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# Electronic structures and magnetic properties of transition metal doped $CsPbI_3$ perovskite compounds by first-principles calculation *

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Transition metal doped cesium lead halide ($CsPbI_3$) perovskite compounds were studied for application in photovoltaic solar cells. Electronic structures, chemical shifts of $^{207}$Pb and $^{127}$I-NMR, vibration modesin infrared and Raman spectra of transition metals ($Mn^{2+}$, $Fe^{2+}$ or $Cu^{2+}$)-doped $CsPbI_3$ perovskite compounds were studied by the first-principles calculation using density functional theory. The $CsPb(Fe)I_3$ perovskite crystals had a slight perturbation of crystal field in the coordination structure.The electron density distribution was delocalized on the 5*p* orbital of I atom, the 3*d* orbital of Fe atom and the 6*p* orbital of Pb atom. The first excited process was based on ligand metal charge transfer from the 5*p* orbital on I atom to the 3*d* orbital of Fe atom. The chemical shifts of $^{127}$I-NM Rwere associated with the electron correlation of electron-nuclear spin interaction and nuclear quadrupole interactions based on electron field graduate. The asymmetric vibrations of Pb-I bonds stretching mode related to electron conductivity with scattering of the carrier diffusion as phonon effectiveness. The slight perturbation of the coordination structure in the $CsPb(Fe)I_3$ perovskite crystal will improve the photovoltaic and optical properties.

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