TECHNISCHE UNIVERSITÄT
CHEMNITZ

Institut für Physik
Physikalisches Kolloquium

Mittwoch, 25.05.2016, um **16:00 Uhr**

Ort: Reichenhainer Str. 90;
Zentrales Hörsaal- und Seminargebäude,
Raum 2/N013

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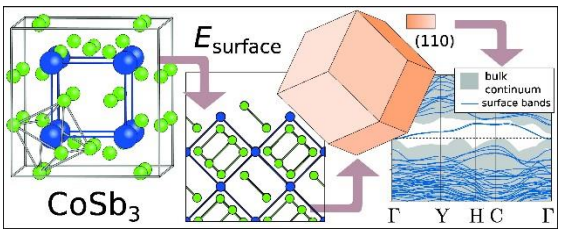
Institut für Chemie und Biochemie

Theoretical material and surface science: From method development to applications

Material properties are mainly determined on the first-principle level applying density-functional methods. In several cases these methods yield sufficient accuracy to predict the most stable allotropes. Here I will present results for aluminium oxide/fluoride mixtures and their interaction with water [1], and for filled and/or doped cobalt-antimon skutterudite [2] as one possible material for thermoelectric applications. Using the results of first-principle calculations and the methods of surface thermodynamics, it is also possible to predict the structure of nanocrystals depending on the pressure and temperature. We apply this method to nanoscopic magnesium fluoride [3].



But there exist materials, where present-day density functionals reveal problems to describe the crystal structures and the cohesive properties. One example are the group-12 metals zinc, cadmium and mercury [3]. The application of the method of increments [4] for the correlation energy in solids based on any size- extensive correlation method like coupled cluster to metals such as magnesium, zinc, and cadmium [5] considerably improved our understanding of binding in these metals compared to the DFT approach.

Another example where density-functional theory can fail is the weak interaction of adsorbed molecules on surfaces. As example the interaction of water with graphene and different carbon nanotubes will be presented [6] applying the method of increments for adsorption energies on the coupled-cluster level.

[1] J. Schacht, J. Wirth, B. Paulus, P. Saalfrank, J. Phys. Chem. C (2016), accepted
[2] L. Hammerschmidt, B. Paulus, Phys. Status Solidi A **213**, 750-757 (2015)
[3] E. Kanaki, S. Gohr, C. Müller, B. Paulus, Surf. Sci. **632**, 158-163 (2015)
[4] N. Gaston, B. Paulus, U. Wedig, M. Jansen, Phys. Rev. Lett. **100**, 226404 (2008)
[5] B. Paulus, Phys. Rep. **428**, 1-52 (2006) review
[6] S. Lei, B. Paulus, S. Li, B. Schmidt, J. Comp. Chem. (2016), in press, DOI: 10.1002/jcc.24342

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

Informationen zum Vortrag erteilt:
Prof. Dr. Michael Schreiber, Tel. 0371 531-21910

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