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A Solution to the Band Gap and Related Problems in Density Functional Theory (DFT).[1] DIOLA BAGAYOKO, Department of Mathematics and Physics, Southern University and AM College, Baton Rouge, Louisiana, 70813, USA — This presentation shows that the attainment of self-consistency, with a single basis set, does not allows one to reach results that possess the physical content of density functional theory (DFT). This fact is amply illustrated in the literature where reported DFT eigenvalues appear not to correspond to actual energy levels in materials under study. Our proof includes an understanding of the second Hohenberg-Kohn (HK) theorem that requires the use of successively larger and embedded basis sets to perform completely self-consistent calculations in order to reach the absolute minima of the occupied energies, i.e., the ground state of the system. Embedding here means that, except for the first one, each basis set is obtained by augmenting the one preceding it with one orbital. We also show that arbitrarily large basis sets, by virtue of the first HK theorem, are over-complete for the description of the ground state: This fact explains the well-known underestimation of energy and band gaps by single basis set calculations for the last 50 years. The non-attainment the ground state et the over-completeness of some large basis set explain the inaccuracy of calculated, optical transition energies, effective masses, dielectric functions and of a host of other computational results.

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