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Bond-orbital models for wurtzite semiconductors WAN-TSANG WANG, IKAI LO, SHIOW-FON TSAY, MING-HONG GAU, JIH-CHEN CHIANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan 80424, Republic of China — A simple theoretical method for calculating electronic band structures of wurtzite materials based on the bond-orbital model is presented. This method can be used to study many problems such as band mixing and effects of external fields (electric field, magnetic field, and unaxial stress, etc.), since it can reproduce fairly accurate lowest conduction-band and top three valence-band structures. This method is very similar to LCAO method; however, it is much simpler and requires less computational effort than LCAO method.

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