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Stability of oxides studied with standard density functional theory.

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Oxides are in general complicated to treat with standard DFT, especially the formation energy of the oxygen molecule and the electron self-interaction for localized d and f electrons are known shortcomings. We present a frame in which it is possible to calculate formation energies of oxides (among those perovskites) based on standard DFT at the GGA level. The idea is to apply a "wet electrochemical reference[1]" this has the advantages that calculation of the oxygen molecule is avoided and that the oxide Pourbaix diagrams come out as a useful side product. We calculate the change in free energy for a reaction e.g:

$A(s)+B(s)+3H_2O \rightarrow ABO_3 + 3H_2$,

where water is applied as reference energy for of the oxygen atoms. Other references can be used by adding the relevant energy difference accordingly.
The calculated formation energies are compared to experimental literature and the absolute mean error is small (always smaller than 0.3eV per formula uint). This allows us to systematic calculate energies for mixed oxides with dopends. The results can be used as a search criteria in designing new perovskite materials with better properties.

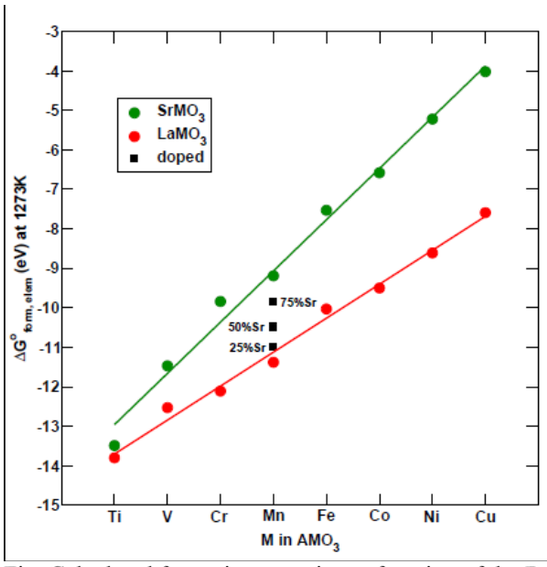

Fig. Calculated formation energies as function of the B atom position is the periodic table. With the A atom being either La or Sr. $La_xSr_{1-x}MnO_3$ formation energies are shown in black.

[1] "Formation energies of rutile metal dioxides using density functional theory" J.I Martinez, H.A. Hansen, J.Rossmeisl, J.K. Nørskov, Physical Review B. 79, 045120, (2009)