

Abstract Submitted  
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**Exploration of Electron Poor Materials and their thermoelectric properties** DARYN BENSON, ULRICH HAUSSERMANN, OTTO SANKEY, Arizona State University — The Electron Poor Materials (EPM); ZnSb, ZnAs which have an average 3.5 valence electrons are explored via ab initio calculations. These materials are of interest for thermoelectric research. The EPM are then compared to valence balanced zinc-blende materials; InSb, GaSb, ZnSe, and ZnTe. Analysis of binding to assess the interesting electronic properties such as the role of non-classical four-center bonds and the thermoelectric Seebeck coefficient are discussed. Bandstructure comparisons to a simple tight-binding model (Linear Combination of Atomic Orbitals (LCAO)) are performed in order to test the effects of the atomic orbitals on the electronic structure.

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