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Sixteen-band atomic bond-orbital model for zinc-blende structures HSIU-FEN KAO, JIH-CHEN CHIANG, W.T. WANG, IKAI LO, Y.C. HSU, C.L. WU, D.J. JANG, Department of Physics, National Sun Yat-sen University, Kaohsiung 80424, Taiwan, MENG-EN LEE, C.Y. REN, YEN-CHIH TSENG, Department of Physics, National Kaohsiung Normal University, Yanchao, Kaohsiung County 82444, Taiwan, CHUN-NAN CHEN, Department of Physics, Tamkang University, Tamsui, Taipei County 25137, Taiwan — We develop a sixteen-band atomic bond-orbital model (16ABOM) which is able to compute the spin splitting induced by bulk inversion asymmetry. This model is derived from the linear combination of atomic orbital (LCAO) scheme such that the characteristics of real atomic orbitals can be preserved for spin-splitting calculations. We derive the Hamiltonian of 16ABOM by performing a similarity transform on the nearest-neighbor LCAO Hamiltonian, followed by taking a second-order Taylor series expansion over k-vector at the Γ point. The spin-splitting energies in bulk zinc-blendes are calculated using this model, and the results are in good agreement with LCAO and first-principles calculations. In addition, it is found the spin-orbit coupling between anti-bonding and bonding p-like states, which can be evaluated directly by this 16ABOM, dominates the magnitude of the spin splitting of the lowest conduction bands in middle-bandgap and wide-bandgap materials.

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