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Understanding the Relativistic Generalization of Density Functional Theory (DFT) and Completing it in Practice. DIOLA BAGAYOKO, Department of Mathematics, Physics, and Science and Mathematics Education (MPSMED) Southern University and AM College, Baton Rouge, LA 70813, USA — In 2014, 50 years following the introduction of density functional theory (DFT), a rigorous understanding of it was published [AIP Advances, 4, 127104 (2014)]. This understanding included necessary steps ab initio electronic structure calculations have to take if their results are to possess the full physical content of DFT. These steps guarantee the fulfillment of conditions of validity of DFT; not surprisingly, they have led to accurate descriptions of several dozens of semiconductors, from first principle, without invoking derivative discontinuity or self-interaction correction. This presentation shows the mathematically and physically rigorous understanding of the relativistic extension of DFT by Rajagopal and Callaway {Phys. Rev. B 7, 1912 (1973)]. As in the non-relativistic case, the attainment of the absolute minima of the occupied energies is a necessary condition for the corresponding current density to be that of the ground state of the system and for computational results to agree with corresponding, experimental ones. Acknowledgments**:** This work was funded in part by the US National Science Foundation [NSF, Award Nos. EPS-1003897, NSF (2010-2015)-RII-SUBR, and HRD-1002541], the US Department of Energy, National Nuclear Security Administration (NNSA, Award No. DE-NA0002630), LaSPACE, and LONI-SUBR.

Diola Bagayoko
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