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STRUCTURAL, ELECTRONIC, AND MECHANICAL PROPERTIES OF NISCTE HALF-HEUSLER COMPOUND

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Abstract

Background: Half-Heusler compounds have attracted significant attention due to their diverse physical properties and potential applications in electronic and functional materials. Among them, Ni-based systems are particularly interesting because of their structural stability and tunable electronic behavior.

Objectives: This study presents a theoretical investigation of the NiScTe Half-Heusler compound using density functional theory (DFT), focusing on its structural, mechanical, and electronic properties.

Methods: Calculations were performed using the WIEN2k package within the framework of DFT. The full-potential linearized augmented plane wave (FP-LAPW) method was employed, and exchange–correlation effects were treated using the generalized gradient approximation (GGA). Structural optimization was carried out to determine the most stable configuration, followed by evaluation of elastic constants and electronic properties.

Results: The results indicate that NiScTe crystallizes in the cubic C1b phase (space group $F\bar{4}3m$) and adopts the most energetically stable configuration. The calculated lattice parameter falls within the typical range for Half-Heusler compounds, confirming the reliability of the findings. The computed elastic constants satisfy mechanical stability criteria, indicating that the compound is mechanically stable. Additionally, the evaluated elastic moduli suggest ductile behavior, while anisotropy analysis reveals direction-dependent mechanical properties. Electronic band structure and density of states (DOS) calculations show metallic behavior, evidenced by the crossing of energy bands at the Fermi level and a finite DOS at the Fermi level, indicating the presence of intrinsic charge carriers without the need for thermal excitation.

Conclusions: The NiScTe Half-Heusler compound exhibits structural stability, ductile mechanical behavior, and metallic electronic properties, making it a promising candidate for applications in electronic and functional materials.

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Keywords: Half-Heusler; FP-LAPW; DFT; Elastic properties; Electronic properties.

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