Ab initio Investigation of Structural, Electronic, Elastic, and Mechanical Properties of New Double Half-Heusler Alloys

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Abstract

Half-Heusler alloys have become an intriguing class of materials with significant potential for various technological applications, thanks to their unique blend of properties. In this research, we performed computational analysis on the double half-Heusler compounds Ti2Pt2ZSb (Z=Al, Ga, In) using two density functional theory (DFT) methodologies: Generalized Gradient Approximation (GGA) and meta-Generalized Gradient Approximation (metaGGA-SCAN).

Investigating double half-Heusler alloys is highly relevant due to their potential for advancing materials science and technology. These alloys exhibit a unique combination of properties, including semiconducting behavior, magnetic properties, and promising thermoelectric performance. Understanding and optimizing these properties can lead to innovative applications in various fields such as energy conversion, spintronics, and thermoelectric devices. Moreover, double half-Heusler alloys offer tunable electronic band structures and can be tailored for specific functionalities through careful material design and synthesis. Investigating these alloys using computational modeling and experimental techniques provides valuable insights into their electronic, magnetic, and structural characteristics, paving the way for the development of next-generation materials with enhanced performance and functionality. Thus, research on double half-Heusler alloys is pivotal for advancing materials design and enabling the realization of novel technologies with improved efficiency and versatility.

The integration of computational modeling techniques, such as density functional theory (DFT), plays a pivotal role in this research by providing insights into the electronic structure, stability, and properties of double half-Heusler alloys. This computational approach complements experimental investigations, enabling researchers to predict and design new alloy compositions with desired properties for targeted applications.

In summary, the investigation of double half-Heusler alloys holds substantial promise for advancing materials science and driving innovation in diverse technological areas, ranging from energy conversion and spintronics to advanced electronic and magnetic devices. Continued research efforts in this field are essential for harnessing the full potential of these intriguing materials and translating them into practical solutions for real-world challenges.

Keywords

Heusler alloys, density functional theory, electronic properties, density of states.