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Understanding Density Functional Theory (DFT) and Completing it in Practice DIOLA BAGAYOKO, Southern Univ & A&M Coll — A brief review of the seminal article by Hohenberg and Kohn leads to two conditions that have to be met by electronic structure calculations in order for their results to represent the physics content of DFT. One of these conditions is often the verifiable attainment of the absolute minima of the occupied energies. *Using the second Hohenberg Kohn theorem, we show that results of calculations that do not meet this condition, when it applies, do not necessarily represent DFT findings.* We illustrate this fact with over 100 calculated band gaps that are much smaller than corresponding, measured ones; in contrast, we list calculations that strictly adhered to the aforementioned conditions and whose results are in excellent agreement with experiment. *We describe two crucial steps in the latter calculations that add to or complete DFT in practice.* Some implications of our findings for academia, industry, and program package developers will be discussed. Acknowledgments: This work was funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award Nos. DE-NA0001861 and DE-NA0002630), LaSPACE, and LONI-SUBR.

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