

# Band Structures of IV-VI Materials From Advanced DFT Calculations

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The discovery of topological insulators is one of the most important recent developments in condensed-matter physics. In these new quantum materials, time-reversal symmetry and strong relativistic (spin-orbit) effects require that the bulk insulating states are accompanied by metallic helical Dirac-like electronic states on the surface of the crystal. These surface states are encoded in topologically non-trivial wave functions of valence electrons. Similar properties could also result from point-group symmetries of the crystal lattice. Materials that have nontrivial topology protected by point-group symmetries, in particular IV-VI narrow-gap semiconductors which host metallic surface states protected by the mirror symmetry of the crystals rock-salt structure, are called topological crystalline insulators [1]. Recently, the discovery that solid solutions of lead and tin chalcogenides (selenides and tellurides) are perfect objects for the study of phase transition between the normal narrow-gap semiconductor state and topological crystalline insulator, started intensive studies of these materials, both experimental and theoretical.

The theoretical description of the behavior of the surface states in the solid solutions of IV-VI materials requires a detailed knowledge of the electronic structure of such ternary alloys. For this purpose the tight-binding approach seems to be the most suitable [2,3], however, in the case of PbSe:SnSe the semi-empirical tight-binding parameterization constitutes a serious problem. Namely, for the tight-binding description of this alloy the band structure of SnSe in rock-salt structure is needed, because all studied mixed crystals with up to 40% of the Sn content have rock-salt structure. However, such band structure cannot be verified experimentally as in reality SnSe itself crystallizes in another, octahedral structure. Thus, it can be only anticipated by first-principle theoretical methods.

The aim of our analysis is to determine the best possible band structure for the rock-salt SnSe crystals. For this purpose we calculate first the band structure of other well-known IV-VI materials, like PbTe, PbSe or SnTe, using various advanced methods based on density functional theory. This includes methods based on modified Becke-Johnson exchange potential, the quasiparticle concept and Green function method (*GW* approximation) as well as on hybrid functionals (in particular Heyd-Scuseria-Ernzerhof screened Coulombic hybrid functional). We compare the obtained results with the known experimentally values of the energy gaps and effective masses for these materials to verify the accuracy of used methods and to choose the most proper one for obtaining band structure of rock-salt SnSe.

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