Halbleiter-Nanophotonik

SFB 787

Einladung

Es spricht: **Keith T. Butler**
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Zeit: **Donnerstag, 05. Februar 2015, 10:00 Uhr**

Ort: **Technische Universität Berlin**
Institut für Festkörperphysik
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Thema: **„Understanding and designing functional materials: the importance of electronic structure in the solid-state"**

Abstract:

Rational design and prediction of materials for technological applications is one of the foremost challenges for contemporary computational science, the proliferation of 'computational materials' screening' programs in the past five years pays testament to the growing importance of this field.

In this presentation I will consider a number of methods for predicting and understanding structure/electronic relationships in crystalline materials. The methods range in complexity from simple models based on local environment and electrostatic potential to state-of-the-art quantum mechanical calculations for studying complex band structures. I will demonstrate how these methods can be applied for understanding and designing new materials for photovoltaics technologies and materials. Specifically I will concentrate on the role of calculation in three key areas of PV design: (i) understanding the electronic structure and operating principles behind the outstanding recent success story of hybrid halide perovskites such as $CH_3NH_3PbI_3$; (ii) predicting new design strategies, based on ultra-thin films for improving band-offsets at materials' hetero-junctions with transparent conductive oxides; (iii) predicting new materials for application as hybrid organic-inorganic ferroelectrics.

Gäste sind herzlich willkommen!
Prof. Dr. A. Hoffmann