Assessing DFT Reproducibility with a Systematic Benchmark: Experimental Variety

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Recently, the precision of 40 different Density Functional Theory (DFT) approaches for periodic solids was assessed in an extensive study (the "Delta Project") using a test set of 71 elemental crystals [1]. To further investigate the question of reproducibility and precision of DFT codes additional benchmark crystals are necessary to capture the vast diversity of real solids and materials.

One step toward a more diverse test set is the addition of "real" experimentally known structures for every element (up to Americium). The cases have been selected in a way that they represent different prototypes of chemical bonding (covalent, ionic, metallic). In order to find such cases the Inorganic Crystal Structure Database (ICSD) [2] was searched for possible candidates. The electronic difference densities of roughly 1450 cases were calculated using WIEN2k [3] which were then used to classify the main bonding type and choose additional test cases.

This presentation will describe the process of making the final selection, summarize the test cases that have been chosen, and address some issues regarding "gaps", where no experimentally known examples could be found.

References

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

[2] https://icsd.fiz-karlsruhe.de

[3] http://www.wien2k.at