Classical Model Potential for Hybrid Perovskite (MYP)

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An interatomic model potential[1] for molecular dynamics is derived from first-principles and used to study the molecular rotations and relaxation times in methylammonium lead halide $CH_3NH_3PbI_3$, here considered as thee prototypical example of a hybrid crystal with a strong reorientational dynamics. Within the limits of a simple ionic scheme, the potential is able to catch the main qualitative features of the material at zero and finite temperature and opens the way to the development of classical potentials for hybrid perovskites. In agreement with experiments and previous theoretical findings, the molecule trajectories exhibit a transition from a dynamics dominated by high symmetry directions at low temperature to a fast dynamics at room temperature in which the molecule can reorient quasi- randomly.

[1] A. Mattoni, A. Filippetti, M.I. Saba, and P. Delugas, J. Phys. Chem. C 119, 17421 (2015).

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