The Delta test revisited

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The Delta test was designed to perform a systematic assessment of precision across density-functional theory codes. It evaluates their agreement based predicted equations of state for the elemental crystals, using the so-called Δ criterion [1]. Thanks to the efforts of a broad collaboration of code developers and expert users, a large data set was established, confirming the excellent precision of recent electronic-structure packages and potentials [2].
In this presentation, I will revisit the results of the original Delta tests, extended with data provided after its publication and available on the Delta project website [3]. It will be shown that different error measures can be used to analyse the results. A direct comparison of equation of state parameters is also possible, but should be done with care, as the sensitivity of the equation of state parameters can be unexpectedly large without actually affecting Δ much [4].

References

[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**, aad3000 (2016).

[3] `https://molmod.ugent.be/deltacodesdft`

[4] K. Lejaeghere, "The uncertainty pyramid for electronic-structure methods" in Uncertainty Quantification in Multiscale Materials Modeling (Eds. Y. Wang and D. McDowell), Elsevier (2019), accepted.