chemisch
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gesellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz,
J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum Vortrag von

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über

Evolutionary crystal structure prediction: methodology and its applications in materials design and study of matter at extreme conditions

am

Dienstag, 20. November 2007, um 17.30 Uhr

Ort: Großer Hörsaal der Experimentalphysik, Universität Wien,
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Abstract:
Crystal structure prediction on the basis of just the chemical formula has long been considered a formidable problem. Being able to solve it would open the possibilities to find new phases of planetary materials at extreme conditions, to solve structures where experimental data are insufficient, and to design new materials entirely on the computer (once the structure is known, it is relatively easy to predict many of its properties). Essentially, the problem can be reduced to the problem of global optimization of the free energy of the crystal with respect to structural parameters. Recently, we addressed this problem and devised a new method based on a specifically devised and carefully tuned *ab initio* evolutionary algorithm, which we implemented in the USPEX code. At given *P-T* conditions, USPEX finds the stable structure and a number of robust metastable structures. USPEX uses *ab initio* free energy as evaluation function and features local optimization and spatial heredity, as well as further operators such as mutation and permutation. This method has been widely tested and applied to solve a number of important problems. It turns out to be extremely efficient for predicting crystal structures with very different geometrical features and types of chemical bonding. This talk will discuss the method and some of its applications to a number of interesting materials (B, C, O, $CaCO_3$, FeS, Xe-C at high pressure and exotic new materials proposed for C, $Al^{12}C$ and $Al^{13}K$ at ordinary conditions) of fundamental or applied interest. Future developments of the method will be outlined as well.

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