

Multiscale Simulation Methods in Molecular Sciences

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Poster Presentations

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Winter School 2009 Multiscale Simulation Methods in Molecular Sciences

	Monday 2 March	Tuesday 3 March	Wednesday 4 March	Thursday 5 March	Friday 6 March
9:00-10:00	9:45-10:00 Opening <i>Thomas Lippert</i>	Density Functional Theory and Linear Scaling <i>Rudolf Zeller</i>	DFT Embedding and Coarse Graining Techniques <i>Mike Payne</i>	Two Topics in Ab Initio Molecular Dynamics: Multiple Length Scales and Exploration of Free-Energy Surfaces Mark E. Tuckerman	Coarse Grained Electronic Structure Using Neural Networks <i>Jörg Behler</i>
10:00-11:00	Large Spatiotemporal-Scale Material Simulations on Petaflops Computers <i>Aiichiro Nakano</i>	QM/MM Methodology: Fundamentals, Scope, and Limitations Walter Thiel	De Novo Protein Folding with Distributed Computational Resources Wolfgang Wenzel	Multiscale Methods for the Description of Chemical Events in Biological Systems Marcus Elstner	Computer Simulations of Systems with Hydrodynamic Interactions: The Coupled Molecular Dynamics – Lattice Boltzmann Approach Burkhard Dünweg
11:00-11:30			Coffee Break		
11:30-12:30	Molecular Dynamics - Extending the Scale from Microscopic to Mesoscopic Godehard Sutmann	Soft Matter, Fundamentals and Coarse Graining Strategies <i>Kurt Kremer</i>	An Introduction to the Tight Binding Approximation – Implementation by Diagonalisation Anthony T. Paxton	Wavelets and Their Application for the Solution of Poisson's and Schrödinger's Equation <i>Stefan Goedecker</i>	Application of Residue-Based and Shape-Based Coarse Graining to Biomolecular Simulations <i>Klaus Schulten</i>
12:30-14:30		•	Lunch Break		•
14:30-15:30	Introduction to Multigrid Methods for Elliptic Boundary Value Problems <i>Arnold Reusken</i>	Introduction to Parallel Computing <i>Bernd Mohr</i>	Strategies for Implementing Scientific Applications on Parallel Computers Bernd Körfgen	Bond-Order Potentials for Bridging the Electronic to Atomistic Modelling Hierarchies Ralf Drautz	
15:30-16:30	Eletronic Structure: Hartree -Fock and Correlation Methods <i>Christof Hättig</i>	Adaptive Resolution Schemes Luigi Delle Site	Practical Session	First-Principles Statistical Mechanics Approaches to Surface Physics and Catalysis Karsten Reuter	
16:30-17:00			Coffee Break		
17:00-18:00	Monte Carlo and Kinetic Monte Carlo Methods – A Tutorial <i>Peter Kratzer</i>	Multiscale Modelling of Magnetic Materials: From the Total Energy of the Homogeneous Electron Gas to the Curie Temperature of Ferromagnets <i>Phivos Mavropoulos</i>	Practical Session	First-Principles Based Multiscale Modelling of Alloys <i>Stefan Müller</i>	
Evening	Reception and Get-Together	Poster-Session I	Poster-Session II	Conference Dinner	

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Modeling the Magnetic Properties of the Wheel-Shaped Tungstophosphate Cu₂₀

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In this work we report the magnetic properties of the large wheel-shaped tungstophosphate $[Cu_{20}Cl(OH)_{24}(H_2O)_{12}(P_8W_{48}O_{184})]^{25-}$

 $(Cu_{20}P_8W_{48})$, in short Cu_{20} which was synthesized in $2005^{1,2}$ The theoretical model we adopt for describing the magnetic molecule of Cu_{20} is the Heisenberg spin Hamiltonian, together with a Zeeman term of an applied magnetic field along the z-axis. The numerical exact diagonalization method has been used to calculate the energy spectrum and the eigenstates of the compound. The results of these energies have been used to get some deeper understanding of the magnetic properties in this material.

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Structural and Dynamic Properties of Porous Coordination Polymers: A Molecular Dynamics Investigation

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Porous Coordination Polymers (PCPs) are a class of functional materials, which are assembled in a "toolkit" approach from different building units. Due to their modularity a wide range of networks are possible with an enormous structural diversity. But for an efficient application of these polymers a knowledge of both structural and dynamic properties on a molecular and atomic level is crucial.

We present here our results for PCP systems using Molecular Dynamics Simulation techniques. The investigated systems range over different PCP subclasses - like Metal-Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs). From the methodological point of view, we used force fields, due to the size of the periodic systems, which are parametrized based on ab-initio calculations of non-periodic model systems. In this regard, for example, our recently parametrized force field for MOF-5 allows the description of structural parameters, elastic and thermal properties and normal modes of the framework¹. Based on this work, we were able to investigate the diffusion of benzene molecules within the pores^{2,3}. Since the diffusion process is essential for the loading and activity of the host-guest systems, we followed this work by analyzing dynamic properties of different host-guest systems systematically (e.g. different aromatic guest molecules in MOFs). Furthermore, we investigated the structure of some PCPs like IRMOFs (Isoreticular Metal-Organic Frameworks)⁴ or COFs, in which different conformational isomers are possible, in principle. This study is not possible experimentally, due to synthetic difficulties, yet. Thus the theoretical approach allows a different insight compared to experimental methods and provides the knowledge needed to design these functional materials. In addition, we studied based on these results the influence of the topology modification of the network on the mobility of the guest molecules.

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Isolated and Adsorbed NaCl Clusters

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Recent experimental and theoretical results suggest that surface atoms are transferred onto the tips of Atomic Force Microscopes (AFM) when scanning ionic surfaces. Different low energy tip structures were calculated and used to find the preferred orientations and structures of $(NaCl)_4$ clusters adsorbed on the apex of the tip. The calculations were performed with the BigDFT density functional theory program using a wavelet basis set¹.

The silicon tips for the simulations were obtained in a systematic way by using the minima hopping method $(MHM)^{2,3}$. In the Molecular Dynamics part of the MHM the temperature was limited to some value used in experiments⁴. A Tight-Binding scheme was used to evaluate energy and forces of silicon and hydrogen atoms in the MHM.

Ground state configurations for several neutral NaCl clusters with up to 512 atoms were found using the MHM. The energy and forces were evaluated with two different force fields and the BigDFT program. Our results confirm that cuboid structures and the formation of the $\{100\}$ surfaces are preferred for isolated neutral NaCl clusters. However, when $(NaCl)_4$ clusters are adsorbed on silicon tips both NaCl cubes and well-oriented NaCl dimers are favored.

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Coupling Atomistic Simulations and the Phase Field Method in Solidification Modelling

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Mechanical performances of alloys depend on their microstructure, thus understanding the solidification process is a fundamental step to obtain the desired properties. Phase Field Modelling (PFM) has proved a reliable technique to this purpose but its predictions depend on input parameters such as interface free energy and partition coefficients. We show here how it is possible to calculate these parameters using atomistic simulations, improving the predictivity of the PFM approach.

References

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Conformations and Mechanical Properties of Single Polymers - Langevin Dynamics Studies

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The mechanical properties of single biopolymers have recently become experimentally accessible with the development of tools such as AFM and Optical Tweezers. In particular the force-extension behaviour of polysaccharides has drawn attention as it deviates from the predictions of existing standard statistical mechanical models. In particular, enthalphic extensions depending on the fine structure of the polymer chain can be observed in addition to the standard entropic restoring forces.

In our earlier work, using AFM experiments and DFT calculations, we recorded and modelled the stretching of a single chain of pectin, an important plant polysaccharide and a component of plant cell wall, which exhibits two enthalphic extensions in its force-extension profile¹. More recently we have turned our attention to models that might be extended in order to incorporate more experimental details such as pulling speed, solvent quality or even associations of chains. Brownian dynamics simulations offer one such avenue^{2, 3}.

Herein, we examine the conformation and stretching behaviour of different statistical chains, both flexible and semi-flexible using Langevin dynamics simulation techniques.

Acknowledgments

We acknowledge Royal society of New Zealand- Marsden grant for funding the project.

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Adaptive Molecular Dynamics

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Modeling and simulation of natural or artificial nanosystems is still a challenging problem, however, for at least three reasons: (a) the number of involved atoms may be extremely large (liposomes, proteins, viruses, DNA, cell membrane, etc.); (b) some chemical, physical or biological phenomena have large durations (e.g. the folding of some proteins); and (c) the underlying physico-chemistry of some phenomena can only be described by quantum chemistry (local chemical reactions, isomerizations, metallic atoms, etc.). The large cost of modeling and simulation constitutes a major impediment to the development of nanotechnology.

Our group develops novel multiscale, adaptive modeling and simulation methods, which automatically focus computational resources on the most relevant parts of the nanosystems under study^{1,2}.

This poster will present the basis of the adaptive simulation framework being developed in the group, as well as some of the results which have been obtained with SAMSON, our software platform for modeling and simulation of nanosystems (SAMSON: System for Adaptive Modeling and Simulation Of Nano-objects).

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A High-Dimensional Neural Network Potential-Energy Surface for Zinc Oxide

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Oxides play an important role in many technical applications, for example as support materials in heterogeneous catalysis. Studying many interesting processes like structural phase transitions and the mechanisms of these transitions, the formation of defects, as well as the stabilization of surfaces by reconstructions requires long simulations of large systems. These simulations are often beyond the capabilities of present-day supercomputers, if computationally demanding electronic structure methods like density-functional theory (DFT) are used. In order to address these problems, more efficient but sufficiently accurate potentials are required.

A promising step towards the construction of such potentials has been the introduction of artificial Neural Networks (NN) to represent first-principles potential-energy surfaces (PES)^{1,2}. This method has recently been extended to high-dimensional PESs now enabling simulations of condensed systems^{3,4}. The NN potential is based on electronic structure calculations, but once it has been constructed, it can be evaluated several orders of magnitude faster, while the accuracy is essentially maintained. This enables routine applications in molecular dynamics simulations of large systems, but so far the method has been applicable only to elemental systems. By combining the flexibility of the NN approach with physically motivated terms we are now able to include long-range interactions. This is a necessary condition for studying binary systems like oxides and general multicomponent systems with significant charge transfer. The capabilities of the method are demonstrated for zinc oxide as a benchmark system. We show that the structural and energetic properties of various phases of zinc oxide predicted by the NN potential are in excellent agreement with reference density-functional theory calculations.

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Simulation of Organic Nanoelectronic Devices - From Molecular Devices to Thin Films

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In the last years the field of organic electronics has been suffering a huge development due to the unique electronic properties of these materials that allow their application as active components in electronic and optoelectronic devices. Nevertheless, the efficiency of these devices is limited by the molecular properties or the arrangement of the molecules inside thin films as a result of the deposition conditions. At experimental level it is possible to study this type of devices, however, it is very difficult to understand the effect of the morphology at nanoscale and the molecular properties separately.

It is in this context that computational modelling reveals to be a powerful tool to understand the influence of these two factors on the physics processes that are behind the functioning of these type of devices. In this communication we will present some of our latest research results on molecular devices made of small conjugated molecules (with and without spatial symmetry) bond to two metallic electrodes¹, using a suitable quantum molecular dynamics method, and the influence of the morphology at nanoscale in thin films of conjugated polymer diodes^{2–4}, using a mesoscopic model based on a generalized Monte Carlo method.

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Constrained Geometric Simulation of Diffusive Motion in Proteins

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Conventional molecular dynamics (MD) simulations are highly demanding computationally relative to biological timescales. These methods solve Newton's equations of motion for all the atoms in the system. Obtaining an accurate trajectory by these methods involves a timestep of approximately femtosecond length, demanding computationally for problems of biological relevance.

A prominent example of this is the behaviour of proteins. Here, the ability of the proteins to undergo sizeable conformational changes can be vital to understanding the system. Rather than employing a Newtonian dynamical approach, it is possible to use a Lagrangian constraint based approach. Instead of producing a trajectory progressing in time, a collection of conformers satisfying various constraints is generated.

This approach is embedded in the software packages FIRST/FRODA^{1,2}, as created by Thorpe, Wells et al. FIRST performs rigidity analysis in order to provide the input information as to what constraints each conformer has to meet so as to be considered valid. This considers the protein as a network in which all covalent bond lengths and angles are fixed, along with identified hydrophobic interactions and hydrogen bonds. The rigidity of the protein is then determined by balancing constraints against degrees of freedom, which is done by use of the "pebble-game algorithm". FRODA then uses this information to explore the resultant mobility possible from the proteins rigidity.

Human serum albumin (HSA) is the most abundant protein in the bloodstream and, as such, is typically the first to adsorb on implanted surfaces. Here, I use the FIRST/FRODA programs, in conjunction with classical molecular dynamics, to investigate HSA adsorption and subsequent deformation on a hydrophobic graphene sheet.

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An Efficient and Tunable Colored-Noise Thermostat

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When performing constant-temperature molecular dynamics, thermostat efficiency affects the time required for equilibration and the ergodicity of the sampling, which depends on the ability of the dynamics to generate uncorrelated configurations of the system. Stochastic thermostats are known to bear good ergodicity properties¹, but - in their most common forms - are poorly tunable. For example, a conventional Langevin thermostat cannot be used in Car-Parrinello-like simulations, as it would apply high-frequency noise to the ionic degrees of freedom, causing the breakdown of adiabatic separation with the electronic modes.

A thermostat based on a non-Markovian, generalized Langevin equation is presented, which combines the efficiency of white-noise stochastic thermostats with a high degree of tunability.² Most importantly, the response of the system to the thermostat can be estimated analytically, so that the parameters can be chosen without the need to perform time-consuming test runs. The behavior of the thermostat is demonstrated for the Car-Parrinello molecular dynamics of a heavy water molecule in vacuum, and is compared to white-noise Langevin and Nose-Hoover chains thermostats³.

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Structural Relaxation Properties of Polymer Electrolytes Based on PEO and Ionic Liquids Derived from Imidazolium Cations: A Computer Simulation Study

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Dynamical properties of polymer electrolytes based on poly(ethylene oxide) PEO and ionic liquids (ILs) of 1-alkyl-3-methylimidazolium cations were calculated by molecular dynamics simulations with previously proposed model¹. The effect of changing the ionic liquid concentration, temperature, and the 1-alkyl chain lengths, [1,3-dimethylimidazolium]PF₆ and [1-butyl-3-methylimidazolium]PF₆ (dmim[PF₆] and bmim[PF₆]), was investigated. Cation diffusion coefficient is higher than those of anion and oxygen atoms of PEO chains. Ionic mobility in PEO/[bmim]PF₆ is higher than in PEO/[dmim]PF₆, so that the ionic conductivity of the former is approximately ten times larger than the latter. The ration between and its estimate from Nernst-Einstein equation / NE, which is inversely proportional to the strength of ion pairs, is higher in ionic liquid polymer electrolytes than in polymer electrolytes based on inorganic salts with Li+ cations.² Calculated time correlation functions corroborate previous evidence from the analysis of equilibrium structure that the ion pairs in ionic liquid polymer electrolytes are relatively weak. Structural relaxation at distinct spatial scales is revealed by the calculation of the intermediate scattering function at different wavevectors. These data are reproduced with stretched exponential functions, so that temperature and wavevector dependences of the best fit parameters can be compared with corresponding results for polymer. This work revealed the dynamical consequences of the equilibrium structures in PEO/[dmim]PF₆ and PEO/[bmim]PF₆ reported in Ref 1. and it also provided atomistic details on the ternary systems defined as PEO/ILs/lithium salt. Clear indications of reduced strength in ion correlations are the distinct time evolution of van Hove correlation functions for anions and cations and the higher κ/κ_{NE} ratio in comparison with, for instance, the PEO/LiClO₄ polymer electrolyte.^{2,3}

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OGOLEM: Global Optimization of Heterogeneous Clusters of Flexible Molecules Using Genetic Algorithms An Object Oriented, Massively Parallel Approach

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Determining equilibrium structures of global minimal energy is one of the central problems in simulating and understanding molecular aggregation processes, self-organizing nano materials and molecular docking in biochemical systems¹. Since the problem is *NP complete*, a deterministic *Ansatz* is not feasible but a couple of stochastic-heuristic approaches have proven their potential during the last decades. Besides the approach of *evolutionary algorithms*² followed here, *basin hopping*³ and *simulated annealing*⁴ have been applied to a broad range of problems⁵.

Using the experience gained in previous work by our group⁶, a new development of a program suite for global geometry optimization, OGOLEM, was started from scratch. It unifies the advantages of pure object oriented design with a massively parallel pool algorithm. The communication layer is a library following the MPI standard, $MPJexpress^7$. An even higher scalability will be achieved in the next development stage by making use of additional lightweight threading.

Since the general problem of finding a structure of minimal energy on the hypersurface can be logically separated into two parts, the global search for basins of attraction and the local search of the minima therein, the program suite can make use of existing program packages for either gradient and energy calculations or complete local optimizations such as MOLPRO and Mopac.

The present stage of development has been applied to a typical benchmark system, Lennard-Jones clusters, and is currently used for research on the aggregation of Kanamycin. Ongoing work is the implementation of more elaborate global optimization algorithms, an approach to so-called cultural algorithms to reduce the search space size and the possibility to globally optimize molecules with internal degrees of freedom.

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Magnetism and Magnetic Anisotropies of Small Organic Molecules

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The ability to enhance and tailor the magnetism of small atomic cluster and molecules will determine whether nanospintronics can be used as a storage tech- nology. We present here our ab initio studies on the magnetism of small organic molecules containing transition metal atoms. We focus specially on 5d atoms like gold, platinum and iridium. These have a large spin- orbit interaction, which generates large magnetic anisotropies in small atomic clusters¹. The work uses a previous simplification of the calculation of the Spin-Orbit in a self-consistent way² that has been successfully applied to chains³ and clusters¹. Work supported by MICINN, project no. FIS2006-12117.



Figure 1. Charge and Spin densitities of Gold Phtalocianine

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Microscopic Modeling of the Behaviour of Self Assembly of Surfactants

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The stability and microstructure of self assembled surfactant solutions for technologically relevant systems are studied based on the use of the 'Single Chain Mean-Field Theory'. Microscopic models and computer simulation programs are developed capable of predicting and explaining the link between molecular details and the formation of self-assembled microscopic structures. Such a link would be highly advantageous in the optimisation of molecular structure for current applications and the possibility to design tailor-made molecules for specific purposes. For example, in the exploration of new applications, such as nanotechnological applications where self-assembled structures are being used as microreactors in order to form nanoparticles or as templates to form nanomaterials which are of importance for a number of technological applications, including detergency, catalysis, pharmaceutical, food and cosmetics formulations, mineral processing and petroleum industries etc. The main idea behind the SCMF theory is to consider a single chain with all its intramolecular interactions explicitly taking into account, within the chosen model to treat the molecules, while the intermolecular interactions are considered within a meanfield approximation. The probability distribution function (pdf) of the chain conformations, the distribution of solvent molecules within the aggregate and free energy of micellisation associated with transferring a surfactant molecule from the bulk solution into micelles are determined by the theory. Other properties of surfactant solutions including the critical micelle concentration (cmc) and cluster size distribution are also predicted. The cmc is compared with literature Monte Carlo results for the same lattice model and the results are in good agreement.

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Stability and Dynamics of Droplets

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Liquid droplets are very important in many scientific research branches and their study has attracted much interest for a long time. In this work we investigate the behavior of droplets via a mesoscale computer simulation approach, the Lattice Boltzmann method^{1–3}. The model employed in the present studies is based on a Cahn-Hilliard type free energy functional, the link to the LB method being provided by the pressure tensor^{4–6}.

In the first part, we consider the stability of a droplet and its saturated vapor inside a finite volume, an issue of considerable importance in nanotechnology^{7,8}. Results obtained within our simulations show the same system size dependence as obtained via analytic approximations to the underlying free energy functional as well as independent numerical solutions of the problem. In particular, we find a certain critical radius below which a liquid droplet becomes unstable and evaporates.

A second topic of fundamental interest is the behavior of droplets on superhydrophobic substrates^{9–12}, which are widely known for their remarkable self-cleaning properties. We investigate, for the first time, the case where the droplet is of comparable size to the roughness scale. A simple analytical free energy model is presented that can explain all the essential results of our simulations. Most interestingly, we are able to observe a new generic metastable state of partial impalement that is different from the known Cassie/Baxter or Wenzel states. Furthermore, we study the stability of the Cassie/Baxter state and its dependence on the substrate geometry, contact angle and droplet size.

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Atomic Scale View on Partially Molten Rocks

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The presence of melt or fluid in rocks has significant influence on their physical and chemical properties. The electrical conductivity of a partially molten rock is influenced by many factors, including melt conductivity, conductivity of the solid phases, and melt fraction, each of which is influenced by temperature. Grain boundaries are known to play an important role in the diffusive, mechanical and electrical properties of partially-melted rocks. Grain boundaries are usually assumed to enhance conductivity since the transport of charge carriers (ions) along the grain boundaries is faster than through the lattice. They are also important pathways for chemical transport in a rock.

Molecular dynamics simulation may provide a picture of the underlying processes at a molecular and atomic level, something that experiments often cannot produce. We construct interfaces between mineral and melt with different crystal orientation and 'measure' various properties in the simulation. We use polarizable ion potentials to describe the particle interactions.¹ We examine how these properties differ between bulk melt, bulk crystal and interface. Here we discuss structural and transport properties of MgSiO₃ melt, forsterite (Mg₂SiO₄) crystal and the respective mineral-melt interface at T=2000 K.

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Shallow Donor States Near a Semiconductor-Insulator-Metal Interface

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Recently there has been an increased interest in the study of shallow donor impurities near an interface because of its importance in nanoelectronics. For the case of a semiconductor/ metal interface the energy spectrum was recently investigated in Ref.¹ using the finite element technique. In² the ground state energy of a donor localized in Si near a semiconductor/dielectric interface was studied using a variational approach.

Due to the increased miniaturization the oxide layer between the semiconductor and the metallic gate is strongly reduced in thickness. Therefore, it becomes important to include the screening effect of the metallic gate on the impurity states. This motivated us to develop a variational approach for shallow donor states localized in a semiconductor at a semiconductor-insulator-metal interface. The image charge problem in this case leads to an infinite series of images. We introduce a term in the variational wave function that is responsible for the interaction of the electron with these images, which leads to a considerable lowering of the energy, especially when the impurity is located very near the interface.

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Membrane Curvature Effects and Excitonic Properties of the Bent *Rhodobacter Sphaeroides* RC-LH1-PufX Dimer

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Photosynthesis is initiated when photon is absorbed by peripheral light-harvesting (LH) proteins, which then transfer their excitation energy to a reaction center (RC), where charge separation is started. Among LH proteins, the light-harvesting complex 1 (LH1) directly surrounds the RC, forming the RC-LH1 complex, which can dimerize when an additional polypeptide PufX is present. Although there is currently no high resolution structure for LH1, electron microscopy and atomic force microscopy studies have shown that the RC-LH1-PufX complex of *Rhodobacter sphaeroides* is an S-shaped dimer highly bent at the dimerization interface. We have obtained a structural model for the RC-LH1-PufX dimer using a new fitting protocol, the molecular dynamics flexible fitting method, based on the recent 3D EM density map. The model elucidates the organization of the pigment array within the RC-LH1-PufX dimer, and allows calculation of the excitonic properties of the dimeric RC-LH1-PufX complex. The structural model also provides a basis for studies on the membrane-bending effects of the RC-LH1-PufX dimer, and simulations showed that the bent dimer curves its surrounding membrane environment, with the resulting membrane curvature agreeing to that of the native tubular photosynthetic membrane.

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Mechanical Properties of Hybrid Inorganic-Organic Materials

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Hybrid inorganic-organic framework compounds form an important class of materials intensively studied in the last few years due to their potential applications in catalysis gas separation and storage.¹ However, the study of their mechanical properties has been so far limited to MOF-5 and related structures for which experiment and simulations exist. These study show that MOF-5 is an isotropic material with a bulk modulus of 18 GPa and a C11 elastic constant of 29 GPa.² We present a detailed computational study of the elastic properties of a new porous framework material Zinc-phosphate-phosphonoacetate hydrate.³ In contrast with MOF-5 this material is anisotropic. With our calculation we have been able to correlate its elastic anisotropic behaviour to its properties such as density, presence of transition metal complexes and porosity. We show that the conventional approach of applying a finite strains to calculate the elastic constants, which for instance has been applied to MOF-5, can fail badly. To remedy this shortcoming, we use here an alternative and successful approach of application of a stress in either x, y or z directions. Finally, we calculate the elastic behaviour of another 6 framework non porous materials, some of them have similar density to that of the porous Zinc-phosphate-phosphonoacetate hydrate. Surprisingly, the calculated bulk modulus of the porous and non porous materials was calculated to be very similar, 30 GPa.

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Bottom-up Approach for Modeling Blood Flow in Microscale Vessels

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Blood is a complex fluid with multiscale properties. While on large scales blood can be modeled by a Newtonian fluid with effective viscosity, at small scales (< 30μ m) its particulate nature has to be taken into account explicitly. It is known that the deformability and the large packing fraction of the red blood cells (RBC) result in effects like shear thinning, Fahraeus and Fahraeus-Lindqvist effects or blunt velocity profiles. A bottom-up approach for modeling blood flow in microscale vessels can be realized by using a discretized membrane spring model for the cells, the lattice Boltzmann method (LBM) for the fluid flow and the immersed boundary method (IBM) for the coupling of the liquid and the cellular phases.

The LBM^{1,2} is a relatively new approach for solving the Navier-Stokes equations. Its advantages are the possibilities to massively parallelize the code and to include complex boundaries and large volume fractions of immersed particles. The discretized membrane spring model³ is an efficient way to describe the cell membrane dynamics with high accuracy and at the same time simulate many cells simultaneously. The IBM⁴ has proven to be a fast and straightforward method coupling the motion of deformable particles to the circumfluent fluid.

Combining those three ingredients, it is possible to efficiently simulate the 3D flow of a dense suspension of RBCs. Such simulations are very important for medical applications: The influence of vessel abnormalities (stenosis, aneurysm) or medication (changing the hematocrit or RBC deformability) can be tested in silico, whereas experiments are often very difficult to perform.

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Ab Initio Ring Polymer Molecular Dynamics for the Calculation of Gas Phase Reaction Rates

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In this work, we aim to establish a methodology based on the Ring Polymer Molecular Dynamics method (RPMD)¹ to compute accurately quantal canonical reaction rates for simple chemical reactions in gas phase, such as $H + H_2$ or $H_2 + OH$.

It is recognized that the RPMD constitutes an efficient way of recovering most of the quantum effects associated with the nuclear motion. This is achieved by computation of the classical dynamics of a ring polymer of beads with fictitious masses coupled by simple harmonic potentials, what is known as the classical isomorphism.² Moreover, its intrinsic versatility can be largely enhanced by the combination of the RPMD scheme with *ab initio* calculations.³ In this approximation each quantum particle (*i.e.* nucleus) is represented by a harmonic ring polymer subject to an external *ab initio* potential provided by a suitable Electronic Structure code.

The calculation of the reaction rates is carried out by means of the Bennett-Chandler approach, for which a precise location of the transition state is not necessary.⁴ The ring polymers are evolved according to a Velocity Verlet algorithm⁵ on an *ab initio* Potential Energy Surface. Since the most expensive stage is the computation of the forces acting on each bead at every time-step,³ the trajectories are not propagated on the actual Potential Energy Surface but on a second order expansion of it, as previously suggested.^{6,7} *Ab initio* energy and two first derivatives are computed only at reference points around which the second order expansion is set. Thus, up to a certain *trust* region, forces can be computed analytically.⁸ Once the boundary of the trust region is reached a new reference point is set and the procedure is repeated until the trajectory is finished.

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Ultrafast Sequential Double Proton Transfer in Excited State 2,2'-[Bipyridyl-]-3,3'-diol

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With two intramolecular hydrogen bonds, 2,2'-[Bipyridyl-]-3,3'-diol has the capability to perform double proton transfer in the excited state. It is known from the experiment that within 100 fs after UV excitation both the single-transfer mono-keto (MK) and the double-transfer di-keto (DK) tautomers are formed.¹ With a characteristic time of 10 ps MK is converted to DK.² A vibrational signature of these processes is found in the time-dependent transient.¹ To get more insight on this process, mixed quantum-classical dynamics simulations at the RI-CC2 and TDDFT/B3LYP levels have been performed.

Contrary to the prevalent experimental interpretation which considers a branched reaction path with either direct MK or DK formation¹, MK was almost exclusively found as an intermediate even in sub 100 fs DK formation. This observation can be understood by a ridge on the potential energy surface when symmetry is conserved. A barrierless symmetry-breaking di-enol (DE) \rightarrow MK pathway gave rise to a 7 fs first proton transfer (RI-CC2). The MK-DK barrier of about 0.1 eV allowed for a sub 100 fs second transfer and even the reverse reaction. The TDDFT/B3LYP results were similar but small changes in the relative energies caused reduced DK formation.

To get a better comparison with the experimental results, the dynamics have been analyzed in terms of normal mode motions. Strong coherent activity was found in the same modes that the experiment¹ observed. In particular it was noted that activity of a symmetric mode was not in contradiction to a symmetry breaking process.

To get more insight on the double proton transfer process, the results are compared to the analogue 2,2'-[Bipyridyl-]-3,3'-diamine.



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Polystyrene/Gold Nanoparticle Interfaces: All Atom Structures from Multiscale Molecular Dynamics Simulations

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Polymer nanocomposites based on nanometer-size metal particles are experiencing an explosive growth during the last years due to their technological applications. Low fabrication costs, high mechanical flexibility, 3D tracking capability, good scalability and versatility of chemical structure are advantages at the base for the development of polymeric materials-based memories. With the development of facile routes of synthesis, gold nanoparticle coated with surface thiol layers are used extensively as building blocks for such mesoscopic structures. Programmable electrical bistability was observed in devices made up with a polystyrene film containing gold nanoparticles and 8-hydroxyquinoline sandwiched between two metal electrodes.¹ Understanding and possibly manipulating structural organization at the interfaces level is the key for a "bottom-up" fabrication approach to the development of nanoscale devices. A key issue to rationalize the behavior and then, hopefully, to improve the performances of these nanomaterials is a fundamental understanding of the effects of various molecular parameters on the interfaces structure. With this purpose, using coarse–grain simulations² joined with reverse mapping techniques³, multiscale simulations have been performed in order to obtain detailed all-atom models of the interface between polystyrene and a gold nanoparticle. Results of simulations of systems containing a gold nanoparticle coated by 1-dodecanthiols and non-coated

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Theoretical Study of Electron Transfer in Polypyrrole Molecular Nanowires Placed between Platinum Electrodes and on the Hydrogen Passivated Diamond Surface

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Over the last decade, the interest in organic materials has significantly increased. It is due to their wide spectrum of use in electronic and microelectronic devices. They are mostly used as a very cheap screens, thin-film transistors and photovoltaic cells¹.

The objective of this work is to obtain complex information about the interface between Pt(111) surface and Ppy chain, diamond(111)-H surface and Ppy chain respectively. It should support the present experiments, where Ppy wires are formed via CVD between platinum or microelectrodes.

The theoretical calculations based on Density Functional Theory (DFT). The transport properties of the interface between polypyrrole (Ppy) wire and platinum (111) surface will be presented in conjunction with the comparison of transport properties of polypyrrole-platinum interface and the polypyrrole-diamond(111)-H interface. We perform the to-tal energy calculation of selected structures using fast local-basis set DFT FIREBALL code^{2, 3}. Based on these calculations, the electron structure of the studied Pt(111)-Ppy and C(111)-Ppy interfaces was obtained, especially the mechanism of charge transfer over this interfaces through projected density of states (PDOS) and the real-space density of states (RDOS). The study of the electron transport and I/V-characteristics was calculated via the Green function method for selected configurations of studied systems.

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Reconstruction of Atomistic Details from Coarse Grained Simulations

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We present a method to reintroduce atomistic (AA) details to the structures obtained with lower resolution models (CG). Our idea is based on simulated annealing, heuristic optimization technique, designed to find a global minimum configuration by lowering system temperature in successive steps. Here searching process is steered by restraints, that transfer information from CG level onto positions of AA atoms. We show that after parameterization of annealing procedure, it is possible to generate correct ensemble of AA structures, that fully satisfies CG restraints. The influence of CG model resolution on quality of reconstructed structures is also investigated. Next, we show that the method can be applied for complex biomolecular systems, as an example helical WALP peptide in DPPC bilayer is back-transformed to AA representation. Correct secondary structure of the peptide is generated in reproducible way.

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A Parallel 2-Dimensional Wavelet Transform on the Cell/BE

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Long range interactions often play an important role in atomistic simulations, e.g. molecular dynamics or Monte Carlo simulations. They are always apparent for charged or polar systems, composed of ions or molecules with partially charged interaction sites. Usually, for the full determination of the electrostatic energy and forces the computational cost is of the order $O(N^2)$, since all pair contributions have to be considered. Because of its importance for a broad class of different applications, e.g. biophysics, chemical physics, material sciences or soft matter, there is strong interest to develop fast methods, which reduce the complexity to $O(N \log N)$ or even O(N).

Based on a Wavelet representation, a method was proposed in Ref.¹, where the distance matrix $A_{ij} = 1/||\mathbf{r}_i - \mathbf{r}_j||_2$ is discretized on a fixed grid, onto which particle charges are sampled. Since this matrix may be precomputed with a 2-dimensional Wavelet transform, the remaining problem during a simulation is reduced to Wavelet transform a charge vector, from where a potential vector may be obtained via matrix-vector product in wavelet space $(\tilde{\Phi} = \tilde{A} \tilde{Q})$ and a back transform of the potential vector ($\Phi = \mathbf{W}_l^T \tilde{\Phi}$). In order to get a fast algorithm, a threshold value is introduced for \tilde{A} , below which elements are set to zero and which leads to a sparse representation of the distance matrix in Wavelet space. Consequently, the matrix-vector product, which has to be computed during a simulation is not $O(N^2)$ anymore.

Since the distance matrix $\mathbf{A} \in \mathbb{R}^{N_g \times N_g}$, where $N_g = n_x n_y n_z$ and n_α is the number of space discretisation points in a cartesian direction, gets rather large, a computationally expensive part is to generate the Wavelet transform of this matrix. Although, in principle, this must only be done once, it is nevertheless a challenge for memory demands and computing time. Therefore, it is worthwhile to have an efficient parallel implementation of a 2-dimensional Wavelet transform. Notewhorthy to say that if one has such an implementation, a versatile tool is set up also for a variety of different applications, e.g. digital image processing. The 2-dimensional Wavelet transform can be calculated via a triple-matrix-product $\tilde{\mathbf{A}} = \mathbf{W}_l \mathbf{A} \mathbf{W}_l^T$, where \mathbf{W}_l contains all wavelet and scaling coefficients for a Wavelet transform of level l.

To accelerate the calculation of the triple-matrix-product, the Cell Broadband Engine (Cell/BE) is considered here as target platform for a parallel implementation. The Cell/BE is a heterogeneous multi-core processor consisting of multiple heterogeneous execution units, SIMD processing engines, fast local storages and a software-managed memory-hierarchy. An efficient implementation of the Wavelet transform is developed by considering the architectural requirements of Cell/BE. Via this implementation, the difficulties and problems in porting code to Cell/BE and using sparse linear algebra operations on the processor are assessed².

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Ab Initio Based Study of Antisite-Precipitates in B2-CoAl

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It is well-known that for high temperatures around 1500K the B2-phase of CoAl up to about 70% Co is stabilized by the existence of so called antisite atoms [1]. By quenching the crystal to low temperatures, this phase separates into an ideal B2-CoAl crystal and precipitates consisting of Co antisites only. By the combination of a density functional theory based cluster expansion Hamiltonian with Monte-Carlo simulations it will be demonstrated that these Co clusters show a characteristic size-shape-temperature dependence. Furthermore, we find a flattening of the precipitates at low temperatures due to the anisotropy of the interfacial energy which is wiped out at higher temperature by entropy. A detailed knowledge of the structure of these nanoclusters is of special importance as they lead to local magnetism in a non-magnetic intermetallic compound. Supported by Deutsche Forschungs-Gemeinschaft.

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Accurate Description of π -Conjugated Aggregates and Crystals with Optimized General Force Fields

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One of the most demanding scientific challenges is to make accessible renewable energy sources – particular solar light – to bulk energy production. A major bottleneck is the high production costs for the presently available, mostly inorganic solar cells. Alternatives, like the much cheaper organic heterojunction solar cells, are not yet competitive due to their low energy conversion efficiency.

A combined experimental and theoretical study¹ of the latter type of solar cells shows that the efficiency crucially depends on the exciton energy transfer, i.e. the transport process of excited states within the solid organic material. This can be evaluated with recently established approaches^{2, 3}, which apply quantum chemical methods on different levels of approximation and accuracy for dye molecules with up to 100 atoms. In the context of the research training school (Graduiertenkolleg) 1221, new materials for solar cells are investigated. In a recent work of our group it was shown that the quenching mechanism of the exciton transfer depends strongly on changes of the aggregate geometry in perylenebisimde systems⁴. Presently we develop a protocol for the optimization of general force fields, which will enable us to find promising dyes for solar cells. Recently it was shown that it is possible to predict the crystal structure of the perylenebisimde PR179 with the simple Williams99 force field, which contains only three terms⁵. Therefore, it is promising to test the common general force fields for their ability to describe crystals of π -conjugated materials with known crystal structures⁶.

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Multi-Particle Collision Dynamics Coupled to Molecular Dynamics on Massively Parallel Computers

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Mesoscale simulations of hydrodynamic media have attracted great interest during the last years in order to bridge the gap between mircoscopic simulations on the atomistic level on the one side and macroscopic calculations on the continuum level on the other side. Various methods have been proposed which all have in common that they solve the Navier-Stokes equations in different types of discretizations, e.g. Lattice-Boltzmann simulations^{1,2} on a spatial grid or Multi-Particle Collision Dynamics (MPC) — also called Stochastic Rotation Dynamics (SRD) — using discrete particles^{3,4}. In the latter approach, pseudo-particles are considered to carry both hydrodynamic information and thermal noise. With a small set of parameters (particle density, scattering angle, mean free path of a particle) it is possible to reproduce hydrodynamic behavior. In particular, the regime of small Reynolds numbers has been investigated in detail, e.g. Poiseuille flow, shear flow, vortices or hydrodynamic long time tails, to name a few^{4,5}.

One advantage of the MPC method is that a coupling to atomistic simulations can be established in a simple way. The main characteristic of MPC is that particles are sorted into the cubic cells (with lattice constant a) of a randomly positioned collision grid. Different variants of MPC vary in the way how the momentum exchange between particles within a collision cell is performed. In the SRD-version of MPC, relative velocities are rotated randomly by a given angle around a randomly chosen direction, which mimics collisions between solvent molecules. If coupled to atomistic simulations of solute particles, e.g. by molecular dynamics (MD), the MD-particles are sorted together with fluid particles into collision cells and their velocities are included into the stochastic rotation step. Because atomistic time scales are typically smaller than hydrodynamic time scales, MD-particles are basically simulated according to their force-fields. In order to establish a coupling to the hydrodynamic medium, they are included every n-th step into a stochastic rotation together with the solvent particles.

Since in typical simulations of colloidal suspensions or semi-diluted polymer systems, fluid particles are 1-5 orders of magnitude more numerous than MD-particles, system sizes get very large in simulations of $10^4 - 10^6$ MD-particles. Therefore, although mesoscale hydrodynamics techniques are algorithmically simple, the computational demand to study large system sizes on long time scales requires an efficient parallel implementation of the simulation code.

In the present work, a highly scalable implementation of the MPC algorithm, coupled to MD is presented⁶. The current version uses a domain decomposition approach, based on MPI. For the SRD part communication between processors is basically reduced to nearest neighbor exchange of collision cell information. The MD part is implemented via an eighth shell (ES) communication for the force computation and a minimum transfer scheme for the particle export/import. It is demonstrated that the program scales for the SRD part to the full capacity of the BlueGene/P architecture at JSC, i.e. 65536 compute cores. This particle based multiscale implementation, including various types of boundary conditions, offers the large scale simulation of microscopic systems coupled to a mesoscopic flow model on extended time scales.

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DFT Studies of The Magnetic Interactions in the Chromium-Based Molecular Rings and Adsorption of Sulfar at Surface on Gold

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We present an ab-initio investigation by means of density functional theory (DFT) simulation techniques of the electronic and magnetic properties of the antiferromagnetic Cr_8 molecular ring (i.e. $[Cr_8F_8Piv_{16}]$, where HPiv - pivalic acid, trimethyl acetic acid). The all-electron linearized augmented plane wave method (LAPW) implemented in the Wien2k package¹ is used to calculate the electronic states, exchange coupling parameters and magnetic anisotropy of Cr_8 , using an infinite chain model². We demonstrate how the chain models mimic with good approximation the electronic and magnetic properties of the original Cr_8 , and offers the reduction of the computational effort, for carrying out extensive investigations of molecules belonging to the Cr-based molecular rings family.

We also present adsorption of sulfur at (100) surface of gold analyzed with a help of the DFT (SIESTA code^{3,4}). Potential energy surface for a single S atom at Au(100) surface is computed and a simple analytical formula was found to reproduce the ab-initio results with a good accuracy. The vibration frequencies of the adsorbed S atom are computed using the harmonic approximation and a contribution of zero-point motion to the adsorption energy is evaluated. The role of effects of the surface Au atoms relaxation in the sulfur adsorption is analyzed. The interactions between S atoms adsorbed in the nearest and the next nearest equivalent adsorption sites is computed and used to define an effective Hamiltonian to describe the interactions between the adsorbed sulfur atoms.

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Ground-State Configurations and Melting of Two-Dimensional Non-Uniformly Charged Classical Clusters

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We consider classical two-dimensional Coulomb clusters¹ consisting of two species² containing five particles with charge q_1 and five with charge q_2 , respectively. The particles are subject to the Coulomb forces and the parabolic confinement potential. The subject of the study is interesting due to some fundamental aspects of the system dynamics and a number of classical and quantum realizations.

We investigate the dependence of the ground state and metastable configurations as well as radial and angular displacements of particles at finite temperature on the ratio $q = q_2/q_1$, using Monte Carlo (MC) and molecular dynamics (MD)¹ simulations and a new genetic algorithm (GA) based approach³. At T=0 the ground state configurations were generated applying the MC simulation and their stability with respect to temperature was analyzed within the MD method. We found a new multi-step melting behavior for q sufficiently different from the uniform charge limit q = 1. The melting scenario is rich and depends on the q value. There are domains where the radial melting precedes the angular melting or vice versa.

Due to some discrepancies present in the previous MC determination of the ground state configurations and the limited accuracy of the simulation, the geometrical structures and structural phase transitions have been analyzed within the GA approach. The recent literature results for T=0 (and these exploited in our MD simulations) have been qualitatively confirmed but the global minima and localization of a second-order phase transition point have been estimated more accurately.

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First-Principles Study of the Growth Kinetics of 1D Pd Islands on SnO₂

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The vapor deposition of Pd on a reduced $\text{SnO}_2(101)$ surface leads to the formation of onedimensional (1D) nanowires. Scanning tunneling microscopy reveals the growth of islands with a monoatomic height and a width of 5 Å and a length of up to 350 Å¹. Nanowires and 1D conductors are potential building blocks of nanoscale devices. For the design of nanowires with specific properties it is essential to fully understand the atomistic processes that lead to this for metal oxide substrates unusual overlayer growth. In order to gain insight into the energetics and the kinetics of the growth of Pd islands on $\text{SnO}_2(101)$ surfaces, the system has been studied by first-principles DFT slab calculations¹ as well as by kinetic Monte-Carlo (kMC) simulations. It is found that a pronounced 1D diffusion, combined with a strong interaction of Pd with the surface Sn atoms and the lack of stable binding sites at the sides of the nanowires are responsible for the formation of the 1D islands.

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Molecular Dynamic Simulations of Static and Kinetic Friction in Extended Tribological Problems

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Numerical simulations can be extensively used in tribological studies, not simply as a mean of supplementing experimental investigations, but as a powerful tool for gaining unique insight into the relevant processes, sometimes even overturning conventional wisdom regarding the nature of friction. If it is not yet possible to fully treat all the characteristic length scales that mark the dynamical mechanisms entering the friction coefficient of engineering materials, a rising number of efforts are nowadays successfully devoted to increase cleverly the accessible timescale and the possibility to simulate really extended systems. Here, we make use of the powerful molecular dynamics code LAMMPS¹, developed at Sandia National Labs, to tackle two distinct challenging tribological problems in extended systems: i) the Kr/Pb(111) island system with reference to the QCM instrument²; ii) the dynamics of a confined boundary lubricant under shear and the peculiar transition between the high dissipative stick-slip motion and the smooth sliding regime.³

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Quantum Monte Carlo Simulations of Molecular Aggregates

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Systems of molecules embedded in superfluid helium clusters are of high interest, since the helium clusters provide a unique matrix^{1–5}. Rotational bands of embedded molecules can be resolved in IR-spectra. These spectra are similar to the gas phase with a renormalized moment of inertia which can be understood as a solvation shell of non-superfluid helium being dragged along^{6,7}. In previous theoretical investigations the solvated molecule is only described as either rigid or with simple force fields^{8,9}. We aim at a better description of the embedded molecule by using DFT as provided by CP2K^{10,11}. This gives us a flexible model for a wide range of embedded molecules including the possibility of reactions inside the droplet.

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Ewald-Summation for the Rotne-Prager Tensor: Error Analysis and Parameter Optimisation

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If no screening effects occur, hydrodynamic interactions are intrinsically of long range nature. Therefore, simulation of dissolved particles in a fluid, which is treated on a hydrodynamic level, leads to a similar problem as in electrostatics, where the Coulomb potential has to be summed up in order to calculate the potential energy and forces on a given particle. In hydrodynamics it is the velocity field, which is created by a particle, onto which a force is acting. In the idealized case of an uncompressible liquid, this particle creates instantaneously a velocity field in the whole system, which gives rise to an effective force onto other particles, prescribed by Stokes law, $\mathbf{F} = 6\pi\eta a\mathbf{v}$, which relates the frictional force to the velocity of the fluid via the viscosity η of the liquid and the radius a of the particle.

In order to take hydrodynamic interactions between dissolved particles into account, an established approximation is the treatment of hydrodynamic effects with the Rotne-Prager tensor¹, which is a positive definite extension of the Green's function of the creeping flow equations, the Oseen tensor. To simulate systems in an infinite system, i.e. not taking into account explicitly surface effects, simulations are usually performed for periodic boundary conditions. In analogy to electrostatic problems, a formulation for an absolutely converging Ewald sum was presented in Refs.^{2,3}. Applying this technique e.g. to Brownian dynamics in the formulation of Ermak and McCammon⁴, the computation becomes very expensive, since every tensor element of a $3N \times 3N$ matrix has to be calculated separately. Therefore a most efficient implementation in terms of parameters, which control (i) the error tolerance and (ii) the run-time behavior seems to be crucial. To our best knowledge there is no consistent error estimate for the Rotne-Prager Ewald summation. In order to optimise the method for a given error tolerance, parameters for the cutoff radius R_c , maximal wavenumber k_{max} and splitting parameter ξ are selected which (i) give rise to the same error threshold in the real- and reciprocal-space sum and (ii) lead at the same time to a minimum in the execution time.

An analytical framework is presented for the error estimates in the Ewald sum for the Rotne-Prager tensor, which is also valid in the limiting case of $a \rightarrow 0$ for the Oseen tensor. Both numerical and model results are presented for parameter optimisations to minimise the execution time. For all particle densities and error tolerances, the splitting parameter is found to be $\xi \approx 2.5 / L$, where L is the boxlength.

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Adsorption Processes on the Glass Surface Simulated by First-Principles and Kinetic Monte Carlo

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In recent experimental work, Gross, et al.¹ observed that upon adding organic acids into the aqueous solution the dissolution rate of glass cations was lower than what is predicted by thermodynamic models. In this work, we investigated the strategies of inhibiting glass dissolution in the presence of oxalic acid by first-principles and kinetic Monte Carlo simulations.

In order to understand at the atomic scale the experimentally observed glass corrosion protection by oxalic acid, we have performed a systematic study of the silicate minerals diopside (CaMgSi₂O₆) and åkermanite (Ca₂MgSi₂O₇), using *ab initio* density functional theory simulations. Surface structure, hydroxylation of surfaces, and chemisorption of oxalic acid molecules on these hydroxylated surfaces were modeled and studied. In the previous work it was observed that the silicate mineral surfaces created by cutting the crystalline solid are easily hydroxylated due to the interaction with water molecules present either in the aqueous solution or in the atmosphere^{2,3}. The behavior of the three different surface cations Si, Mg and Ca in the above processes has been investigated. It was observed that the surface Si atom (for diopside) and the surface Si and Mg atoms (for åkermanite) after surface relaxation as well as after hydroxylation have the same coordination numbers as in bulk crystals. The surface Ca atom was not fully saturated. The oxalate or bioxalate ions of oxalic acid bond to yet unsaturated surface Ca and/or Mg atoms, keeping the saturation of Si (and possibly Mg) unaltered. The surface complexes that are created this way form a hydrophobic layer on the surface and thus protect the leaching of metal cations from the multicomponent glass surface. This provides a description of the mechanism of glass corrosion inhibition at the atomic level: the chemisorption energy of oxalic acid being larger than the physisorption energy of water, the former is the process that will actually happen. The developed KMC algorithm is an efficient method for the investigation of adsorption processes for various multi-component systems. The developed algorithm allows to simulate non-equilibrium processes and to add dynamics to the existing thermodynamic models.

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Vortex Configurations in Mesoscopic Superconducting Triangles: Finite-Size and Shape Effects

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Triangular-shaped mesoscopic superconductors are consistent with the symmetry of the Abrikosov vortex lattice resulting in a high stability of vortex patterns for commensurate vorticities. However, for non-commensurate vorticities vortex configurations in triangles are not compatible with the sample shape. Here we present the first direct observation of vortex configurations in μm -sized niobium triangles using the Bitter decoration technique, and we analyze the vortex states in triangles by analytically solving the London equations and performing molecular-dynamics simulations. We found that filling rules with increasing vorticity can be formulated for triangles in a similar way as for mesoscopic disks where vortices form shells.

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