

Towards ultimate precision in density-functional theory

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A large part of studies in modern solid-state physics and materials science relies on density-functional theory (DFT). It is implemented in diverse codes, and many of them rely on pseudopotentials, compact basis sets or other features. Their purpose is to improve computational performance, but it comes at the price of reduced precision. Therefore, it is important to be able to verify and systematically improve such approaches, which, in turn, requires indisputable reference data. We address ultimate precision in DFT by employing the full-potential linearized augmented plane waves + local-orbitals (LAPW+LO) method implemented in **exciting** [1]. We calculate total energies of atoms and 55 molecules of the G2-1 set using LAPW+LO and unrelated numerical approach that is based on the multi-resolution analysis [2]. The results obtained with these two methods agree within $\sim 1 \mu\text{Ha}/\text{atom}$, which demonstrates that LAPW+LO attains the complete-basis limit within this error margin [3]. For periodic systems, there are no such reference tools for crosschecking the LAPW+LO method. We therefore use the duality of the LAPW+LO basis and variable atomic-sphere sizes to show that the $\sim 1 \mu\text{Ha}/\text{atom}$ precision is attained also for solids.

References

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