ASSESSING DFT REPRODUCIBILITY WITH A SYSTEMATIC BENCHMARK: CHEMICAL VARIETY

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Recently the precision of 40 numerical methods has been assessed for a test set of 71 elemental crystals [1]. Despite already being a large project by itself, this was only the first step on a long way towards finally answering the ubiquitous question of reproducibility and precision of DFT. One step on the roadmap of the "Delta 2.0" project is extending the benchmark set by diatomic materials in order to assess the quality of predictions for a wide range of chemically more diverse environments.

In order to scan chemical diversity in a systematic way, we examined for every element X (where X runs from Hydrogen to Curium) six different cubic oxides with stoichiometries that are chosen in such a way that the formal oxidation state of element X varies from +1 to +6. This presentation will showcase some first insights gained from the extended test set. In particular the focus will be on the transferability of conclusions from the initial 71-element delta test set and the sensitivity of the extended test set.

References

[1] K. Lejaeghere, *et al.,* Science **351,** 6280 (2016).