Post synthesis Mn-Doping in $CsPbI_3$ nanocrystals to stabilize black perovskite phase

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Abstract: Superior thermal stability of $CsPbI_3$ makes it more desirable for optoelectronic applications including solar cells. But optoelectronically active black perovskite phase of $CsPbI_3$ is thermodynamically not stabile at room temperature. Replacing Pb partially (~ 10 %) with Mn has been suggested to improve the stability of $CsPbI_3$ black perovskite phase of nanocrystals (NCs). Here, we addressed this issue by post synthesis Mn-doping and examined the structural stability at room temperature. Post-synthesis doping neglects additional effects of size/shape, surface energy, and ligand shell of host NCs allowing us to study effect of dopant in a more controlled manner. As a result doping Mn in black perovskite phase of $CsPbI_3$ NCs improves structural stability significantly from few days to more than one month under ambient. The prolonged stability of Mn-doped $CsPbI_3$ NCs is realized only in presence of Mn and least to surface passivation driven phenomenon. Both lattice contraction and higher bond dissociation energy of Mn-I compared to Pb-I in Mn-doped $CsPbI_3$ NCs increases the surface energy key to improve its structural stability.

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