TECHNISCHE UNIVERSITÄT
CHEMNITZ

Institut für Physik
Physikalisches Kolloquium

Mittwoch, 31.05.2017, um **16:00 Uhr**

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

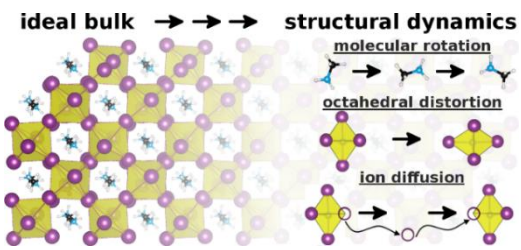
Dr. David A. Egger

Institut für Theoretische Physik,
Universität Regensburg

Lead-Halide Perovskites on the Move: Insights from First-Principles Calculations

Power-conversion efficiencies of lead-halide perovskite (LHP) solar cells have improved at record pace and are currently above 22%. It is of both fundamental and practical importance to examine phenomena that contribute to, or limit, these impressive efficiencies. To this end, a lattice of ions displaced from their static positions only by harmonic vibrations is often invoked when understanding charge-transport and light-absorption in the semiconducting material. However, recent studies suggest that such a picture is not sufficient for LHPs, in which different structurally dynamic effects, going strongly beyond small harmonic vibrations, arise already at room temperature.

After providing an introduction to LHP-based solar cells, I will discuss our recent results on structurally dynamic effects in LHPs, using first-principles calculations based on density functional theory. Starting from the canonical band structure picture, the impact of ionic diffusion, optical phonons, and dynamic polar distortions will be presented. From this discussion, open questions with relevance for charge-carrier dynamics in LHPs will be addressed.



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

Informationen zum Vortrag erteilt:
Prof. Dr. Carsten Deibel, Tel.: 0371 531-34878