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Investigation on Structural, Electronic and Thermoelectric Properties of Half-Heusler Compounds TiXSb (X = Si, Ge) under Pressure Based on Density Functional Theory (DFT)

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Structural, electronic, and thermoelectric properties of TiXSb (X = Si, Ge) at 0, 5, 10, and 15 GPa pressures based on density functional theory have been investigated. Structural properties at 0 GPa are in accord with other theoretical and experimental works. In electronic properties at 0 GPa, Ti-d^2 orbitals have main contributions near the Fermi energy in valence band and in conduction band. According to our calculations in diagrams of electronic density of states at different pressures, by increasing pressure, peaks in the valence band move to more negative energies. However, in the conduction band, they move to more positive energies. This occurs as a result of decreasing stability of the system due to increase in pressure. In this study, we also calculated the thermoelectric properties such as Seebeck coefficient electronic thermal conductivity divide by relaxation time, electrical conductivity divide by relaxation time and figure of merit by ignoring low contribution of phonon thermal conductivity at pressures 0, 5, 10, and 15 GPa, in the temperature range of 100−900 K.

Keywords: thermoelectric properties, half-Heusler compounds, density functional theory, electronic properties