



Dienstag, 10. Dezember 2019 13:00 Uhr

ZNN, Seminarraum EG 0.001

"Theory of functional energy materials – Prospects and challenges"

Energy materials are active compounds in devices for energy conversion or storage, e.g., semiconductors in solar cells or solid ion conductors in batteries. In my group, we use theoretical calculations to investigate these systems, in order to derive structure-function relations for optimizing their macroscopic properties and invent new compounds with superior characteristics for device applications. In this presentation, I will provide an overview of our activities, ranging from characterizing charge transport and nuclear disorder in halide perovskite solar materials to predicting energy level diagrams at nanoscale interfaces. Recent progress in theory method development will be summarized to address prospects and challenges of the state-of-the-art, which will lead to an improved understanding of what theory can do for experiments and vice versa.

> Prof. Dr. David A. Egger Department of Physics Technical University of Munich Garching, Germany