Highlights

Other Materials - 2015

Ferroelectric Polarization of $CH_3NH_3PbI_3$: A detailed Study Based on Density Functional Theory and Symmetry Analysis

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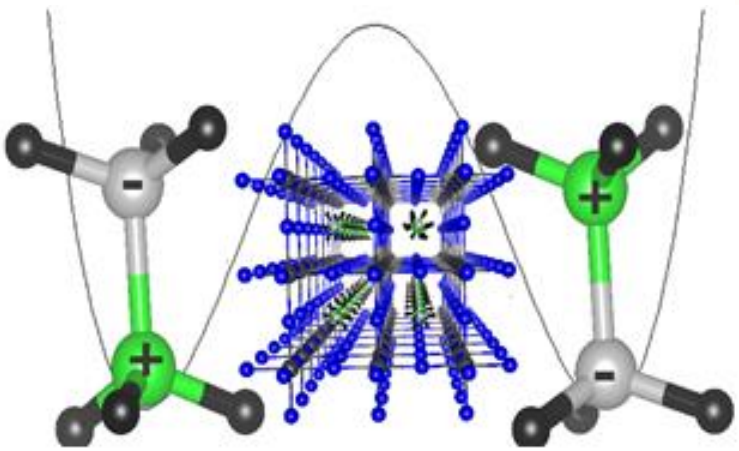
Ferroelectricity in halide perovskites currently represents a crucial issue, as it may have an important role for the enhancement of solar cells efficiency. Simulations of ferroelectric properties based on density functional theory are conceptually more demanding compared with “conventional” inorganic ferroelectrics due to the presence of both organic and inorganic components in the same compound. Here we present a detailed study focused on the prototypical $CH_3NH_3PbI_3$ perovskite. By using density functional theory combined with symmetry mode analysis, we disentangle the contributions of the methylammonium cations and the role of the inorganic framework, therefore suggesting possible routes to enhance the polarization in this compound. Our estimate of the polarization for the tetragonal phase at low temperature is ~4.42 μC/cm², which is substantially lower than that of traditional perovskite oxides.



Possible dipole ordering at low temperature in perovskite halides.