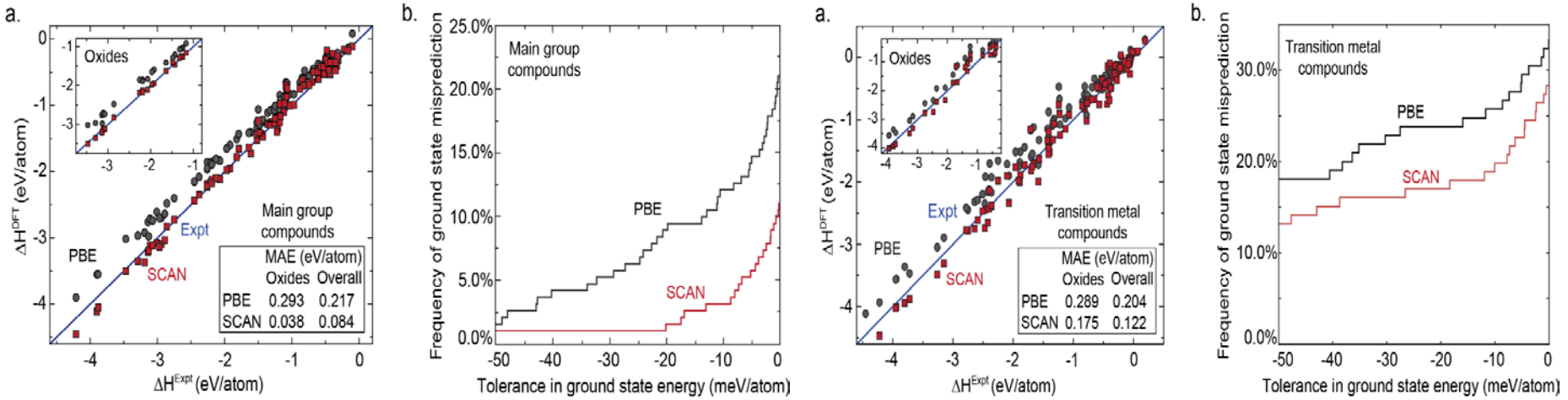
Efficient first-principles prediction of solids stability: Towards chemical accuracy



Formation enthalpy and ground state structure selection errors from SCAN and PBE for main group compounds (left) and transition metal compounds (right).

Research Details

- Formation enthalpy of 196 binary solids, including 102 main group compounds and 94 transition metal compounds, were calculated using PBE and SCAN.
- Relative stability for 297 binary solids, including 191 main group compounds and 106 transition metal compounds, with about 10 structures for each binary were calculated for the ground state structure selection

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Work was performed at Tulane, Temple, and Berkeley

Scientific Achievement

The strongly-constrained and appropriately-normed (SCAN) density functional significantly improves over the standard PBE GGA, approaching the chemical accuracy for solid stability.

Significance and Impact

The question of material stability is of fundamental importance to any analysis of system properties in condensed matter physics and materials science. SCAN offers a robust model for a significant portion of the periodic table, presenting an opportunity for the development of novel materials and the study of fine phase transformations even in largely unexplored systems with little to no experimental data.

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