CP2K users' and developers' meeting

Sponsored by CCP5, CCP9 and UKCP, IOP Computational Physics Group and EPSRC

Friday 14 June 2019

Molecular Sciences Research Hub (MSRH), Room G23/25,
White City Campus, Imperial College London, UK

Web: https://www.ccp5.ac.uk/cp2kmeet2019

11:30	Registration and Lunch
12:20	Welcome *Dr. Clotilde Cucinotta (ICL)*
12:30	Molecules at the solid/liquid interface: understanding experiments with simulations **Marcella Iannuzzi**, University of Zurich (CH)
13:00	Controlling the preferential motion of chiral molecular walkers on a surface **Lev Kantorovich**, King's College London (UK)
1330	Electrochemistry and Molecular Electronics from Projector Operator-based Diabatization (POD) **Jochen Blumberger**, University College London (UK)
14:00	Coffee Break
14:30	Reflections on 10 years of PLUMED **Gareth Tribello**, Queen's University Belfast (UK)
15:00	The time-dependent electronic response of liquid water to energetic ionic projectiles **Bin Gu**, Queen's University Belfast
15:30	The Role of Cation-Vacancies and Terminations for the Electronic and Optical Properties of Aluminosilicate Imogolite Nanotubes: A Non-local, Linear-Response TDDFT Study **Emiliano Poli**, ICTP (IT)
16:00	Flash presentations
16:15	Wine and Cheese
	Discussion (future plans/ build network)
17:30	Close

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Abstracts

Molecules at the solid/liquid interface: understanding experiments with simulations
Marcella Iannuzzi

The fundamental understanding of interfaces at the atomic level would greatly help in predicting the stability and reactivity of materials and eventually would lead to the rational tuning of the different components for example for heterogeneous catalysts, nano-electronics, photocatalysis. Most of the relevant processes in an electrochemical cell occur at solid/liquid interfaces. Unfortunately, the direct observation of these processes and the characterisation of the interfaces under operating conditions are still challenging for both experimental and modeling approaches. However, by developing efficiently scaling computational strategies, modelling of materials properties and processes from first principles is becoming sufficiently accurate as to facilitate the design and testing of new systems in silico. We present a few examples where computational materials science turns out to be valuable and necessary for developing novel functional materials.

Controlling the preferential motion of chiral molecular walkers on a surface
Lev Kantorovich

Molecular walkers standing on two or more "feet" on an anisotropic periodic potential of a crystal surface may perform a one-dimensional Brownian motion at the surface-vacuum interface along a particular direction in which their mobility is the largest. In thermal equilibrium the molecules move with equal probabilities both ways along this direction, as expected from the detailed balance principle, well-known in chemical reactivity and in the theory of molecular motors. For molecules that possess an asymmetric potential energy surface (PES), we propose a generic method based on the application of a time-periodic external stimulus that would enable the molecules to move preferentially in a single direction thereby performing as Brownian ratchets. To illustrate this method, we consider a prototypical synthetic chiral molecular walker, the 1,3-bis(imidazol-1-ylmethyl)-5(1-phenylethyl)benzene, diffusing on the anisotropic Cu(110) surface along the Cu rows. As unveiled by our kinetic Monte Carlo simulations based on the rates calculated using ab initio density functional theory, this molecule moves to the nearest equivalent lattice site via the so-called inchworm mechanism in which it steps first with the rear and then with the front foot. As a result, the molecule diffuses via a two-step mechanism, and due to its inherent asymmetry, the corresponding PES is also spatially asymmetric. Taking advantage of this fact, we show how the external stimulus can be tuned to separate molecules of different chirality, orientation and conformation. The consequences of these findings for molecular machines and the separation of enantiomers are also discussed.

Electrochemistry and Molecular Electronics from Projector Operator-based Diabatization (POD)

Jochen Blumberger

Abstract: One principal parameter determining electrochemical electron transfer rates and current-voltage characteristics is the electronic coupling between the electrode and the molecule that is adsorbed on it. Here I will describe the implementation of a simple method for the calculation of these matrix elements in the CP2K package, termed Projector Operator-based Diabatization (POD)\cite{1}. In the POD approach the self-consistent Kohn−Sham Hamiltonian of the full system is partitioned in donor (e.g., molecule) and acceptor (e.g., metal) blocks which are block-diagonalized\cite{2}. The coupling matrix elements between donor and acceptor states are simply identified with the matrix elements of the off-diagonal block. We will discuss several applications: electron injection from a dye molecule to TiO_2, electron transfer from a molecule, that forms self-assembled monolayers, to metallic Au(111)\cite{1} and the all-QM calculation of the current-voltage response of a full redox protein sandwiched between two gold elecrodes (~20,000 electrons) demonstrating that POD is a useful and cost-effective tool for estimation of electronic coupling across heterogeneous interfaces.

Reflections on 10 years of PLUMED

Garreth Tribello

PLUMED is an interoperable and open-source plugin that can be used with many molecular dynamics codes. You can use PLUMED to analyse trajectories and to perform enhanced sampling calculations. We have now been working on PLUMED for the last 10 years. During this time there have been huge changes in the way that we and others develop code and share that code with others. During my talk I will discuss what some of what I think are the most important of those changes. In other words, I will explain what we have learned by developing and maintaining PLUMED for the last 10 years. Furthermore, I will also discuss the challenges that I believe the future holds and why we have created the PLUMED consortium to try to address those challenges

The time-dependent electronic response of liquid water to energetic ionic projectiles

Bin Gu and Jorge Kohanoff

The study of stopping of ions in liquid water, the most crucial and abundant substance in living cells, is important for our understanding of radiation induced damage to biological systems, as in current and future space and planetary missions and in the field of radiotherapy as well. In this talk, we show some tests on calculations of electronic stopping of proton and alpha-particle in liquid water with the state-of-the art non-equilibrium ab initio simulations at the level of all-electron Time Dependent Density Functional Theory (TD-DFT) with Gaussian and Augmented Plane Wave (GAPW) basis sets, which has been

implemented in CP2K. Such approach allows us to study the real-time dynamics of the system, taking into account the details of the structural and electronic properties of the system. Some technical problems which we are faced with in the calculations are also given for discussion.

The Role of Cation-Vacancies and Terminations for the Electronic and Optical Properties of Aluminosilicate Imogolite Nanotubes: A Non-local, Linear-Response TDDFT Study

Emiliano Poli, J.Elliott, S. Chulkov, M. Watkins, G. Teobaldi

In this presentation we report the combined non-local (PBE-TC-LRC) Density Functional Theory (DFT) and linear-response time-dependent DFT (LR-TDDFT) study of the structural, electronic, and optical properties of the cation-vacancy based defects in aluminosilicate (AlSi) imogolite nanotubes (Imo-NTs) that have been recently proposed on the basis of Nuclear Magnetic Resonance (NMR) experiments. These defects are found to introduce both shallow and deep occupied states in the pristine NTs' band gap (BG). These BG states are highly localized at the defect site. LR-TDDFT simulation of the defects reveal increased low-energy optical absorbance for all but one defects due to the appearance of optically active excitations at energies lower than for the defect-free NT. On the basis of these results we propose a tentative interpretation of the low-energy tail in the experimental UV-vis spectra for AlSi NTs. The PBE TC-LRC-approximated exciton binding energy for the defects' optical transitions is found to be substantially lower (up to 0.8 eV) than for the pristine defect-free NT's excitations (1.1 eV). In addition we show preliminary results regarding the electronic, and optical termination-induced effects in finite aluminosilicate, and aluminogermanate (AlGe) NTs. Following the determination of the smallest finite-sized model that allows for the simultaneous description of the NT-ends and bulk-like NT-core the electronic properties and optical absorption of different NT-terminations are discussed. The simulations of finite NTs uncover the presence of longitudinal band-bending brought about by structural relaxation of the NT-ends. This longitudinal band-bending is accompanied by occurrence of appealing core-periphery VB ad CB edge separations, which could suggest the possibility of a mechanisms for the separation of photo-generated e*-h pairs along the NT.

Flash presentations

Nourdine Zibouche
Insights into electronic properties of 2D halide perovskites for photovoltaics

Laia Delgado Callico
Nanoproperties of Ni_{19}

Manasi R Mulay
Interaction of anatase with water pollutants

Arno Proeme
BioExcel: CP2K and QM/MM for biomolecular modelling & simulation Talk Abstract: to be determined

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