Error overload? Dealing with DFT uncertainty

Density-functional theory (DFT) offers a perfect description of many-particle systems, but when it is used to predict the macroscopic behaviour of real materials, errors start accumulating. Things go wrong as soon as the theoretically exact formalism is implemented in a computer code: continuous variables need to be discretized, approximations are required to mitigate computational cost, ... It is no surprise that each DFT code comes with its own set of *numerical* errors. In addition, the DFT Kohn-Sham equations have conveniently hidden away all nastiness in a single quantity: the exchange-correlation functional. Its shape is not known, so an educated guess is needed. Materials properties determined from DFT calculations therefore suffer from errors *intrinsic* to the chosen functional. These errors can be separated into a predictable component and residual contributions. Finally, periodic DFT is a zero-kelvin theory for perfectly ordered materials, while most relevant materials science pertains to disordered and/or microstructured materials at temperatures around 300 K or even far beyond that. Whether high-quality approximations or simple semi-empirical relations are used, they remain approximations and introduce *model* errors of their own.

This talk will discuss each of these levels of errors, focusing on some interesting case studies. Numerical errors are assessed by comparing predictions of elemental equations of state (EOS) between different DFT codes and pseudopotentials [1,2]. Intrinsic errors are illustrated by means of EOS parameters (using LDA, PBE and HSE functionals) [1] and surface properties (using PBE) [3]. Model errors are demonstrated for the thermal expansion coefficient (using PBE) [4]. In addition, it is shown how errors on EOS parameters depend on the particular shape of that equation of state [5].

[1] K. Lejaeghere, V. Van Speybroeck, G. Van Oost and S. Cottenier, *Crit. Rev. Solid State* **39**, 1-24 (2014).

[2] K. Lejaeghere et al., *Science* **351** (6280), aad3000 (2016).

[3] S. De Waele, K. Lejaeghere, M. Sluydts and S. Cottenier, submitted.

[4] K. Lejaeghere, J. Jaeken, V. Van Speybroeck and S. Cottenier, *Phys. Rev. B* **89**, 014304 (2014).

[5] K. Lejaeghere, L. Vanduyfhuys, T. Verstraelen, V. Van Speybroeck and S. Cottenier, *Comput. Mater. Sci.* **117**, 390-396 (2016).