# Benchmarking DFT and beyond-DFT methods for thermodynamics and electronic properties

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From a tool of understanding and rationalization, ab initio techniques have clearly become a tool for predictive materials design. However, these techniques rely on approximations that are sometimes difficult to a priori evaluate. Rules of thumbs exist and the expert will be able to qualitatively assess the performance of a method for a specific property. However, statistically sound and unbiased benchmarks are required if true predictive materials design is to be performed.

I will use examples of benchmarks studies especially focusing on thermodynamic quantities such as formation energies or electronic properties such as band gap.[1,2] I will highlight the importance of having a clear assessment of the error bar of a property for a given technique but also stress general challenges in terms of size, curation and chemical diversity of the experimental data or automatic convergence of the computations.

# References

[1] G. Hautier, S.P. Ong, A. Jain, C.J. Moore, G. Ceder, Accuracy of density functional theory in predicting formation energies of ternary oxides from binary oxides and its implication on phase stability, Phys. Rev. B. 85 (2012) 155208.

[2] M.J. van Setten, M. Giantomassi, X. Gonze, G.-M. Rignanese, G. Hautier, Automation methodologies and large-scale validation for GW : Towards high-throughput GW calculations, Phys. Rev. B. 96 (2017) 155207.