

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**Evaluating density functionals: case study for organic perovskites**

MENNO BOKDAM, JONATHAN LAHNSTEINER, BENJAMIN RAMBERGER, TOBIAS SCHÄFER, CHRISTOPH DELLAGO, GEORG KRESSE, University of Vienna, Faculty of Physics and Center for Computational Materials Sciences, Vienna, Austria — The precise ordering of the molecules in organometal halide perovskites at elevated temperatures is difficult to determine. Density functional theory (DFT) calculations proposes ordering patterns, but they depend on the type of exchange-correlation functional used. Van der Waals interactions are important in this system and require an accurate description, which goes beyond choosing the "best" density functional based on common reasoning. Here we use the random phase approximation (RPA) to evaluate various density functionals for the perovskites, specifically MAPbI<sub>3</sub>. The evaluation is done by first creating finite temperature ensembles for small supercells of MAPbI<sub>3</sub> using a beyond DFT approach, and then evaluating the variance between the random phase approximation and various approximate density functionals for these ensembles. The finite temperature ensembles are generated using hybrid Monte-Carlo techniques as well as finite temperature RPA molecular dynamics. We will present an overview of various density functionals and how well they correspond with the random phase approximation applied to the perovskites.

Menno Bokdam  
University of Vienna

Date submitted: 20 Nov 2016

Electronic form version 1.4