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Study on the anharmonicity of the lead-halide bond and effective pair potentials of chlorine-substituted CH3NH3PbI3

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Research interest has increasingly focused on hybrid perovskites MABX3 like [CH3NH3]+ (MA), B = Pb and X = I or Cl as a future photovoltaic material. There is a strong demand to better understand the possible impact of various entropy contributions (stochastic structural fluctuations, anharmonicity and lattice softness) on the optoelectronic properties of halide perovskite materials and devices.1 There are essentially two sources of dynamic disorder in halide perovskites. One is the motion of the organic cations. FTIR [2] and quasi-elastic neutron scattering (QENS) [2] studies showed that chlorine substitution has a large influence on the rotational dynamics of the MA molecule in MAPbI3-xClx perovskites[3] since the chlorine substitution leads to a weakening of the hydrogen bridge bonds (these bonds connect the MA molecules with the [PbX6]- octahedra host structure).[3] Another source of dynamic disorder is the anharmonic motion of the halide atom. The analysis of the Pb L3-edge EXAFS Debye-Waller factor of chlorine-substituted MAPbI3 allows a direct determination of the influence of chlorine substitution on the anharmonicity of the lead-halide bond. This allows quantitative statements to be made about the effective pair potentials of the bond. The experimentally determined potential parameters can then be compared with computational results obtained, for example, from ab initio molecular dynamics simulations.

[1] Katan, C. et al, Nature Materials 2018, 17, 377
[2] G. Schuck, et. al., J. Phys. Chem. C, 2018, 122, 5227
[3] G. Schuck, et. al., J. Phys. Chem. C, 2019, 123, 11436

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