Abstract Submitted
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**Accurate Electronic and Transport Properties of Bulk wurtzite Beryllium Oxide (w-BeO)**[1] CHEICK BAMBA, LASHOUNDA FRANKLIN, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Southern University 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 states, effective masses, and bulk modulus. Our calculated band gap of 10.29 eV, using an experimental lattice constant of 2.6979 at room temperature is in agreement with the experimental value of 10.6 eV.

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