

**VSC School**  
**The Delta Project – Toward a Precision**  
**Benchmark Set for Solid State DFT**

**T. Ruh<sup>a,b</sup>, K. Lejaeghere<sup>b</sup>, S. Cottenier<sup>b</sup>, and P. Blaha<sup>a</sup>**

<sup>a</sup>*Institute of Materials Chemistry, TU Wien*

<sup>b</sup>*Center for Molecular Modeling (CMM), Ghent University*

Density Functional Theory (DFT) is the basis of many different methods that use the electronic density to describe a material and subsequently calculate its properties from quantum mechanical simulations.

Considering the large number of methods (each with its own approximations) and different implementations of DFT in various codes like WIEN2k [1] it is necessary to verify that results that were obtained with different methods or different codes agree with each other.

The Delta Project is an ongoing project that extends a previously devised procedure [2] to assess reproducibility and precision of different solid state DFT methods beyond elemental crystals that were used initially.

The ultimate goal is the creation of a benchmark set that includes a broad range of different structures in order to not only compare different DFT methods (implemented in a variety of codes) with each other but also to validate improvements (e.g. newly developed pseudopotentials for core treatment) in a way that reflects the large diversity of real solids in terms of their vastly different chemical environments.

On the one hand such a set has to contain enough different cases to reproduce as much of this diversity as possible – on the other hand the set should not be too large and contain cases that are easy to calculate to allow for fast calculation. Therefore, the design of the set and the choice of the included has to be conducted very carefully.

The foundation of the benchmark set consists of crystals of the elements up to an atomic number of 95 in different structural settings in order to capture structural diversity. In addition six different oxides per element – with the element in different oxidation states – will be used to account for different chemical environments.

In order to supplement the mainly hypothetical structures, avoid oxide-bias, and most importantly add some experimental bias to the test set, a third part of the benchmark set is going to be comprised of experimentally found, binary structures for all the elements already in the set.

These cases are chosen in a way that they cover different bonding scenarios (covalent, ionic, metallic) to additionally enforce chemical diversity of the whole benchmark set; and will be taken from the Inorganic Crystal Structure Database (ICSD) [3].

For the creation of this experimental part of the benchmark set it is going to be necessary to perform a large number of calculations to assess possible candidates and to optimize the chosen cases, so that proper input structures can be provided. A single calculation of this type usually takes only a few minutes on a single core, however, the sheer number of needed calculations makes an efficient, highly parallel execution crucial.

## References

[1] Blaha, P., et al., [www.wien2k.at](http://www.wien2k.at).

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

[3] <https://icsd.fiz-karlsruhe.de/>