Checking the engines: quantitative error bar assessment for DFT-based property predictions

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Resume : Whereas first-principles calculations used to be primarily employed to understand materials, they are nowadays being applied increasingly often to design new materials. To date, this evolution has culminated in the construction of large databases with ab initio computed materials properties. One of the side effects of this change in focus is a renewed interest in assessing the error bars that are associated with DFT-based property predictions [1-4]. Indeed, when interacting with industry-minded materials engineers, the need arises to replace hand-waving statements as ?it is commonly known that GGA slightly overestimates the lattice parameter? by more quantitative confidence intervals. In the present contribution, we review three sources of errors for DFT-based property predictions: code-related numerical errors [1,3], functional-related intrinsic errors [1] and model-related errors [4]. For each of these, procedures will be discussed to obtain quantitative error bar information. We will inspect a few case studies, and will present a status report on an on-going community-wide effort to crosscheck the validity and accuracy of mainstream DFT codes. [1] K. Lejaeghere et al., Crit. Rev. Solid State Mater. Sci. 39, 1-24 (2014) [open access, dx.doi.org/10.1080/10408436.2013.772503] [2] F. Jollet et al., Comp. Phys. Commun. (2014) dx.doi.org/10.1016/j.cpc.2013.12.023 [3] https://molmod.ugent.be/deltacodesdft [4] K. Lejaeghere et al., Phys. Rev. B (2014) accepted