Session 4: beyond total energies

A discussion develops on 'do we need to test properties beyond total energies?' Many properties do depend on total energy differences, even complex ones as a phonon band structure. It makes most sense to do this for properties that do not depend (entirely) on the total energy, such as magnetism.

We cannot test all properties thoroughly, hence it is important to choose wisely which one. Proxies should be used wherever possible (e.g. band structure as a proxy for magnetism). Or rather than calculating an entire phonon spectrum, the forces after a simultaneous random displacement of all atoms can be compared across codes. When prioritizing the properties for which a bench mark set will be developed, it could help to select those properties first that matter for applications.

Another discussion starts from the deliberately provocative question whether ever an ideal pseudopotential will be found. The puristic answer is: no. Eventually, there will always be a point at which the scattering properties of the nucleus matter, and a pseudopotential has no info on this. Also the PAW scheme has its limitations, due to the frozen core. When relaxing the core, the PAW scheme becomes de facto an all-electron method.

An interesting insight is that there is no need to invest too heavily into very precise pseudopotentials, because our calculations are anyway not yet sufficiently accurate (=close to experiment). What is the value to be able to reproduce – at high cost – an all-electron calculation exactly, if the predictions that are based thereupon are considerably different from the experimental values due to limitations of the XC-functional?

Are there alternatives to the use of pseudopotentials and plane waves? If we would allow to use other basis sets than plane waves, one could work with much harder pseudopotentials. Multiresolution basis sets behave differently near the nucleus and far away from it, and are becoming available for periodic calculations as well. One drawback is that it is (and always will be) more difficult to develop other features on top of this, in that respect a plane wave basis set is much easier to work with.

Work along such lines require a lot of human effort, beyond what is possible for one PhD. Concerted actions and stimulating the development of joint libraries (libxc, ESL,…) are very much needed.

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).