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Structural, elastic, electronic, bonding, and optical properties of PtBiTe and PtBi₂ structures.

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In recent days, semimetals have become an active branch of materials research. The Platinum Group Mineral (PGM) semimetal Insizwaite (PtBi₂) and Maslovite (PtBiTe) are polymorphic systems with interesting electronic properties. Here we report the optimised crystals belonging to the pyrite-type cubic structure which are important electronic systems to investigate both from the point of view of fundamental physics and prospective applications. We have employed the density functional theory (DFT) to investigate the structural, elastic, mechanical, electronic, bonding and optical properties of PtBi₂ and PtBiTe. Calculations of elastic constants and moduli indicated that PtBi₂ and PtBiTe possess a low level of elastic anisotropy, reasonably good machinability, mixed bonding characteristics with ionic and covalent contributions, brittle nature and relatively high Vickers hardness with a low Debye temperature. The mechanical stability conditions were fulfilled. Analysis of bond population supported the bonding nature as indicated by the elastic parameters. The bulk electronic band structure revealed clear semi-metallic features with signature Dirac cone-like dispersions near the Fermi level. A pseudo gap in the electronic energy density of states at the Fermi level separating the bonding and the antibonding peaks point towards significant electronic stability of cubic of PtBi₂ and PtBiTe. The Fermi surface mostly consisted of electron-like sheets with very few small hole pockets. The band structures were isotropic in the k-space. The optical constants indicated interesting characteristics. Furthermore, all the energy-dependent optical parameters exhibited clear metallic signatures and were in complete accord with the underlying bulk electronic density of states calculations. we calculate the electronic band structure using the obtained structure parameters. These findings warrant further research using a broader array of experimental techniques.

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No

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