MM 2: Invited Talk: R. de Souza

Time: Monday 9:30–10:00 Location: H10

Invited Talk MM 2.1 Mon 9:30 H10

Probing Ion Migration in ABX_3 Perovskite Compounds: Five Fallacies of Simulations — •Roger De Souza — Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany

Simulation studies play a central role, in interpreting and explaining experimental data on ion transport, in providing insights at the atomic scale, and in predicting data for new systems. Ion migration in ABX_3 perovskites has been examined with both molecular-static and molecular-dynamic calculations, employing classical pair potentials, reactive force-fields or quantum-mechanical calculations.

In this contribution, taking ion migration in $BaTiO_3$, $CaTiO_3$, and $MAPbI_3$ as examples, I draw attention to problems that may arise when using molecular-static calculations to obtain activation barriers for higher symmetry perovskite phases. In general, a far more critical consideration of simulation results in the literature is required.