Error quantification for density-functional theory calculations of surface energy and work function

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Density-functional theory (DFT) predictions of materials properties are becoming ever more widespread. With increased use comes the demand for estimates of the accuracy of DFT results. In view of the importance of reliable surface properties, this presentation discusses the calculation of surface energies and work functions for a large and diverse test set of crystalline solids. This set consists of all elementary metals and metalloids up to bismuth, except for the lanthanides. They are compared to experimental values by means of a linear regression. This results in an estimate for the uncertainty on the DFT value and enables the separate determination of a predictable and stochastic uncertainty contribution. Two of the most prevalent functionals, the local density approximation (LDA) and the Perdew-Burke-Ernzerhof parametrization of the generalized gradient approximation (GGA-PBE), are evaluated and compared. It is found that both LDA and GGA-PBE yield accurate work functions with error bars below 0.3 eV, which is comparable to the experimental precision. LDA also provides satisfactory estimates for the surface energy with error bars smaller than 10%, but GGA-PBE significantly underestimates the surface energy for materials with an important correlation energy contribution.

References

[1] S. De Waele, K. Lejaeghere, M. Sluydts, and S. Cottenier, Phys. Rev. B **94**, 235418 (2016).