ab-intio study of anisotropic properties in isomorphic TiX2 (X=S, Se, Te)

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Abstract

Isomorphic titanium dichalcogenide TiX2 (X=S, Se, Te) compounds exhibit very diverse and anisotropic chemical and physical properties. The temperature dependent electrical resistivity of TiSe2 was found to exhibit anomalous behavior at low temperatures (< 200 K) which was connected to the emergence of a unique charge density wave (CDW), which was explained on the basis of 2a0×c0 superstructure formation, whereas bulk TiS2 and TiTe2 do not exhibit CDW instability. In order to understand their diverse nature, we have systematically investigated the electronic structure of titanium dichalcogenides by using the FPLAPW and PAW methods based on the density functional theory (DFT). The energy bands calculated by implementing the latest generalized gradient approximation (GGA) with PBE and TB-mBJ potentials confirm the semiconducting nature of TiS2 and metallic nature of TiSe2 and TiTe2, however the Wu-Cohen potentials show a semi-metallic nature for all three dichalcogenides. The diverse properties of TiX2 are governed by two bands, S/Se/Te p-band close to the Γ-point and Ti 3d-band around M (L)-points. The presence of electron and hole pockets at the Fermi energy level have been previously confirmed experimentally, although our calculated size and extent of overlap of these pockets was overestimated compared to experiments. Various physical parameters such as electrical conductivity, Seebeck coefficient etc. which depend sensitively on nature of states at the Fermi level also amply illustrate the diversity of the compounds. The electron localization function and Bader charge partitioning illustrate the increasing covalency with varying chalcogenide atom, which is consistent with the spectral features observed in the DOS. The lattice dispersion of the titanium dichalcogenides are calculated by using the PAW method with PBE potentials. The phonon band structure is correlated to the electronic band structure in order to explain the occurrence of CDW. In TiSe2, the presence of a phonon mode with imaginary frequency indicated lattice instability against distortion. The displacements of Ti-Se atoms of this phonon mode allows the mixing of states of the electron and hole pockets, which leads to lattice distortion i.e. a CDW structure which lowers the energy of the system. Although there is a weak imaginary mode, the mixing of states is absent in TiS2 due to absence of electron or hole pockets, whereas TiTe2 is structurally most stable.

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