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Accurate Electronic, Transport, and Bulk Properties of Wurtzite Beryllium Oxide (BeO) CHEICK OUMAR BAMBA, YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813 — We present *ab-initio*, self-consistent density functional theory (DFT) description of electronic, transport, and bulk properties of wurtzite Beryllium oxide (w-BeO). We used a local density approximation potential (LDA) and the linear combination of atomic orbitals (LCOA) 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 our local density approximation (LDA) calculations – as per the derivation of DFT [AIP Advances, 4, 127104 (2014) We report the band gap, density of states, partial density of state, effective masses, and the bulk modulus. Our calculated band gap of 10.29 eV, using an experimental, room temperature lattice constant of 2.6979 A at room temperature is in agreement with the experimental value of 10.6 eV. Acknowledgments**:** This work was funded in part the US National Science Foundation [NSF, Award Nos. EPS-1003897, NSF (2010-2015)-RII-SUBR, and HRD-1002541], the US Department of Energy, National Nuclear Security Administration (NNSA, Award No. DE-NA0002630), LaSPACE, and LONI-SUBR.

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