

Abstract Submitted
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Electric polarization of $CH_3NH_3PbI_3$ and enhancement by Cl substitution¹ WEN-LI YAN, Beihang University, University of Utah, GUANG-HONG LU, Beihang University, FENG LIU, University of Utah — As a prototype of organic-inorganic hybrid perovskite, $CH_3NH_3PbI_3$ has attracted extensive attention recently due to its applications in high power-conversion-efficiency solar cells. In comparison with its inorganic perovskite counterparts such as $CsPbI_3$, the organic cation $CH_3NH_3^+$ is expected to play multiple important roles in distorting crystal structures and thus band structures as well as creating local electrically polarized domains to help separate charge carriers. Using first-principles method and berry phase theory, the electric polarization vectors of $CH_3NH_3PbI_3$ have been calculated. The off-center displacement of Pb within the PbI_6 octahedral is shown to introduce major intrinsic polarization, with additional contributions from off-center displacement of $CH_3NH_3^+$ within PbI_3 cage and charge polarization within the organic cation. With chlorine substitution of iodine, the electronegativity difference between halogen and Pb becomes larger, and the lattice distortion and hence the electric polarization increases, which provides a possible mechanism to further assist charge carrier separation in solar cell devices. This is consistent with enhanced photovoltaics properties of $CH_3NH_3PbI_{3-x}Cl_x$ found in recent experiments.

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