Investigation of Stability Improvement of $FAPbI_3$ Through Cs Doping via DFT Calculation

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Perovskite solar cells (PSCs) are receiving much attention due to their increasing power conversion efficiency and low-cost materials. Nevertheless, PSCs are still not used commercially because of their low stability. Widely studied formamidinium (FA) perovskite has a problem that the photoactive black phase is thermodynamically stable only above 160 ℃. To solve this problem, researchers have studied mixed cation perovskite such as Cs doped FA perovskite and found it has high efficiency and good thermal stability. However, theoretical analysis on the effect of Cs doping has not been sufficiently done. Thus, this study was designed to identify the role of Cs doping using the density functional theory calculation. First, to investigate the stabilization of black phase $FAPbI_3$ through Cs doping, the difference of the formation energy between desired photoactive black phase and photoinactive yellow phase was compared by increasing Cs doping content. Then, the trap states were investigated by calculating the charged defect formation energy. Through this study, we proposed the most appropriate Cs doping content to improve the stability of PSCs by finding the origin of the trap states.