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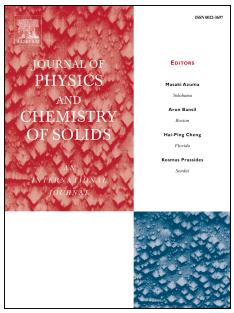

Analysis of electronic, thermal, and thermoelectric properties of the half-Heusler CrTiSi material using density functional theory

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Analysis of Electronic, Thermal, and Thermoelectric Properties of the Half-Heusler CrTiSi Material using Density Functional Theory

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Abstract

In this study, we investigated the electronic structure, thermal, and thermoelectric properties of half-Heusler CrTiSi based on first-principles calculations. CrTiSi is an indirect band gap semiconductor with a band gap of 0.65 eV in the spin-up state. The presence of flat energy bands along the L and X directions indicates large effective masses for the charge carriers. CrTiSi has promising thermoelectric properties according to the high Seebeck coefficient, very larger power factor, and moderate thermal conductivity at room temperature with values of ~128 μV K^{-1}, 0.3 (10^{12} Wm^{-1} K^{-2} s^{-1}), and 1.25 W mK^{-1}, respectively. The effects of high pressure up to 35 GPa were determined on thermal properties comprising the crystal volume, thermal expansion coefficient, heat capacity, and Grüneisen parameter. Our results demonstrate that CrTiSi is a strong candidate for use in thermoelectric applications over an extensive temperature range.

Keywords: Grüneisen parameter; Lattice thermal conductivity; Power factor; Seebeck coefficient

Introduction

Thermoelectric materials directly convert waste thermal energy into useful electrical energy and they could have crucial roles in averting the energy crisis, as well as in decreasing the emissions of greenhouse gases, i.e., by serving as green energy sources [1-4]. Many materials have been designed with high conversion efficiency for use in automobiles and Peltier coolers [5-6]. However, the main issue that prevents increases in the efficiency of these materials is the dependency of their properties on each other because there are tradeoff relationships between various properties. In general, the efficiency of a thermoelectric material is represented by the figure of merit (*ZT*) [7-9]:

$$ZT = S^2\sigma T/\kappa$$