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Bonding, magnetic properties and stability of the half-Heusler alloys LiMnZ (Z=N, P, Si)[1] LIAM DAMEWOOD, BRIAN BUSEMEYER, C.Y. FONG, University of California, Davis, MICHAEL SHAUGHNESSY, Sandia National Laboratories at Livermore — We examined the bonding and magnetic properties, as well as the stability, of three magnetic half-Heusler alloys, namely LiMnZ, with Z=N, P or Si, in the three different atomic ordering of the $C1_b$ crystal structure (i.e. α, β, and γ phases). Using LiMnP as a prototype, we examined the bonding properties of the three phases and found, at the optimized lattice constant, each phase is a ferromagnetic metal. Assuming a proper matching substrate could be found, we found that α-LiMnN, LiMnSi in the β and γ phases, and LiMnP in the α and β phases can be ferromagnetic half-metals at lattice constants larger than the optimized values. Volume stability studies showed that the β phase is the most stable for these materials. In our search for more half-metals, we found that β-$Li_{0.75}$MnSi, β-$Li_{0.75}$MnP and γ-$Li_{0.75}$MnN can be half-metals at the respective LiMnSi half-metallic lattice constants. By comparing β-LiMnP to the metastable zinc blende phase of MnP, the role of Li in the structure, with respect to the elastic stability, electronic properties, and magnetic properties, was studied. Finally we examined the possibility of a compensated half-metallic phase in these materials.

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