Theoretical Study on Effect of Methylammonium Chloride Additive on Crystallinity of *α*-phase $FAPbI_3$ Perovskite for High-performance Solar Cell

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Organic-inorganic lead halide perovskite has received much attention for high-performance solar cell (*i.e.*, $>23\%_{efficiency}$). For achieving the high-performance, high crystallinity of cubic-phase (*α*-phase) perovskite structure should be obtained. Experimentally, by adding methylammonium chloride (MACl) additive, high crystalline *α*-phase $FAPbI_3$ perovskite was obtained, resulting in the very high-performance of solar cell (*i.e.*, $23.48\%_{certified\ efficiency}$). In this study, we investigated the roles of MACl additive in the formation of *α*-phase $FAPbI_3$ perovskite through density functional theory calculation. We found that MA and Cl thermodynamically stabilized the *α*-phase perovskite by enhancing the interaction between FA and I in cubo-octahedral structure composed by Pd and I in the *α*-phase perovskite. Moreover, the optimal concentration of MACl additive was traced for obtaining the high crystalline *α*-phase perovskite by calculating the doping formation energy of MACl into the perovskite and the formation energy of the perovskite including MAI. To this end, we revealed the roles of MACl additive in the formation of *α*-phase perovskite for high-performance solar cell.