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A Mathematical Solution to the Theoretical Band Gap Underestimation: Predictive Calculations of Properties of Semiconductors[1]

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Most density functional theory (DFT) calculations find band gaps that are 30-50 percent smaller than the experimental ones, as illustrated in this presentation that recalls some popular explanations of this band gap problem, i.e., self-interaction effects and derivative discontinuities of the exchange correlation energy. A survey of the increasingly numerous approaches aimed at resolving the theoretical underestimation follows these explanations. These approaches include the Green function and screened Coulomb approximation (GWA), time dependent density functional theory (TDDFT), the exact exchange and screened exchange methods, and the use of local density approximation (LDA) potentials plus additional potentials located at atomic sites. 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 the Hamiltonian. We present the Bagayoko, Zhao, and Williams (BZW) method [Phys. Rev. B 60, 1563 (1999); PRB 74, 245214 (2006); and PRB 76, 037101 (2007)] that follows from the description of the aforementioned effect and that 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, InAs, and AlN. We conclude with a request to revisit beliefs relative to actual limitations of DFT and of schemes purporting to correct it or to go beyond it.

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