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Accurate Electronic, transport, and Related Properties of Wurtzite Beryllium Oxide (w-BeO)[1] CHEICK BAMBA, RICHARD INAKPENU, YACOUBA DIAKITE, YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, DIOLA BAGAYOKO, Department of Mathematics and Physics, Southern University and AM College, Baton Rouge, LA 70813, USA — We present ab-initio, self–consistent density functional theory (DFT) description of electronic and related properties of wurtzite beryllium oxide (w-BeO). We used a local density approximation (LDA) potential and the linear combination of atomic orbitals (LCAO) formalism. Our implementation of the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF), ensures the full, physical content of the results of our calculations [AIP advances, 4, 127104 (2014). We report the band gap, the total and partial densities of states, and effective masses. Our calculated, direct band gap of 10.29 eV, using experimental lattice constants of a = 2.6979 and c = 4.3772 at room temperature, agrees with some experimental ones of 10.3 eV and not with others (7.8, 8.8, 9.6 10.45, and 10.6 eV).

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