Testing the hell out of DFT codes with virtual oxides

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If you use DFT to predict a property of a crystal, how confident can you be that the prediction is computed in a bug-free way? And if your DFT-code uses pseudopotentials, can you trust that the pseudopotential does not modify your predictions? Answering such questions has been the goal of a study a few years ago, in which 71 unary crystals were examined in exactly the same way by 40 different DFT methods and codes [1]. In a next step, a consortium of 45 scientists has done a similar exercise for a much larger pool of crystals: all elements of the periodic table up to Z=96, each in 10 different crystal structures, most of them being (virtual) oxides that sample a range of chemical bond types. In this presentation, we will discuss the reasons to choose these crystals, the different quality criteria by which results can be compared, and we will demonstrate how this exercise leads to more precise and more trustworthy pseudopotential libraries.

References

1. https://doi.org/10.1126/science.aad3000