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Localized electron basis sets and the electronic properties of novel materials PABLO RIVERO, University of Arkansas, VICTOR MANUEL GARCIA-SUAREZ, JAIME FERRER, Universidad de Oviedo, KYUNGWHA PARK, Virginia Tech, SALVADOR BARRAZA-LOPEZ, University of Arkansas — Density functional theory algorithms based on localized electron basis sets permit calculation of material properties with modest computational cost, provided quantitative benchmarks against known properties available. Within the SIESTA computational package, we present a pragmatic and quantitative method to optimize basis sets and pseudopotentials of ordinary and novel materials. The method gives us a solid foundation to explore the electronic properties of new materials such as the strong topological insulator Bi_2Se_3.

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