Mechanical Engineering Thesis Defense

Quantum Mechanical Study of the Electronic Structure and Thermoelectric Properties of Heusler Alloys

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Abstract

Heusler alloys were discovered in 1903, and materials with half-metallic characteristics have drawn more attention from researchers since the advances in semiconductor industry. Half-metallic materials are useful in semiconductor chip design as they can be used as gated layers due to their tunable electrical conductivities to control the electrical current in the semiconductor wafers. In this work, the electronic structures, phonon dispersion, thermal properties, and electrical conductivities of seven novel alloys (AuCrSn, AuMnGe, PdMnSn, Au2MnSn, Cu2NiGe, Pd2NiGe and Pt2CoSn) along with their magnetic moments are studied using ab-initio calculations to understand the roots of half-metallicity in these alloys of Heusler family. From the phonon dispersion, the thermodynamic stability of the alloys in their respective phases is assessed. Phonon modes were also used to further understand the electrical transport in the crystals of these seven alloys. This study evaluates the relationship between materials' electrical conductivities and bandgaps at the Fermi level in minority spin configuration of band structure, and it provides suggestions for selecting constituent elements when designing new half-metallic Heusler alloys of C1b and L21 structures.

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