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Abs-initio, Predictive Calculations for Optoelectronic and Advanced Materials Research[1]

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Most density functional theory (DFT) calculations find band gaps that are 30-50 percent smaller than the experimental ones. Some explanations of this serious underestimation by theory include self-interaction and the derivative discontinuity of the exchange correlation energy. Several approaches have been developed in the search for a solution to this problem. Most of them entail some modification of DFT potentials. The Green function and screened Coulomb approximation (GWA) is a non-DFT formalism that has led to some improvements. Despite these efforts, the underestimation problem has mostly persisted in the literature. Using the Rayleigh theorem, we describe a basis set and variational effect inherently associated with calculations that employ a linear combination of atomic orbitals (LCAO) in a variational approach of the Rayleigh-Ritz type. This description concomitantly shows a source of large underestimation errors in calculated band gaps, i.e., an often dramatic lowering of some *unoccupied energies* on account of the Rayleigh theorem as opposed to a physical interaction. We present the Bagayoko, Zhao, and Williams (BZW) method [Phys. Rev. B 60, 1563 (1999); PRB 74, 245214 (2006); and J. Appl. Phys. 103, 096101 (2008)] that systematically avoids this effect and leads (a) to DFT and LDA calculated band gaps of semiconductors in agreement with experiment and (b) theoretical predictions of band gaps that are confirmed by experiment. *Unlike most calculations, BZW computations solve, self-consistently, a system of two coupled equations.* DFT-BZW calculated effective masses and optical properties (dielectric functions) also agree with measurements. We illustrate ten years of success of the BZW method with its results for GaN, C, Si, 3C-SIC, 4H-SiC, ZnO, AlAs, Ge, ZnSe, w-InN, c-InN, InAs, CdS, AlN and nanostructures. We conclude with potential applications of the BZW method in optoelectronic and advanced materials research.

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