DFT and experiment: a match made in heaven or in hell?

Kurt Lejaeghere[1], Louis Vanduyfhuys[1], Veronique Van Speybroeck[1], and Stefaan Cottenier[1,2]

[1] Center for Molecular Modeling, Ghent University
Technologiepark 903, 9052 Zwijnaarde, Belgium
[2] Department of Materials Science and Engineering, Ghent University
Technologiepark 903, 9052 Zwijnaarde, Belgium

In the last decades, density-functional theory (DFT) has become one of the most popular tools to model materials at the atomic scale. It is even used to predict the properties of hitherto undiscovered compounds, yielding unprecedented insights long before the first sample is manufactured. The combination of theory and experiment in materials design is therefore often depicted as a match made in heaven. But is it really, or are we inavertibly heading for an ugly divorce?

This talk will show that compared to experiment, DFT predictions of thermal properties are affected by three levels of errors: numerical errors [1], intrinsic errors [1] and semi-empirical errors [2]. By focusing on the thermal expansion coefficient and the melting temperature, each of these effects will be explained and quantified using a benchmark set of 71 elemental crystals.

In addition, we will have a closer look at how the error on an equation of state depends on the shape of that curve. This makes it possible to differentiate between different materials, whereas the first part of the talk focuses on average error properties. Using both an analytical and a Monte-Carlo-based approach, the errors on the equilibrium volume, bulk modulus and bulk modulus derivative are found to depend on these properties themselves [3].

Finally, this systematic analysis of DFT errors concludes that there is nothing going on between DFT and experiment that a bit of marriage counselling cannot fix.

[1] K. Lejaeghere, V. Van Speybroeck, G. Van Oost, and S. Cottenier, Crit. Rev. Solid State **39**, 1-24 (2014).
[2] K. Lejaeghere, J. Jaeken, V. Van Speybroeck, and S. Cottenier, Phys. Rev. B **89**, 014304 (2014).
[3] K. Lejaeghere, L. Vanduyfhuys, V. Van Speybroeck, and S. Cottenier, *in preparation.*