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FIRST PRINCIPLES INVESTIGATION OF ENERGY HARVESTING MATERIALS FOR GREEN ENVIRONMENT

by

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Abstract

The cutting-edge research of materials enables the discovery of novel energy harvesting materials. In this project the structural, electronic, magnetic, thermodynamic, thermoelectric, and optical properties of different energy harvesting materials are studied. The main objective of this work is primarily to study thermoelectrically efficient Half-Heusler and photovoltaically active Perovskites. Variant schematics of innovative compounds with defect introduction are investigated. The compositionally altered compounds designed by introducing crystallographic defects in terms of substitutional or interstitial dopants, offer new trends of material properties. To accomplish the task, Density Functional theory based computational packages (VASP and Wein2K) are used. Using defect and strain engineering, this study explores thermoelectric and photovoltaic properties. Our goal is to computationally design and study half-Heusler and perovskite for thermoelectric, solar applications, and green energy productions. The computational simulations, along with the obtained results are consistent with the previous studies to give a better understanding of the perovskites and half-heuslers.

Keywords: Density functional theory, Half-Heuslers, Perovskites, Solar Cells, Dopants