Virtual oxides as a test bed for DFT methods and codes

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Some years ago, a community-wide benchmarking effort of +40 DFT methods and codes demonstrated that modern mainstream DFT codes are in good agreement with one another [1]. 71 elements of the periodic table were represented in this test, each as an elemental crystal. A next step in the process is to study all elements (Z=1 to Z=95, no gaps) in a series of very different environments. These environments are provided by 6 binary oxides for every element, chosen in such a way that the element under consideration is forced in 6 different formal oxidation states. This represents a strong transferability test for pseudopotentials. When compared with all-electron results, cases can be found which passed the simpler test but fail on the oxides. We will have a look at preliminary conclusions from this exercise, and I will formulate some caveats on the extent to which DFT codes can be meaningfully compared to each other.

[1]. K. Lejaeghere et al., Science 351 (2016) aad3000.