

Abstract Submitted
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Exploring Half Metals in Li-based Half Heusler Alloys¹ B. BUSEMEYER, University of California, Davis, CA 95616, M. SHAUGHNESSY, Sandia National Laboratories, Livermore, CA 94551, C. Y. FONG, University of California, Davis, CA 95616 — We examine the electronic and magnetic properties of three Li-related half Heusler alloys, namely LiMnN, LiMnP, and LiMnSi in a structure close to the well-known zinc-blende structure in the attempt to search for new half metallic materials. If they do demonstrate half metallic properties, this will open new grounds for finding half metallic spintronic materials. Our results will furnish guidelines for future exploration of alkali-related half metals. Using the primitive cell LiMnSi is a half metal, while the pnictides are not. However when the conventional cell is used, we find that $\text{Li}_3\text{Mn}_4\text{P}_4$ and $\text{Li}_3\text{Mn}_4\text{N}_4$ are half metals. The physical reason for these two pnictides to be half metallic and for their magnetic moment per unit cell will be presented.

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