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Effects of van der Waals Interaction on Structural and Electronic Properties of Methylammonium Lead Iodide Perovskites

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Methylammonium lead iodide ($MAPbI_3$) belongs to perovskite material class with chemical formula ABX_3, with A and B representing cations and X as anions. Ideal perovskite has cubic crystal structure with corner-sharing BX_6 octahedral network and A at the center of the octahedral cage. This hybrid organic-inorganic perovskite has recently gained intensive research interests due to their high efficiency as photovoltaic materials.

Our study employs density functional theory (DFT) to study the structural and electronic properties of cubic $MAPbI_3$. It has been shown in earlier studies that van der Waals interaction is crucial to DFT calculation accuracy regarding structural property determination. We investigate the importance of this non-local interaction and determine which van der Waals functional is suitable for DFT study $MAPbI_3$ systems.

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