Bond-orbital models for wurtzite semiconductors

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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 struc-
tures. 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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Date submitted: 01 Dec 2004
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