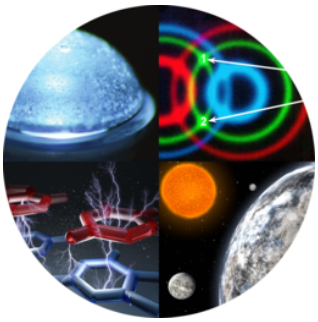

Münchner Physik-Kolloquium

Winter 2019/20

Dynamic properties of energy materials from first-principles

Prof. Dr. David Egger, *Technische Universität München, Garching*

Monday, 3 February 2020, 17:15 h
Hörsaal H 030, Fakultät für Physik der LMU, Schellingstraße 4, München

Energy materials are crucial components in devices for energy conversion or storage, such as solar cells and batteries. Since these devices must operate efficiently around room temperature to be technologically relevant, one must understand how microscopic effects in these compounds give rise to macroscopic properties, such as charge transport, around RT. To address the impact of nuclear dynamics on functional properties of energy materials, I will present our recent theoretical results that were obtained using first-principles and force-field based molecular dynamics simulations. It will be shown that traditional models based on harmonic approximations of nuclear dynamics – a cornerstone of solid-state physics for understanding materials at elevated temperatures – cannot describe some of the most important properties in pertinent solar and ion-conducting materials. From this, it will be discussed that impacts of unusual nuclear dynamics in energy materials cannot be neglected when understanding them microscopically and designing new functional compounds for energy conversion and storage.

Student event: Meet the speaker

*We invite you to a **student-only** discussion-round with Prof. Dr. David Egger before his Munich Physics Colloquium talk.*

Be curious and feel free to ask any question.

Monday, 3 February 2020, 16:00 h,
Room H 522 (5th floor), Fakultät für Physik der LMU, Schellingstraße 4, München