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### Ab-initio study of van der Waals forces in metallo-organic interfaces

Gregor Feldbauer

The interactions between organic molecules and metallic surfaces are crucial for various technological purposes. In particular the interplay between fuels or lubricants and iron based alloys is of high industrial interest. Van der Waals (vdW) interactions play a decisive role in such processes due to their long range nature together with their collective effect. However, the description of vdW forces from first principles has proven to be challenging. To model these systems, we simulated the adsorption of ethanol and isooctane on a bcc Fe (100) within the framework of the density functional theory (DFT). These species were chosen to be rather simple prototypes for polar and non-polar molecules, which are common in many technological applications. Furthermore, the effect of a mono-layer of water on top of the surface on the adsorption process was examined. The generalized gradient approximation (GGA) and vdW density functionals are compared and their effects on adsorption energies, equilibrium structures and charge distributions are presented. The results demonstrate the importance of a proper treatment of vdW forces in such systems. Moreover, the water mono-layer is found to form a 'zig-zag' structure on this Fe surface influencing the adsorption geometries of the molecules and reducing the adsorption energies.

### The correlated semiconductor CrSb<sub>2</sub>

Anna Galler

Intermetallic-based correlated semiconductors display an intriguing temperature dependence in their physical properties: while at high temperatures a Curie-Weiss-like susceptibility develops, a regime of notably large thermopower is found at low temperatures. Between the two regimes optical spectra exhibit large transfers of spectral weight. Here, we present a theoretical many-body study for a member of this class of materials: CrSb<sub>2</sub>. We compute interaction matrix elements from first principles using the constrained random-phase approximation (cRPA) and study many-body spectra and response functions within LDA+DMFT (local density approximation combined with dynamical mean field theory).

### Combination of DFT with multi-orbital VCA for SO-coupled systems

Faruk Geles

Correlation effects show fascinating phenomena in many compounds, especially in materials with partially filled d- and f-bands. Since band theory within the density-functional theory fails to describe the electronic

states in these materials, in some cases even qualitatively, many-body methods have to be applied to deal with the electronic correlations. In this work, we use the variational cluster approach (VCA) for this problem. Starting from density-functional theory calculations, we construct a low-energy model by Wannier function construction. Adding multi-orbital Coulomb interactions, we arrive at a many-body Hamiltonian which is solved within the VCA. As a benchmark of the method, we compare our results with continuous-time quantum Monte Carlo (CTQMC) calculations for the intensively studied vanadate  $\text{SrVO}_3$ . Compared to CTQMC, the VCA has the advantage that its applicability and performance only slightly depends on the actual structure of the local interacting Hamiltonian. Therefore, full rotational invariant interactions as well as spin-orbit coupling can be treated much more efficiently. Applying this method, we will investigate the influence of spin-orbit coupling on the electronic band structure and Fermi surfaces in ruthenates, e.g.  $\text{SrRuO}_3$ .

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### Hidden Scale Invariance in Metallic Elements

Simple liquids or strongly correlated liquids (SCL) exhibit identical thermodynamical behaviour up to unit scaling for states on isomorph curves. Melting lines and lines of constant excess entropy follow isomorph curves for simple liquids. We performed ab-initio calculations for all metal melts at the triple point, testing the degree of isomorphic behaviour. We find that most melts are indeed simple to a high degree, at least at PBE-DFT level. We also show that an inverse-power-law (IPL) model - forming fully correlated liquids - give an excellent approximation for thermodynamic properties of the simple metal melts. For those metals, the IPL approximation even allows to predict the ambient pressure crystal structure solely from liquid data.

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### Nucleation of Hard Colloidal Cubes

Carina Karner

Currently, research on hard anisotropic colloids is receiving a lot of attention from various experimental and theoretical groups in the soft matter community, partly due to the emergence of new fabrication techniques making it possible to produce colloidal particles with various anisotropic shapes or interactions [1]. Recent results obtained from computer simulations and theory indicate that many three dimensional hard anisotropic particles of polyhedral shape exhibit a first order phase transition from an unordered fluid to an ordered crystal. Unlike hard spheres, the simple cubic crystal lattice of hard cubes exhibits a reasonable amount of vacancies near coexistence. Smallenburg et al. [2] showed that this finite vacancy concentration in fact stabilizes the crystal and by doing so, lowers the melting point. In addition to the high vacancy concentration, the crystal is characterized by relatively fast diffusion near coexistence. Hence, coming from the liquid phase, hard cubes will nucleate into this dynamic, vacancy rich crystal. In this poster we will present the dynamics of the freezing transition of hard colloidal cubes. To study the properties of the transition we used kinetic Monte Carlo, combined with rare event sampling techniques such as Transition Interface Sampling.

[1] Stefano Sacanna and David J. Pine. Shape-anisotropic colloids: Building blocks for complex assemblies. *Current Opinion in Colloid & Interface Science*, 16(2):96–105, 2011.

[2] Frank Smallenburg, Laura Filion, Matthieu Marechal, and Marjolein Dijkstra. Vacancystabilized crystalline order in hard cubes. *Proceedings of the National Academy of Sciences*, 109(44):17886–17890, 2012.

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### Transition path sampling with core-modification aimless shooting for a homopolymer chain

Christian Leitold

We investigate the crystallization of a single, flexible homopolymer chain using transition path sampling (TPS). The chain consists of  $N$  identical spherical monomers evolving according to Langevin dynamics. While neighboring monomers are coupled via harmonic springs, the non-neighboring monomers interact via a short-ranged attractive potential. For a sufficiently small interaction range  $\hat{\mathbf{r}}$ , the system undergoes a first-order freezing transition from an expanded, unordered phase to a compact crystalline state. Using a new shooting move tailored for polymers combined with committor analysis we study the transition state ensemble of the

N=128 chain and search for possible reaction coordinates based on likelihood maximization. We find that typical transition states consist of a crystalline nucleus attached to one or more chain fragments. Furthermore, we show that the number of particles in the crystalline core is not well suited as a reaction coordinate. We then present a better choice for a reaction coordinate, which includes information from both the potential energy and the overall structure of the transition states.

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### **Metal-Insulator Transition in 5d Transition Metal Oxides $\text{Sr}_{n+1}\text{Ir}_n\text{O}_{3n+1}$ ( $n=1, 2$ , and $\infty$ ):**

#### **Effects of Spin-Orbit Coupling and Hubbard Interactions**

Peitao Liu

Ruddlesden-Popper series of perovskite-like iridium oxides  $\text{Sr}_{n+1}\text{Ir}_n\text{O}_{3n+1}$  exhibit exotic physical properties due to the cooperative interplay among the crystalline electric field, spin-orbit coupling (SOC), Hubbard ( $U$ ) and spin-exchange interactions. It was suggested[1] that the electronic correlation coupled with the strong SOC lead to a spin-orbit induced Mott insulator for  $n=1$  ( $\text{Sr}_2\text{IrO}_4$ ) and  $n=2$  ( $\text{Sr}_3\text{Ir}_2\text{O}_7$ ), whereas the three-dimensional  $\text{SrIrO}_3$  remains metallic due to the comparatively larger bandwidth. However, the above picture is only valid when the SOC is enough to split the  $J_{\text{eff}}=1/2$  and  $J_{\text{eff}}=3/2$  bands[2]. In present work, we study the crossover between the metallic/insulating and non-magnetic/magnetic phases in  $\text{Sr}_{n+1}\text{Ir}_n\text{O}_{3n+1}$  by systematically investigating the evolution of the orbital and spin properties as a function of  $U$ , the SOC strength and  $n$ . We provide detailed phase diagram of the metal-insulator transition (MIT) and discuss the intermingled interactions of  $U$  and SOC for  $n=1, 2$  and  $\infty$ . It is found that the stronger the SOC, the smaller is the critical interaction  $U_c$  required for a MIT transition. The onset of the insulating state is controlled by the bandwidth narrowed via the SOC in the strong spin-orbit coupling limit, but is dominated by the magnetic ordering in the intermediate spin-orbit coupling regime.

[1] Moon S. et al., Phys. Rev. Lett. 101, 226402 (2008).

[2] Carter J.-M. et al., Phys. Rev. B. 88, 035111 (2013).

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Mattia Lupetti

We present an alternative formulation of absorbing boundary conditions for Maxwell's equations, which are meant to overcome some of the problems characteristic of Perfectly Matched Layers (PML). The proposed boundary conditions are implemented in the tRecX code.

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### **A Reaction Coordinate for the Sphere- to Slab-Geometry Phase Transition**

Clemens Moritz

Geometric phases are found in systems which exhibit phase separation and are characterized by droplet shapes other than spherical that are stabilized by the use of periodic boundary conditions in simulations. These geometric phase transitions have been observed to cause exponential slowing down in simulations of first order phase transitions [1]. We investigate the phase transition from a spherical cluster to a slab shaped cluster in the 2D Ising model in simulations with constant total magnetization and zero external field. Previously, several order parameters for non-spanning droplets have been proposed [1]. We present the Minimum Distance/Width (MDW) coordinate as a new order parameter that is defined for spanning as well as for non-spanning clusters. We show that at a temperature of 90% of the critical temperature this coordinate alone cannot predict committer probabilities, however by developing a measure for asphericity based on the Fourier transform of a given configuration, which we combine with the MDW coordinate using likelihood maximization [2][3], we can obtain a suitable reaction coordinate. After verifying the performance of this new coordinate by performing a histogram test[4], we use it to calculate the free energy barrier that separates the two geometric states.

[1] T. Neuhaus and J. S. Hager, J. Stat. Phys. 113, 47 (2003), [2] B. Peters and B. L. Trout, J. Chem. Phys. 125, 054108 (2006).

[3] B. Peters, G. T. Beckham, and B. L. Trout, J. Chem. Phys. 127, 034109 (2007).

[4] B. Peters, J. Chem. Phys. 125, 241101 (2006).

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## **DFT studies of the lattice thermal conductivity of thermoelectric materials**

Rene Moser

Thermoelectric materials are of technological and scientific interest because of their ability to convert a temperature gradient directly into electric energy. The efficiency of this process is defined by the figure-of-merit  $Z = T S^2 \sigma / \kappa$  which contains the Seebeck coefficient  $S$ , the electrical conductivity  $\sigma$  and the thermal conductivity  $\kappa$  at a given temperature  $T$ . A large  $Z$  is achieved by a large  $S$  and a small  $\kappa$ , which properties one tries to optimize. The total thermal conductivity  $\kappa = \kappa_{el} + \kappa_{ph}$  is the sum of the electronic contribution  $\kappa_{el}$  and the phonon mediated lattice thermal conductivity  $\kappa_{ph}$ . Here we focus on the first-principles modelling of  $\kappa_{ph}$  by a density functional (DFT) theory approach for the electronic structure and phonon properties in combination with Boltzmann's transport theory. Results are presented and discussed for a selection of thermoelectric materials. Supported by FWF, project nr. P24380.

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## **Cu precipitation in Fe – From first-principles to cluster properties**

Alice Redermeier

Phase decomposition in the binary  $\text{Fe}_{1-x}\text{Cu}_x$  alloy is studied using Monte Carlo (MC) simulations. In this study, we want to use the full information on energy from first-principles calculations as input for the cluster formation, and on the other hand we want to speed up the calculation times. The methodology we use to achieve this goal can basically be divided into the “full-information path” and the “large scale path”.

The “full-information path” starts with density functional theory (DFT) calculations for a temperature of 0 Kelvin for different atomic configurations with system sizes of a few atoms. Phonon calculations provide information on the transition to higher temperatures. In the end, the Cluster Expansion (CE) enables us to get information on various crystal structures. The aim of the “large scale path” is to use efficient pair potentials, in order to speed up Monte Carlo simulations to study phase separation. The pair potentials are fitted to the phase diagram obtained from the DFT-CE results from the full-information path.

On comparison of the MC simulations using the full information and large-scale paths, we observe that both MC approaches provide very similar information on the properties of small clusters, i.e., the size evolution, mean radius, composition as well as interface constitution. However, the large-scale path delivers results in significantly shorter computation time. The full-information path is computationally too expensive to be a useful tool for large-scale simulations of precipitate nucleation and growth.

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## **The charge transfer between a proton and a lithium fluoride surface**

Fran Paul Tiwald

We study the charge transfer from an LiF alkali halide surface to an incident proton on an ab-initio level. Questions to be addressed include the velocity dependence of the charge transfer probability, and the nature of the coupling between the ionic and the charge transfer channels.

We apply high-level configuration interaction methods that allow for calculation of ground and excited states of the quasi-molecule complex ( $\text{H}^+ + \text{LiF}$ ) as well as the non-adiabatic couplings between them. The LiF surface is represented by a small active cluster embedded into a surrounding point charge matrix to account for the extended system. We calculate 3D potential energy surfaces of several electronic states and the couplings between them. These electronic states converge for large distances between projectile and surface to either the  $\text{H}^+ + (\text{LiF surface})$  or to the  $\text{H} + (\text{LiF surface})^+$  configuration. This information serves as input for the calculation of the neutralization dynamics using either full wave packet propagation or Tully's semiclassical surface hopping algorithm.