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Looking at Benchmarks for Density Functional Calculations

Pascal Pernot[1], Andreas Savin[2]

[1]Institut de Chimie Physique, UMR8000 CNRS, Université Paris-Saclay, F-91405, Orsay, France

[2]Laboratoire de Chimie Théorique, CNRS and UPMC Université Paris 06, Sorbonne University, F-75252 Paris, France

*Corresponding author

ABSTRACT

Benchmarks presenting the accuracy of computational methods tend to replace personal experience and study in their choice. This has the advantage of beingadapted to the huge amount of computational material produced through easily available programs, but hide a series of pitfalls. In particular, a more careful look at thebenchmark is needed than just looking at summarizing numbers like the mean absoluteerror.

DOI: 10.21467/abstracts.122 ISBN: 978-81-954993-3-5