SIX INCONVENIENT TRUTHS ABOUT DFT UNCERTAINTY QUANTIFICATION

Uncertainty quantification for density-functional theory (DFT) is a relatively new activity. Although the basic theorems behind DFT were already formulated in the sixties, error characterization has long been limited to defining increasingly large sets of experimental data with respect to which different flavours of DFT could be ranked. The latest decade has introduced a movement against this "mindless" DFT benchmarking. I will present six inconvenient truths that followed from this new line of research and that oppose current traditions:

1) Implementation matters. [1,2]
2) One mean absolute error does not cover everything. [1,3]
3) Beware of hidden model assumptions. [4,5]
4) Errors are correlated. [3,6]
5) DFT uncertainty is highly system- and property-dependent. [1,3,7]
6) Don't trust your reference data too easily. [3,7]

I will illustrate these claims by means of some contemporary illustrations from solid-state materials science.

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