Area: Area 5 Perovskite Solar Cells

ELECTRONIC STRUCTURES AND MAGNETIC PROPERTIES OF TRANSITION METAL DOPED PEROVSKITE COMPOUNDS FOR SOLAR CELL APPLICATIONS

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Perovskite based solar cells have great advantages of the photovoltaic performance with high conversion efficiency and optical properties, as optimizing with chemical elements of perovskite compounds. The elemental parameters of chemical composition ratio, chemical doping using halogen atoms, and crystal phase in the perovskite structures is an important factor to control the photovoltaic performance with high conversion efficiency [1]. Synthesis of photovoltaic materials using manganese (Mn) doped methylammonium lead halide ($CH_3NH_3PbI_3$) and cesium (Cs) lead halide perovskite compounds ($CsPbI_3$) have been studied for application of photovoltaic solar cell and spintronic devices [2].

The purpose of this work is to investigate the electronic structures and magnetic properties of transition metals (Mn^{2+}, Co^{2+}, and Cu^{2+})-doped cesium lead halide perovskite compounds ($CsPbI_3$) for photovoltaic and spintronic application. Roles of metals in the perovskite structure on the electronic structures, crystal structure, chemical shift, and optical absorption were studied by the first-principle calculation using density functional theory. The electronic structures, electron density of distribution, total density of states (DOS), and magnetic parameters of the transition metal-doped $CsPbI_3$ perovskite compounds will be discussed. The perovskite compounds form in a cubic crystal phase with a lattice constant of 6.36 Å. As shown in Fig. 1, the electron density distribution of sp^2 hybrid orbital were delocalized on the iodine halogen-atom at highest occupied molecular orbital (HOMO), and those of sp^2-3d hybrid orbital and sp^2 hybrid orbital were delocalized on metal atom and Pb atom at lowest unoccupied molecular orbital (LUMO). Effect of the crystal phase with varying lattice spacing in the perovskite structures on the band gap and optical absorption will be investigated. The absorption properties in the near-infrared region originated from ligand-metal charge transfer (LMCT) from 5p orbital of I atom to the 3d hybrid orbital in metal atom. The chemical shift in ^{127}I-NMR and magnetic parameters of metal atom depended on electronic correlation between 5p orbital of I atom and the 3d hybrid orbital on metal atom with nuclear quadrupole interaction. The photovoltaic mechanism will be explained by contribution of LMCT and electronic correlation between itinerant electron of 5p orbital in Pb atom and the 3d hybrid orbital of the metal atom. Collaboration of LMCT with magnetic interaction is important factor to develop the photovoltaic solar cell and spintronic devices.

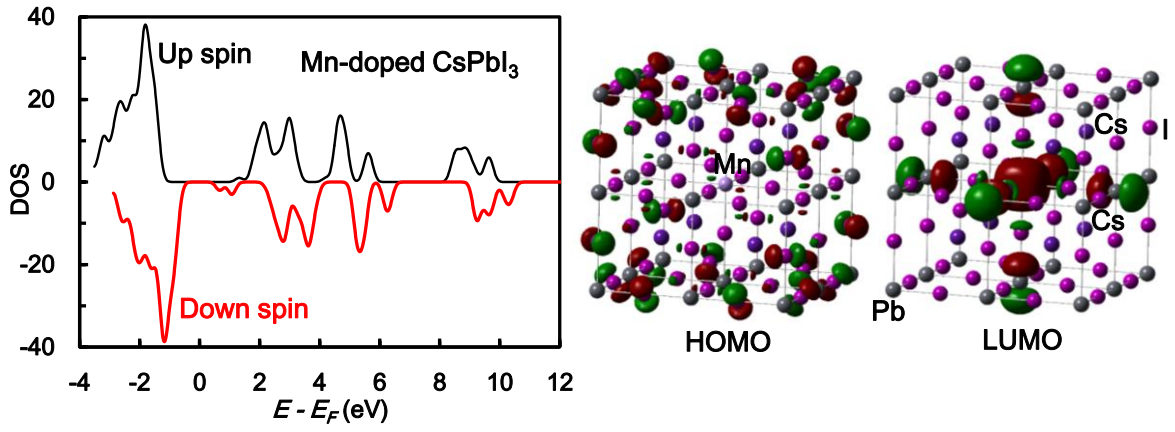

Figure 1. DOS and electron density distribution at HOMO and LUMO of Mn-doped $CsPbI_3$ perovskite compound.

References

[1] H.X. Zhu, J.-M. Li, *Scientific Reports* **6**, 37425 (2016).

[2] B. Náfrádi, P. Szirmai, M. Spina, H. Lee, O.V. Yazyev, A. Arakcheeva, D. Chernyshov, M. Gibert, L. Forró, E. Horváth. *Nature Communications* **7**, 13406 (2016).