Einladung zum Vortrag von

Prof. Stephan Kümmel

Universität Bayreuth

Dienstag, 22. März 2011
Hörsaal Physik, Montanuniversität Leoben
15 Uhr c.t.

Interpreting photoelectron spectra based on DFT - new hope or just hopeless?

Density functional theory (DFT) is widely used to predict the electronic structure of solids and molecules. However, the performance of DFT appears to be erratic, with great successes being accompanied by dramatic failures. This is in particular so with respect to the simulation of photoemission data. With organic semiconductors serving as an important example we discuss when and why DFT is able to predict the electronic structure reliably. We show that the importance of electronic self-interaction, which is a decisive factor in DFT accuracy, can be reliably tested for with a simple criterion, and demonstrate that orbital density functionals can greatly enhance the predictive power of DFT.

Der Vortrag wird vom Lehrstuhl für Atomistic Modelling and Design of Materials im Rahmen der *SimNet Multiscale Lectures* und vom Institut für Physik im Rahmen des *Seminars aus Halbleiterphysik und Nanotechnologie* veranstaltet.