What Can "Quantum-Black-Boxes" Do for the Inorganic Thermochemist?

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Energies of formation and binding energies for molecular systems are now recognized as key quantities to benchmark state-of-the-art quantum mechanical methods and are also important for assessing the available experimental data. For small molecular systems, quantum mechanical simulations, in particular at higher levels of theory, often supersedes the accuracy of experimental data. By contrast, quantum mechanical calculations of energies of formation are much less common for inorganic compounds like ternary oxides. At the same time it is evident that experimental determinations of these quantities are extremely time consuming and high accuracy often requires complex home-made equipment. The aim of the present presentation is to show that theoretical methods and commercial computer software are available at an accuracy level that is useful to the inorganic thermochemist. Such methods have a large potential also from an engineering point of view due to the high speed and low costs involved. The calculation of enthalpies of formation of ABO3 (A = Ca, Sr, Ba; B = Ti, Zr, Hf) from the binary constituent oxides by ab-initio density functional theory is one example presented.