Abstract Submitted
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Ab-initio Computations Of Electronic, Transport, And Structural Properties Of Zinc Blende Beryllium Selenide (Zb-bese).[1] RICHARD INAKPENU, CHEICK BAMBA, IFEANYI NWIGBOJI, LASHOUNDA FRANKLIN, YURIY MALOZOVSKY, GUANG-LIN ZHAO, DIOLA BAGAYOKO, Department of Mathematics and Physics, Southern University and AM College, Baton Rouge, Louisiana, 70813, USA — We report results from several ab-initio, self-consistent computations of electronic, transport and bulk properties of *zinc blende* beryllium selenide (*zb*-BeSe). Our non relativistic calculations utilized a local density approximation (LDA) potential and the linear combination of atomic orbitals (LCAO). The key distinction of our calculations from other DFT ones is our implementation of the Bagayoko, Zhao and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). Our calculated, indirect band gap is 5.46 eV, from to a conduction band minimum between and X, for a room temperature lattice constant of 5.152 Å. Available, room temperature experimental band gaps of 5.5 eV (direct) and 4.0 – 4.5 eV (unspecified) point to the need for additional measurements. Our calculated bulk modulus of 92.35 GPa is in excellent agreement with experiment (92.2 ± 1.8 GPa). Our predicted equilibrium lattice constant and band gap, at zero temperature, are 5.0438 Å and 5.4 eV, respectively.

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