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Density Functional Study of the Electronic Structure and Magnetism of LaFeAsO alloyed with Zn[1] LIJUN ZHANG, DAVID SINGH, Oak Ridge National Laboratory — The effect of substitution of Fe by the non-magnetic $3d$ element, Zn in LaFeAsO is investigated by first-principles supercell calculations. As expected, Zn occurs in a d^{10} configuration, with the d states fully occupied at higher binding energy in $LaFe_{1-x}Zn_xAsO$, similar to the pure Zn compound LaZnAsO. This is highly disruptive to the electronic structure of LaFeAsO near the Fermi energy, which is dominated by the partially filled Fe d shell. Further, this favors localization, the formation of moments on the Fe atoms in proximity to the Zn, and magnetic states that compete with the spin density wave. These results are discussed in relation to experimental observations for Zn substituted LaFeAsO.

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