MM 31: Computational Materials Modelling: Physics of Ensembles 2

Time: Thursday 11:45–13:00 Location: H44

MM 31.1 Thu 11:45 H44

Making low-scaling GW accurate — •Jan Wilhelm[1] and Dorothea Golze[2] — [1]Institute of Theoretical Physics, University of Regensburg — [2]Faculty of Chemistry and Food Chemistry, TU Dresden

In standard GW implementations, the computational cost is growing as $O(N^4)$ in the system size N, which prohibits their application to many systems of interest. I present a GW algorithm in a Gaussian-type basis with a computational cost that scales with N^2 to N^3. It will be shown that large minimax grids and resolution of the identity with the truncated Coulomb metric improve the accuracy of the low-scaling GW algorithm to < 0.01 eV for the GW100 test set. Large-scale applications of low-scaling GW will be discussed.

MM 31.2 Thu 12:00 H44

Atomic cluster expansion parametrization of carbon for a fast, accurate and transferable interatomic potential — •Minaam Qamar, Matous Mrovec, Yury Lysogorskiy, Anton Bochkarev, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany

We present a parametrization of the atomic cluster expansion (ACE) for carbon that can be employed in large-scale atomistic simulations of complex phenomena. The ACE model is parametrized over an exhaustive dataset of important carbon structures at extended volume and energy ranges, computed using highly accurate density functional theory (DFT). Dispersion corrections are explicitly added to properly account for long-ranged van der Waals interactions. A rigorous validation against DFT data reveals that ACE predicts accurately a broad range of properties of both crystalline and amorphous C phases while being significantly more computationally efficient than other popular machine learning models. We demonstrate the predictive power of ACE on two distinct applications: (1) brittle crack propagation in diamond at finite temperature, and (2) evolution of amorphous carbon structures at different densities and quench rates.

MM 31.3 Thu 12:15 H44

Design and analysis of scattering data driven molecular dynamics simulation on the example of water and selected crystals — •Veronika Reich[1], Sebastian Busch[1], and Martin Müller[2] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon, Lichtenbergstr. 1, 85748 Garching bei München, Germany — [2]Helmholtz-Zentrum Hereon, Max-Planck-Str. 1, 21502 Geesthacht, Germany

Molecular dynamics simulations are an indispensable tool to preinvestigate neutron scattering experiments. For many systems reliable force fields have been established and yield to significant simulations. On the other hand a lot of systems still don't have a satisfactory agreement between experiment and simulation.

In this work we compare experimental data to different liquid water model simulations and give an outline to crystal simulations.

We simulate the samples using molecular dynamics simulations using the program LAMMPS. Subsequently we calculate the coherent and incoherent scattering signals using the program SASSENA. Ensuing we compare the outcomes to already existing experimental data and evaluate changes in the underlying force fields in terms of their impact on the behaviour of the simulation. Finally we compare the incoherent calculations to mathematical models, which in turn we later fit to the simulation.

The aim of our work is to create a simple to use workflow of molecular dynamics simulations for scattering experiments.

MM 31.4 Thu 12:30 H44

Approximating nuclear quantum effects in solids by temperature remapping — •Raynol Dsouza[1], Liam Huber[1], Blazej Grabowski[2], and Jörg Neugebauer[1] — [1]Max Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]University of Stuttgart, 70569 Stuttgart, Germany

The quantum nature of solids, which is especially important at low temperatures, is often ignored in finite temperature atomistic simulations. Formulations to estimate quantum anharmonic effects precisely, such as the path integral method, are computationally demanding. Although various acceleration approaches allowing quantum effects to be fully accounted for in systems of hundreds of atoms have been proposed over the last two decades, they can fall short when it comes to modeling defects in solids, which can require significantly larger system sizes. We present a new approach for approximating nuclear quantum effects, exploiting a temperature map between the quantum system and its best classical surrogate. This map is constructed using the internal energies of classical and quantum harmonic oscillators within the Debye model. To a good approximation, our approach captures the impact of quantum effects on lattice constants, internal energies, and heat capacities with almost no additional cost compared to purely classical molecular dynamics simulations. Results for diamond cubic carbon and silicon are in good agreement with available literature values, which use full path integral Monte-Carlo simulations. We also show how this approach can be used to predict phase transition temperatures, e.g. the FCC to BCC transition for calcium.

MM 31.5 Thu 12:45 H44

Sharp phase-field modeling of isotropic solidification with a super efficient spatial resolution — •Michael Fleck and Felix Schleifer — University of Bayreuth, 95447 Bayreuth, Germany

The phase-field method provides a powerful framework for microstructure evolution modeling in complex systems, as often required within the framework of integrated computational materials engineering. However, spurious grid friction, pinning and grid anisotropy seriously limit the resolution efficiency and accuracy of these models. The energetic resolution limit is determined by the maximum dimensionless driving force at which reasonable model operation is still ensured. This limit turns out to be on the order of 1 for conventional phase-field models. Grid friction and pinning can be eliminated by a the restoration of Translational Invariance (TI) in the discretized phase-field equation. This is called the sharp phase-field method, which allows to choose substantially coarser numerical resolutions of the diffuse interface without the appearance pinning. We propose an accurate scheme to restore TI locally in the local interface normal direction. The new model overcomes grid friction and pinning in three dimensional simulations, and can accurately operate at dimensionless driving forces up to the order of 10^4. At one-grid-point interface resolutions, exceptional degrees of isotropy can be achieved, if further the inhomogeneous latent heat release at the advancing solid-liquid interface is mitigated. Imposing a newly proposed source term regularization the new model captures the formation of isotropic seaweed structures without spurious dendritic selection by grid anisotropy.