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How accurate is Density Functional Theory in Predicting Reaction Energies Relevant to Phase Stability? GEOFFROY HAUTIER, SHYUE PING ONG, ANUBHAV JAIN, CHARLES J. MOORE, GERBRAND CEDER, Massachusetts Institute of Technology — Density Functional Theory (DFT) computations can be used to build computational phase diagrams that are used to understand the stability of known phases but also to assess the stability of novel, predicted compounds. The quality and predictive power of those phase diagrams rely on the accuracy of DFT in modeling reaction energies and we will present in this talk the results of a large scale comparison between experimentally measured and DFT computed reaction energies. For starters, we will show that only certain reaction energies are directly relevant to phase stability of multicomponent systems and that very often those reaction energies are not the commonly studied reactions from the elements. Using data from different experimental thermochemical tables and DFT high-throughput computing, we will present the results of a statistical study based on more than 130 reaction energies relevant to phase stability and from binary oxides to ternary oxides. We will show that the typical error are around 30 meV/at and therefore an order of magnitude lower than the errors in reaction energies from the elements. Finally, we will discuss the broad implications of our results on the evaluation of ab initio phase diagrams and on the computational prediction of new solid phases.

Geoffroy Hautier
Universite Catholique de Louvain

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