19

Type: **Talk**

Nanoscale materials and electronic transport: from ballistic to hopping approaches

Thursday, November 8, 2012 4:50 PM (25 minutes)

To support accelerating materials development cycles we have developed simulation approaches for de-novo characterisation and optimisation of materials and device properties with nanoscale constituents. In recent years we have developed simulation methods that describe the conformation and electronic properties of materials built on the basis of well-defined nanoscale constituents. We have applied these methods to describe both ballistic and hopping transport in nanoscale devices. Here we discuss applications on single-molecule electronics, specifically molecular wires (metallic, organic and DNA based) and on the development of an atomic transistor [1,2,3,4]. A second point of emphasis will be the development of methods to describe function of organic light emitting diodes [5] based on detailed atomistic models of their morphology and molecular properties, accent being on the morphology simulations with Monte Carlo methods. Finally I will discuss the integration of these methods into a European framework for multiscale materials modelling in the EU project MMM@HPC, which shall make these and other simulation method accessible to a wide audience of interested scientists and enable exploitation on high performance computing architectures.

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Authors: POSCHLAD, Angela; DANILOV, Denis; KONDOV, Ivan; NEUMANN, Tobias; MEDED, Velimir; WENZEL, Wolfgang

Presenter: MEDED, Velimir

Session Classification: Session: Organic electronics, photovoltaics (Click for details or select 'Detailed view')

Track Classification: Organic electronics, photovoltaics

Contribution ID: 20

Type: **Poster**

Organic Semiconductors For Advanced Electronics” Detailed atomistic simulations of the semi-crystalline nature of Regioregular Poly-3Hexyl-Thiophene (Rr-P3HT)

Thursday, November 8, 2012 6:05 PM (10 minutes)

We investigate the assembling and structure of regioregular poly-3-hexylthiophene (Rr-P3HT) chains using classical molecular dynamics simulations. Taking into account recent experimental findings that give evidence to a semicrystalline ordering of the P3HT system where crystalline lamellae are periodically separated by interlamellar amorphous zones we have carried out detailed atomistic molecular dynamics (MD) simulations of the pure crystalline and pure amorphous phases of Rr-P3HT separately in order to generate fully relaxed configurations of model P3HT system representative of their true morphology (amorphous versus crystalline domains). The effect of temperature and system's molecular weight (MW) is also investigated through a series of MD simulations in a wide range of temperatures from 225K to 600K and for two different P3HT systems (20-3HT and 30-3HT). In the pure crystalline phase the system is found to adopt a noninterdigitated and tilted structure irrespective of temperature and MW consistent with XRD measurements. The inter-chain distance inside the crystal is not dramatically affected with increasing temperature; thus it is expected that temperature will have a minor effect in charge hopping in the direction of π - π stacking.

Authors: ALEXIADIS, Orestis (ICE-HT); MAVRANTZAS, Vlasios G. (ICE-HT)

Presenter: ALEXIADIS, Orestis

Session Classification: Poster Session

Contribution ID: 21

Type: **Poster**

Efficient scheme for modeling of disordered morphologies in organic semiconductors

Thursday, November 8, 2012 5:15 PM (10 minutes)

Organic light emitting diodes (OLEDs) are typically fabricated by vapor deposition or solution processing of organic charge-transport and emitter materials. The typical resulting morphology of the material is an amorphous film. Because of localization, charge transport in the disordered materials takes place by hopping of charge carriers from one molecule to another. As a consequence, the charge transport properties of organic semiconductors are extremely sensitive to the morphology of the material. Therefore, development of efficient simulation approaches for predictive characterization and optimization of the disordered morphologies in organic materials is very important in engineering of new efficient OLED devices. In this work we present a Monte Carlo based approach which generates disordered morphologies using method that simulates vapor physical deposition of molecular films: a single molecule deposition protocol. On a very rugged potential energy surface, such as those induced here by the roughness of the partially deposited film, the simulations can be trapped for long times in metastable conformations. To reduce the trapping of the system in metastable conformations, for each molecule we performed basin-hopping cycles, each of which consisted of a simulated annealing run. The individual steps in the simulated annealing run are standard Metropolis Monte Carlo moves. To increase the computational efficiency, a grid representations for electrostatic and for van der Waals interactions is used. This method leads to linear $O(N)$ dependence of the computational time on the system size N in contrast to $O(N^2)$ scaling for direct full atom-atom evaluation of the interatomic potentials.

Authors: DANILOV, Denis (Karlsruhe Institute of Technology); NEUMANN, Tobias (Karlsruhe Institute of Technology); WENZEL, Wolfgang (Karlsruhe Institute of Technology)

Presenter: DANILOV, Denis

Session Classification: Poster Session

Contribution ID: 22

Type: **Poster**

BigDFT GridBean within the UNICORE framework, a component for fully automated workflows

Thursday, November 8, 2012 5:55 PM (10 minutes)

Density functional theory (DFT) is the fundamental theory used to describe the quantum laws that governs the interactions between atoms and molecules within a molecular system. Realistic simulations requires a large amount of resources, which most often exceed the available resources given at a local site. These simulations belong to a certain class of High Performance Computing (HPC) and can only take place in the world of large scale computing involving several applications linked together via a Grid infrastructure. Furthermore

these simulations requires the use of hybrid machines, that is machine composed of both CPU and GPU accelerators. In this work we describe the work accomplished so far in the GridBean development for a DFT code, that is used within the UNICORE frame work. This GridBean, which we call BigDFTGridBean is then used within UNICORE to create workflows in a Grid computing infrastructure replacing laborious and tedious codes manipulations.

Presenter: BONNET, Frederic**Session Classification:** Poster Session

Contribution ID: 23

Type: **Poster**

Improving the scaling of the BigDFT electronic structure code

Thursday, November 8, 2012 5:45 PM (10 minutes)

The fact that wavelets exhibit at the same time orthogonality and compact support makes them an ideal candidate basis set for $O(N)$ calculations where one has to deal with localized quantities. We are currently implementing a new approach to $O(N)$ DFT using Daubechies wavelets as an underlying basis set. The KS orbitals are expressed via an intermediate basis set which we call trace minimizing basis (TMB) and which adapts itself to its chemical environment. Therefore we can achieve excellent accuracy using only a very small number of these basis functions. In particular we can calculate energies and forces with an accuracy comparable to that of a reference standard DFT code with cubic scaling. We will present preliminary results demonstrating this accuracy for a variety of systems and also demonstrate the ability to reach large system sizes.

Authors: CALISTE, Damien; RATCLIFF, Laura; GENOVESE, Luigi; BOULANGER, Paul; GOEDECKER, Stefan; MOHR, Stephan; DEUTSCH, Thierry

Presenter: RATCLIFF, Laura (CEA Grenoble)

Session Classification: Poster Session

Contribution ID: **24**

Type: **Poster**

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Thursday, November 8, 2012 5:35 PM (10 minutes)

Presenter: POSCHLAD, Angela (Karlsruhe Institute of Technology)

Session Classification: Poster Session

Contribution ID: 25

Type: **Poster**

Multiscale Modelling of Charge Transport in High mobility molecular semiconductor

Thursday, November 8, 2012 5:25 PM (10 minutes)

Recently, much attention has been paid to charge transport of high mobility molecular semiconductors [1]. Solution processed 6,13-bis(triisopropylsilyl ethynyl)-pentacene (TIPS-P) field effect transistors (FET) showed mobilities of up to 4.6 cm²/Vs [2] which is close to the performance of inorganic semiconductors. Until now most of the theoretical effort has been spent on a better understanding of the fundamental transport mechanism in these materials [3]. In this work we will present a multiscale approach to quantify the effect of anisotropy and structural defects on charge transport in high mobility organic materials. We prepared zone casted, large area 2D crystals of TIPS-P which show an anisotropic hole mobility in FET structures. Those TIPS-P crystals are used as a model system with which to test the capabilities of our simulation approach. In our multiscale approach charge transfer integrals and reorganization energies are calculated using semi-empirical quantum chemical methods. Either the Master equation or a Monte Carlo method is applied to estimate mobilities. Results are analysed in comparison with experimental data on TIPS-P FETs. We discuss how studies on this model system help to elucidate the role of anisotropy and structural disorder on charge transport and so help to develop design rules for high mobility molecular semiconductors. References

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Authors: JAMES, David T.; STEINER, Florian; NELSON, Jenny; KIM, Ji-Seon

Presenter: STEINER, Florian

Session Classification: Poster Session