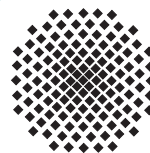# Stuttgarter Physikalisches Kolloquium

Max-Planck-Institut für Festkörperforschung
Max-Planck-Institut für Intelligente Systeme
Fachbereich Physik, Universität Stuttgart

Ansprechpartner: Andreas Schnyder
E-Mail: A.Schnyder@fkf.mpg.de
Telefon: 0711 689-1553

Dienstag, 25. Juni 2019	16.15 Uhr	Hörsaal 2D5

Stuttgarter Max-Planck-Institute, Heisenbergstraße 1, 70569 Stuttgart-Büsnau

Hybrid perovskites: from the random phase approximation to machine learned potentials

Prof. Dr. Georg Kresse,
Universität Wien
in collaboration with: Menno Bokdam and Ryosuke Jinnouchi

Abstract

Reaching predictive accuracy in first principles calculations for complex materials has always been a dream. Here we address this challenge for a very complex highly dynamic material, the hybrid perovskite $MAPbI_3$ a promising new solar cell material.

The first part of the talk addresses the issue, which density functional is the "best" for structure simulations of a particular material? A concise, first principles approach to answer this question is presented [1]. The random phase approximation (RPA)—at least for solids a very accurate many body theory—is used to evaluate and rank various density functionals for $MAPbI_3$. The evaluation is done by first creating finite temperature ensembles for small supercells using RPA molecular dynamics, and then evaluating the variance between the RPA and various approximate density functionals for these ensembles. We find that, contrary to recent suggestions, van der Waals functionals do not improve the description of the material, whereas hybrid functionals and the strongly constrained appropriately normed (SCAN) density functional yield very good agreement with the RPA.

In the second part of the talk, realistic large scale finite temperature simulations of $MAPbI_3$ are presented. To achieve the required long simulation times and large length scales, an on-the-fly machine learning scheme that generates force fields automatically during first principles molecular dynamics simulations is used (relying on the previously determined best functional SCAN). This opens up the required time and length scales, while retaining the distinctive chemical precision of first principles methods and minimizing the need for human intervention. Using machine learned potentials, isothermal-isobaric simulations give direct insight into the underlying microscopic mechanisms of the phase transitions. Although used for $MAPbI_3$ here, the method is widely applicable to multi-element complex systems [2].

[1]. Menno Bokdam, Jonathan Lahnsteiner, Benjamin Ramberger, Tobias Schäfer, and Georg Kresse, Phys. Rev. Lett. 119, 145501 (2017).

[2]. Ryosuke Jinnouchi, Jonathan Lahnsteiner, Ferenc Karsai, Georg Kresse, and Menno Bokdam, Phys. Rev. Lett. in print, selected as Editors' Suggestion.