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First-Principles Study on the Ferromagnetism of Mn-Doped LiZnAs Half-Heusler Compound

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We have investigated the magnetic properties of Mn-doped LiZnAs half-Heusler compound using density functional simulations within the gradient generalized approximation (GGA) with the on-site Hubbard U_{eff} parameter (GGA + U). A detailed study of magnetism in the two compounds GaAs and LiZnAs doped with Mn is presented. A super-cell of 64 and 96 atoms have been built for the zinc blend and the half-Heusler compounds, respectively. GGA + U calculations predict that the ferromagnetic state in LiZnAs : Mn compound with a magnetic moment of 3.51 μB per manganese is more appropriate in energy than the anti-ferromagnetic state. The topological similarity between GaAs and LiZnAs non-magnetic compounds is also confirmed in these Mn-doped systems. The band structures and densities of states show that the Mn-doped half-Heusler LiZnAs has become a dilute magnetic semiconductor with a direct gap of 0.43 eV. The cubic symmetry and distances between the dopant pairs (Mn) are two key factors to predict the character and the magnetic order of Mn-doped LiZnAs system.

Keywords: LAPW + LO, DFT + U, impurity defects, magnetic properties, ferromagnetic semiconductor.