Heats of formation of solids with error estimation - DTU Orbit (05/12/2018)

Heats of formation of solids with error estimation: The mBEEF functional with and without fitted reference energies

The need for prediction of accurate electronic binding energies has led to the development of different schemes for combining density functional calculations, typically at the level of the generalized gradient approximation (GGA), with experimental information. We analyze one such scheme by Stevanovic’ et al. [Phys. Rev. B85, 115104 (2012)PRBMDO1098-012110.1103/PhysRevB.85.115104] for predictions of compound enthalpies of formation using fitted elemental-phase reference energies. We show that different versions of GGA with or without +U and a meta-GGA (TPSS) lead to comparable accuracy after fitting the reference energies. Our results also show that the recently developed mBEEF, a Bayesian error estimation functional, gives comparable accuracy with the other functionals even without the fitting. The mBEEF functional furthermore supplies an ensemble estimate of the prediction errors in reasonable agreement with the actual errors. We also show that using the fitting scheme on the mBEEF ensemble leads to improved accuracy including realistic error estimation.

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