Session 7 : beyond DFT

When considering codes that are even more complex than DFT implementations, the issue of benchmarking becomes ever more important. At one hand, it is for reasons of independence and neutrality not the most ideal situation of code developers run these tests (as has been the case for DFT codes). On the other hand, doing tests for GW calculations can be much more complex than doing a regular GW calculations, such that it should be mandatory done by developers. Can one do this right this from the beginning when developing more complex methods? (no clear answer emerges)

The question is raised what is the level of precision that is useful. In chemistry, there is the concept of 'chemical accuracy'. Being much more precise than that, does not really matter. Can similar targets be formulated for solid state physics? Some arguments were given:

- It depends very much on the property you want to predict.
- The precision one aims for, should not be better than the available accuracy of the method.
- Are relative differences sometimes more relevant than absolute differences? Working with a 20 meV band gap is something different than working with a 3 eV band gap.
- Sometimes people are pragmatic: we know that some methods are intrinsically approximate, yet they agree reasonably well with experiment. Perhaps for the wrong reasons, but if it works, it works.
- When comparing codes, a higher precision is required than when comparing one code with experiment (because in the latter case the experimental uncertainty and de imperfection of the XC-functional are involved as well).

This is a digest of a dedicated discussion session held at PQ-DFT 2019. For other digests, videos of all talks and summarizing recommendations, please visit https://pqdft2019.abinit.org/. To access the videos directly on Youtube, visit http://bit.ly/2XFKUCl. Any comments, thoughts or items you want to discuss? Feel free to contact Stefaan Cottenier (stefaan.cottenier@ugent.be) or Kurt Lejaeghere (kurt.lejaeghere@ugent.be).