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"Study of Thermoelectric Properties of Half-Heusler Phases:
***ab initio* and Machine Learning Analysis"**

Abstract

This doctoral dissertation is a continuation of past theoretical research related to the potential application of half-Heusler (hH) compounds as thermoelectric (TE) materials [1-3].

The high-throughput investigation with the use of Density Functional Theory (DFT) of over 150 hH phases with 18 valence electrons was performed, including two Exchange-Correlation (XC) functional parametrizations: Perdew-Burke-Ernzerhof (GGA) and modified Becke-Johnson GGA (MBJGGA) [4, 5]. Among the initial set of hH phases, over 120 systems were found to be semiconductors, whereas only 34 hH systems have been identified as novel and thermodynamically stable [6]. The detailed analysis of named systems (e.g., electronic structures) and their TE properties (including two XC functional approaches and two types of conductivity regimes) is undertaken in this doctoral dissertation.

The *ab initio* research has been supported through Machine Learning (ML) methods. The analysis and predictions were done for six different targets, including band gaps [7] and TE performance (TE Power Factor for GGA parametrization and p-type regime) [8]. The chemical trends and potential predictors in all the cases were examined in detail.

The overall findings from DFT and ML analysis conducted here on the hH phases infer novel hH phases as candidates for TE materials and some insights into the crucial predictors for their favorable TE performance.