TECHNISCHE UNIVERSITÄT CHEMNITZ

Institut für Physik
Physikalisches Kolloquium

Mittwoch, 31.01.2018, um **16:00 Uhr**
Ort: Reichenhainer Str. 90;
Zentrales Hörsaal- und Seminargebäude,
Raum 2/N013

Prof. Dr. Ralf Drautz
Ruhr-Universität Bochum

From the Atomic Interaction to Thermodynamic and Mechanical Properties of Materials

Density functional theory (DFT) provides a solid basis for the simulation of materials properties. The computational expense of DFT makes the calculation of thermodynamic or dynamic properties of materials difficult. We coarse grain the interatomic interaction from DFT at two levels of approximation to allow for faster and larger simulations. First, a tight-binding model is derived from a second-order expansion of DFT in a minimal basis. The parameters in the tight-binding model are obtained directly from minimal basis DFT calculations. In a second step the tight-binding model is approximated locally and analytically, resulting in the analytic Bond-Order Potentials (BOPs). Because of the derivation of the BOPs from DFT, contributions of magnetism and charge transfer to bond formation are directly taken into account. The BOPs are orders of magnitude faster than DFT and allow for the direct sampling of thermodynamic observables.

I will discuss the application of the BOPs to simulating finite temperature magnetism in iron, in particular the ferromagnetic to paramagnetic phase transformation and the alpha-gamma transition and the prediction of some mechanical properties. I will further discuss atomic simulations for phase stability, nucleation and solid-solid transformations with relevance to high-temperature materials.

Alle Zuhörer sind ab 15:45 zu Kaffee und Tee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt:
Prof. Dr. Sibylle Gemming, Tel. 0351 260 2470

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