MM 48: Methods in Computational Materials Modelling VI: Algorithms

Time: Thursday 10:15–11:30   Location: H 0106

MM 48.1   Thu 10:15   H 0106

Molecular-Dynamics Simulations on Many-Core Processors — •Ralf Meyer and Chris Mangiardi — Laurentian University, Sudbury, Canada

Molecular-dynamics (MD) simulation is one of the most important methods for the numerical studying of materials. This contribution discusses new algorithms for large-scale MD simulations on modern CPUs. Forthcoming many-core processors will soon integrate hundreds of compute cores in a single processor with SIMD units that operate on vectors of 8 or more double-precision numbers simultaneously. However, the full power of these devices will only be accessible with the help of novel algorithms.

The cell task method [1,2] uses a task-based programming approach for the parallelization of MD simulations on multi- and many-core architectures. The method avoids load balancing problems by using a large number of dynamically scheduled small tasks to distribute the workload among the processing cores. Furthermore, a tiling algorithm is used that increases the efficiency of wide SIMD vector units in the simulations.

Results from benchmark simulations on Xeon Phi co-processors are presented. The results show that the cell task algorithm scales well for large numbers of threads. In addition to this, the method outperforms the spatial decomposition approach for simulations of inhomogeneous (e.g. porous) systems.

[1] R. Meyer, Phys. Rev. E **88**, 053309 (2013).
[2] R. Meyer, J. Phys.: Conf. Ser. **540**, 012006 (2014).

MM 48.2   Thu 10:30   H 0106

Studies of thermomechanical properties and nanoscale phase transitions using the universal multiscale computer program MBN Explorer — •Christian Kexel[1,2] and Andrey Solov'yov[1,2] — [1]Department of Physics, Goethe University, 60438 Frankfurt, Germany — [2]MBN Research Center, 60438 Frankfurt, Germany

We present the popular multipurpose computer code MBN Explorer (MesoBioNano Explorer) which allows modeling molecular systems of varied level of complexity. The package is suited to compute system's energy, to optimize molecular structures as well as to simulate many molecular systems with sizes ranging from the atomic to the mesoscopic scales by means of molecular-dynamics and kinetic monte-carlo approach. A distinct feature of the program, which makes it significantly different from existing codes, is its universality and applicability to the description of a broad range of problems comprising atomic clusters, nanotubes, fullerenes, polypeptides, proteins, DNA, composite systems and nanofractals. In particular, we present our research on the thermomechanical properties of various materials and the study of nanoscale phase transitions.

MM 48.3   Thu 10:45   H 0106

A QM/MM method to study solid-solid interfaces — •Sara Panahian Jand[1], Pouya Partovi-Azar[2], Setareh Javadi Dogahe[1], and Payam Kaghazchi[1] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Department Chemie, Technische Chemie, Universität Paderborn, 33098 Paderborn, Germany

The hybrid quantum mechanics/molecular mechanics (QM/MM) approach is a promising method to study large systems on the atomic scale. In this work we present our recently developed QM/MM method that can be used to study solid-solid interfaces. In this method, the QM region is described by density functional theory (DFT). For the MM region we discuss the influence of choosing different classical potentials on the QM/MM results. The point charges which are required for the coulomb interactions as well as van der Waals parameters are obtained independently by fitting the classical potentials to DFT-based electrostatic energies and long-range dispersion energies (calculated by the Quantum Harmonic Oscillator model with Maximally Localized Wannier Functions), respectively. The remaining parameters for the MM region are evaluated by comparing physical quantities calculated with DFT and those calculated with classical potentials. We finally show the application of our QM/MM approach to study solid electrolyte interphases in Li-ion batteries.

MM 48.4   Thu 11:00   H 0106

Ab-initio non-linear optics beyond the long-wavelength limit. — •Klaus-Dieter Bauer, Martin Panholzer, and Kurt Hingerl — Johannes Kepler Universität, Linz, Österreich

In ab-initio methods optical properties are typically evaluated in the long-wavelength limit, which leads to questionable results for absorbing systems in general and specifically predicts zero bulk contribution to second harmonic generation, while experimental results show a bulk contribution from small-wavelength components of the field.

We try to establish how these effects are related to the full microscopic second-order response function $\chi^{(2)}(\mathbf{k}_0, \omega_0; \mathbf{k}_1, \omega_1, \mathbf{k}_2, \omega_2)$ and how to obtain effective local response functions from DFT.

MM 48.5   Thu 11:15   H 0106

Test set for materials science and engineering — Toktam Morshedloo[1,2], •Norina A. Richter[1], Fawzi R. Mohamed[1], Xinguo Ren[3], Sergey V. Levchenko[1], Luca M. Ghiringhelli[1], Igor Ying Zhang[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Ferdowsi University of Mashhad, Mashhad, IR — [3]University of Science and Technology of China, China

Understanding of the applicability and limitations of electronic-structure methods needs detailed comparison with highly accurate data of representative test sets. A variety of highly valuable test sets have been established in quantum chemistry for small molecules. However, for crystalline solids they are still lacking. We present a representative test set for materials science and engineering (MSE) which includes first and second row elements and their binaries, comprising various crystal structures. This allows for unbiased benchmarking for various chemical interactions. In the MSE test set, we consider cohesive energy, lattice constant, bulk modulus, electronic band structures, and phonons etc. A big effort is made to produce systematically converged results with respect to basis set[1] and **k** mesh for a hierarchy of electronic-structure methods, ranging from the local-density approximation to advanced orbital-dependent functionals implemented in the all-electron, full-potential FHI-aims code. Furthermore, we use incremental schemes to obtain benchmark values calculated with coupled-cluster approaches. [1] I. Y. Zhang *et al.*, *NJP* **15** 123033 (2013)