O 10: Methods: Electronic structure theory & Methods: other (theory)

Time: Monday 15:00–17:15 Location: H31

O 10.1 Mon 15:00 H31

The importance of van der Waals dispersion forces in ice — •Biswajit Santra[1], Angelos Michaelides[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany. — [2]University College London, London, UK.

For decades it is known that the condensed phases of water are held together through a combination of hydrogen bonds (HBs) and van der Waals (vdW) dispersion forces. Whilst HBs have received widespread attention, relatively little is known about the importance of vdW forces. Partly this is down to the now most popular electronic structure theory (density-functional theory (DFT)) providing an inadequate description of vdW forces when standard exchange-correlation functionals are used. However, improved semi-empirical vdW corrections to DFT[1] and the non-local vdW functional[2] mean that it is now possible to shed light on this issue. Here, we report simulations on a range of ambient and high pressure phases of ice to understand the delicate interplay of HBs and vdW. We find that the proportion of the lattice energy coming from vdW forces monotonously increases as the density of the ice phases increases, and as a consequence vdW plays a crucial role in determining the relative stabilities of the high density phases of ice. In addition, our calculations show that the effective volume of the water molecules is reduced when vdW is accounted for and provide general insights into the importance of vdW forces in other condensed phases of water. [1]Tkatchenko *et al.*, PRL **102**, 073005 (2009), [2]Dion *et al.*, PRL **92**, 246401 (2004).

O 10.2 Mon 15:15 H31

Density functional calculations for thousands of atoms: KKRnano - recent developments and first applications — •Alexander Thiess[1,2], Rudolf Zeller[2], and Stefan Blügel[2] — [1]German Research School for Simulation Sciences, 52425 Jülich, Germany — [2]Institut für Festkörperforschung and Institute for Advanced Simulation, Research Center Jülich, 52545 Jülich, Germany

KKRnano is a new massively parallel DFT-algorithm in the framework of the KKR Green function method [1] we have developed for large-scaled applications on state-of-the-art supercomputers. The advantageous scaling of our code enables to exceed the limits of most of today's DFT-algorithms of hundreds of atoms per unit cell by one order of magnitude. In order to deal with the enormous computational requirements of such calculations we have parallelized our code in real space, spin space, over energies and with respect to angular momentum. This allows for an efficient use of hundreds of thousands of processors. We present recently developed extensions as a fast parallel Lloyd's formula algorithm, real space calculation of Liechtenstein's formula and preconditioning techniques leading to a significant speed-up. First applications considering complex disordered systems of thousands of inequivalent atoms illustrate the strength of our method.

[1] R. Zeller, J. Phys.: Condens. Matter **20**, 294215 (2008).

O 10.3 Mon 15:30 H31

Using the kinetic energy density in local density functionals — •Georg Madsen[1], Lara Ferrighi[2], and Bjork Hammer[2] — [1]ICAMS, Ruhr Universität Bochum, Germany — [2]Department of Physics and Astronomy, Aarhus University, Denmark

Recent developments in local functionals including the kinetic energy density, so-called meta-generalized gradient approximations (MGGAs), are described. It is shown how MGGAs can solve the longstanding problem of the cross over between 2D and 3D structure for cationic and anionic gold clusters. The MGGAs stronger tendency towards 3D structures lies in their smaller gradient enhancement, but contrary to GGAs with smaller gradient enhancements, MGGAs do not overestimate the atomization energy. Furthermore, we find that closed shell interactions are fingerprinted in the kinetic energy density and that MGGAs have enough flexibility to treat correctly both the covalent and the dispersive interactions in layered solids such as Graphite, h-BN and MoS_2. It is shown how MGGAs thereby potentially can give a consistent improvement over the GGAs for the adsorption on metal surfaces.

Ferrighi, Hammer, Madsen, J. Am. Chem. Soc. **2009**, *131*, 10605
Madsen, Ferrighi, Hammer, J. Phys. Chem. Lett.

O 10.4 Mon 15:45 H31

Adsorption behavior of super-heavy elements from 112 to 118 on inert and metal surfaces — •Josef Anton and Timo Jacob — Institut für Elektrochemie, Universität Ulm, 89069 Ulm

One of the very interesting but also rather challenging topics in modern chemistry are the properties of super-heavy elements at the edge of the periodic table [1]. Due to their very short life times (usually $< 1\,\mathrm{s}$) one is only able to perform extremely short (before the decay of the nucleus) experiments on one atom at a time. Therefore, most standard techniques of "traditional" chemistry are not applicable, leaving only a few possibilities. One of these is the gas-phase thermochromatography [1,2], where the desorption temperature of a species is measured and afterwards analyzed to obtain different element properties such as the volatility.

For the theoretical calculation of the properties of these super-heavy elements as well their adsorption behavior on the detector material (e.g. gold or quartz), a fully-relativistic description of all electrons is required. Therefore, using our four-component DFT code [3], we determined the adoption energies of elements 112 to 118 and their homologues on different metal surfaces. In this presentation we will discuss these results, compare them to available experiments, and provide predictions for future measurements.

O 10.5 Mon 16:00 H31

Real-Space DFT for large Molecules on Surfaces — •Paul Baumeister[1], Daniel Wortmann[1], Tomoya Ono[2], and Stefan Blügel[1] — [1]Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich — [2]Dept. of Precision Science and Technology, Osaka University, Japan

Electronic structure calculations within the framework of density functional theory (DFT) has turned out to be the most powerful tool for a reliable determination of ground state properties of large structures such as big organic molecules on surfaces. Especially complicated systems containing far beyond several hundreds of atoms become move with increasingly into the focus of research. We present a real-space grid density functional simulation code that has been developed in Osaka and Jülich. It combines the flexibility of arbitrary boundary condition with the strength of nearly perfect parallel efficiency on massively parallel computers. The projector augmented wave (PAW) method, proposed by Blöchl[1], provides an accurate description for reproducing the chemical behavior of valence states with a reasonable number of grid points. Grid based methods tend to show Pulay-like forces depending on the atomic position with respect to the nearest grid points, sometimes referred to as egg-box effect. These oscillations of forces and total energies endanger the reliable convergence of structural relaxation. We will discuss how to apply the double grid technique[2] and pre-filtering in Fourier space to avoid this problem.

[1] P.E. Blöchl, PRB 50, 17953 (1994)
[2] T. Ono, K. Hirose, PRB 72, 085115 (2005)

O 10.6 Mon 16:15 H31

Van der Waals forces in solids: Challenges for density functionals — •Guo-Xu Zhang, Alexandre Tkatchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

While the importance of van der Waals (vdW) forces for binding between molecules is well established, their influence on the cohesive properties of solids remains to be quantified from first-principles. In particular, most state-of-the-art density functionals yield systematic deviations for the lattice constants, cohesive energies, bulk moduli and transition pressures for a range of solid-state systems. We evaluate the long-range C_6 dispersion coefficients for ions in solids and use them to assess the effect of the long-range vdW forces on the abovementioned cohesive properties of ionic (NaCl, AgCl, MgO) and semiconductor (Si, GaAs) solids. For all of these systems, we obtain consistently accurate results by coupling the long-range C_6R^{-6} dispersion energy with the Perdew-Burke-Ernzerhof functional for the short range. We compare our results for the cohesive properties with recently developed functionals for solids.

O 10.7 Mon 16:30 H31

Exchange an Correlation effects in the electronic properties

of transition metal oxides: the example of NiO — •Matteo Guzzo[1,3], Matteo Gatti[2,3], and Lucia Reining[1,3] — [1]LSI - ETSF, Ecole Polytechnique, Palaiseau CEDEX 91128, France — [2]Nano-bio group - ETSF, Universidad del Pais Vasco, San Sebastian, Spain — [3]European Theoretical Spectroscopy Facility (ETSF)

This contribution has been rescheduled to O 55.9.

O 10.8 Mon 16:45 H31

Determination of structural and electronic properties of different titanates by means of XANES — •Stephan Borek[1], Remya Govind[1], Martin Trautmann[1], Franziska Steudel[1], Michael Huth[1], Liudmilla Makhova[2], Joachim Gräfe[2], Daniel Wett[2], Karl-Michael Schindler[1], Reinhard Denecke[2], and Angelika Chassé[1] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Wilhelm-Ostwald Institute for Physical and Theoretical Chemistry, University Leipzig, Germany

Starting from SCF potentials we have calculated near edge XAS spectra on the perovskites $BaTiO_3$ and $SrTiO_3$, both in the cubic and in the tetragonal phase. The resulting spectra could be explained by comparing with the calculated DOS in terms of the dipole-approximation. It has be shown that the observed differences in the XAS spectra for the O K-edge, the Ti $L_{2,3}$-edge and the Ba and Sr $M_{4,5}$-edge, between the cubic and tetragonal phase, may be related to the differences in the calculated DOS. Furthermore we investigate the effect of iron-multilayers on the electronic, e.g. the spectroscopical properties of the different titanates, and compared our calculations with experimental results, measured on the beam-line of BESSY.

O 10.9 Mon 17:00 H31

Particle redeposition and the non-local damping term in the Kuramoto-Sivashinsky equation — •Nils Anspach and Stefan Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Deutschland

Ion-beam erosion processes have recently regained the focus of both experimental and theoretical physicists due to the fact that they can induce the formation of regular and well-ordered patterns on surfaces under low-energy ion bombardement. The so far most promising model for the evolution of the surface's height profile under normal ion incidence is the non-local Kuramoto-Sivashinsky equation (KSE) which is able to reproduce the experimentally observed structures. However it is still unclear what the physical origin of the non-local damping term in the KSE might be. Motivated by some speculation in the literature that redeposition of eroded particles back to the surface could possibly be the relevant mechanism here, we have developed a conceptually simple one-dimensional model that catches the essence of a potential redeposition process while simultaneously neglecting all other surface effects included in the KSE. This model and its inherent properties are investigated in considerable detail [1]. After that, the obtained results are then compared to the non-local damping term in order to discuss the potential role of particle redeposition as the driving force behind this term.

[1] N. Anspach, S. J. Linz, submitted for publication.