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A First-Principles Study of the Structural, Mechanical, Dynamical and Electronic properties of HfSnPt: Half-Heusler Structure

The density functional theory (DFT) is applied to systematically investigate the geometrical structure, electronic, mechanical, vibrational, and optical properties of half-Heusler HfSnPt in its cubic phase. To the best of one's knowledge, many physical properties of this compound are still not well established or not yet investigated; such as phonon properties, mechanical behavior, thermal properties, and so on. In this work, the stability of HfSnPt is explored by looking at its thermodynamical behavior through calculation of formation energy, cohesive energy, and phonon dispersion. HfSnPt compound shows a negative heat of formation, indicating thermodynamic stability, which is consistent with it's cohesive energy. Its mechanical properties are examined based on various characterization descriptors such as the independent elastic coefficients, bulk, shear, and Young's modulus, ratios such as Pugh and Poisson's, Kleinnman parameter, Zener anisotropy factor, Debye temperature, and melting temperature. The equilibrium elastic constants satisfy all the mechanical stability criteria for cubic crystals. The analysis of band structures, along with total and partial density of states, reveals that HfSnPt structure is semiconductor with indirect band gaps of 0.910 eV for HfSnPt. Finally, the phonon calculations confirm that HfSnPt is dynamically stable. This compound exhibits thermodynamic, mechanical, and dynamic stability, along with a high melting point, making it a strong candidate for high-temperature structural applications.

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