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A Correct, Density Functional Description of Semiconductors[1] D. BAGAYOKO, G. ZHAO, L. FRANKLIN, H. JON, Southern University and A&M College — The profusely reported inability of some density functional calculations to describe correctly the band gaps of semiconductors has been ascribed to the derivative discontinuity of the exchange correlation energy, the self-interaction associated with approximate potentials, and other factors, i.e., pd repulsion in the case of wurtzite InN. From 1998 to present, we have studied several semiconductors with local density approximation (LDA) and generalized gradient approximation (GGA) potentials. Upon applying the Bagayoko, Zhao, and Williams (BZW) method to the implementation of the linear combination of atomic orbital (LCAO) formalism, we have obtained band gaps and electron effective masses in excellent agreement with experiment for $BaTiO_3$, GaN, GaAs Si, Ge, 3C-SiC, 4H-SiC, ZnSe, ZnO, carbon nanotubes, InN, and AlAs among others. This ab-initio method avoids a basis set and variational effect inherently associated with LCAO calculations – irrespective of the selected potential. We present a summary of the BZW method and of the aforementioned results, including *the correct description of low-lying conduction bands as verified by agreements with measured optical transition energies and dielectric functions.* These results clearly point to an urgent need to revisit (a) the above presumed causes of reported failures of DFT and (b) computational methods suffering from the identified and well-defined basis set and variational effect.

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