MS14-2-8 Predictive modelling of order-disorder phase transitions in hybrid organic materials with machine learning force fields
#MS14-2-8

R. Tranås [1], E.D. Sødahl [1], J.M. Carrete [2], G. Madsen [2], K. Berland [1]
[1]Norwegian University of Life Sciences NMBU - Ås (Norway), [2]TU Wien - Vienna (Austria)

Abstract
The caloric and ferroic properties of hybrid-organic materials make them attractive environmental-friendly materials for a range of technological applications, including actuators, sensors, energy harvesting, and solid-state refrigeration. However, progress in the development of such materials is hampered by the huge computational costs of ab-initio molecular dynamics modelling at finite temperatures which is required for predictive modelling of dynamical properties including phase transition temperatures. However, recent advances in machine-learning force fields (ML-FF) hold a promise of providing first-principles accuracy of dynamical properties at a fraction of the computational costs while retaining high accuracy. In this case study, we use the recently developed NeuralIL [1] ML-FF software to provide microscopic insight into the barocaloric (CH3)2NH2Mg(HCOO)3 system [2]. The simulations reveal the important role of methyl side group rotations in the vicinity of the phase transitions. The predictive phase transition temperature is also in close agreement with the experimental predictions, highlighting the potential of the method.

References
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