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The Physical Content of Eigenvalues from Density Functional Theory (DFT) D. BAGAYOKO, L. FRANKLIN, Department of Physics, Southern University and A&M College, C. EKUMA, Department of Physics and Astronomy, Louisiana State University, Y. MALOZOVSKY, Department of Physics, Southern University and A&M College — The density functional theory (DFT) of Hohenberg and Kohn rests on the energy functional $E_v[n]$ assuming its minimum for the *correct density* n(**r**), with the admissible functions restricted by the condition$N[n] = \int n(r)dr = N$, where N is the number of particles in the system under study. We show that, for such a system, there is an infinite number of basis sets (of localized orbitals) for which N is fixed while the density is not necessarily the correct one. Consequently, the eigenvalues obtained with self consistent DFT calculations using a single basis set do not necessarily have any particular physical content. The physical content is ensured only by the search and utilization of *the optimal basis set* that yields *the minima of the occupied energies* and physically meaningful values of low laying unoccupied energies. Further, by virtue of the Rayleigh theorem, there exist many basis sets larger than the optimal one [and that contain it] for which some unoccupied energies are lowered on account of a mathematical artifact. We illustrate these points in the cases of ZnO, TiO_2, and $SrTiO_3$. The calculated band gaps and other properties of these materials are in excellent agreement with experiment. Work funded by in part by the National Science Foundation, through LASiGMA [NSF AwardEPS-1003897, No. NSF (2010-15)-RII-SUBR, and No. HRD-1002541], LONI [Award No. 2-10915], and the Louisiana Space Consortium (LaSPACE).

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