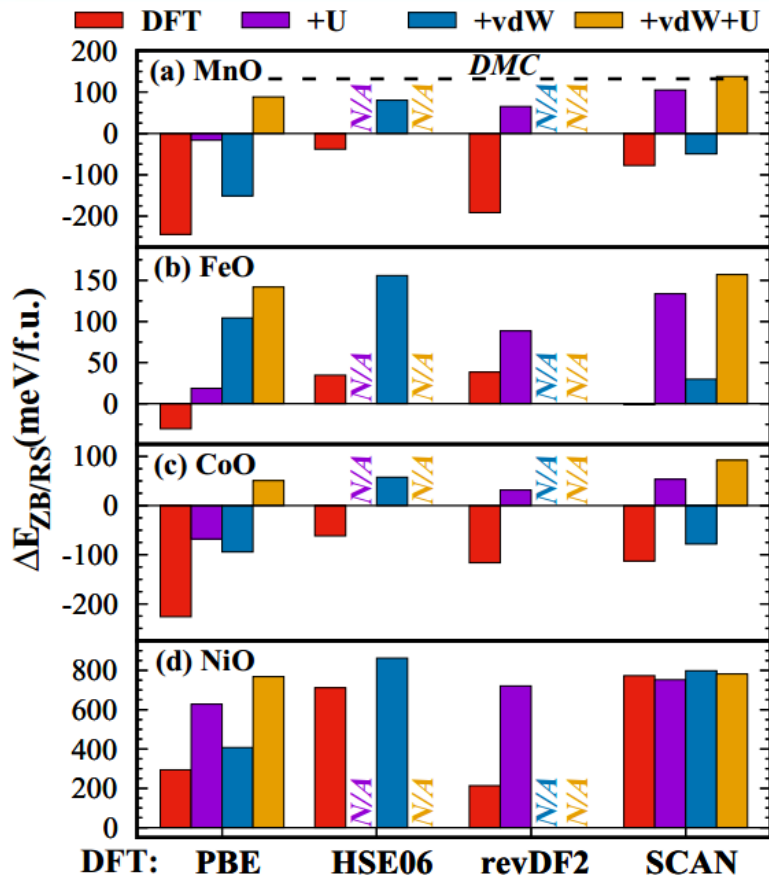


Synergy of van der Waals Correction and Self-Interaction Correction in Transition-Metal Monoxides



Energy difference between the zinc-blende (ZB) and rock-salt (RS) phases of four transition-metal monoxides, from four different flavors of density functionals, with or without van der Waals (vdW) and/or self-interaction corrections.

Haowei Peng and John P. Perdew, Phys. Rev. B 96, 100101 (2017)
DOI: 10.1103/PhysRevB.96.100101

Scientific Achievement

We pointed out the otherwise overlooked importance of van der Waals (vdW) interactions in determining the ground-state structure of transition metal monoxides, in addition to the well-known self-interaction correction (SIC), and proposed and tested SCAN+rVV10+U as an accurate and computationally efficient method for this problem.

Significance and Impact

Our work illustrates the ubiquity of vdW interactions, even in conventional *hard bulk* materials. Our work further provides an accurate and efficient computation method for energetics and structural properties of transition-metal compounds, in particular, metastable structures and alloys for Li-ion battery and other functional materials.

Research Details

We calculated the energy difference between the ZB and the true ground-state RS phases for MnO, FeO, CoO, and NiO using different flavors of density functionals and corrections (PBE-GGA, HSE06 hybrid, revDF2 vdW-DF, and SCAN meta-GGA for the former, TS-vdW, vdW-DF2, rVV10 for vdW, and Hubbard U from linear response and exact exchange in HSE for SIC).

Work performed at Temple University. Supported as part of the Center for the Computational Design of Functional Layered Materials, an Energy Frontier Research Center funded by DOE BES under Award # DE-SC0012575.



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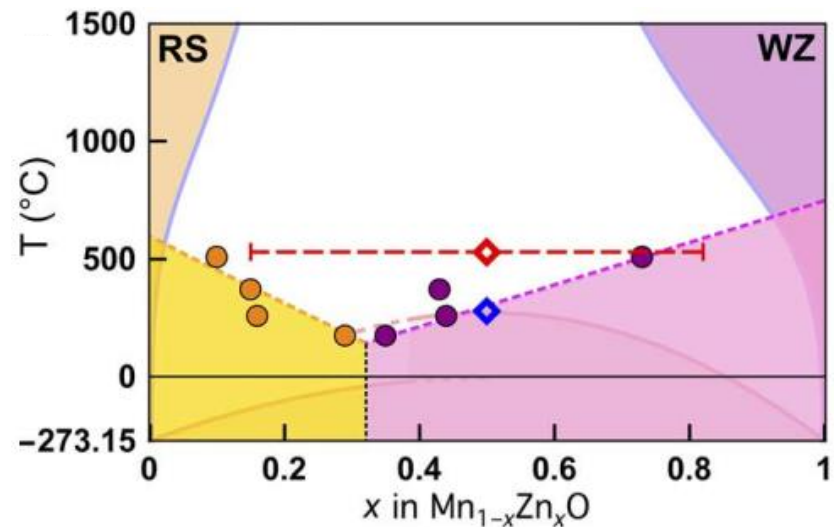
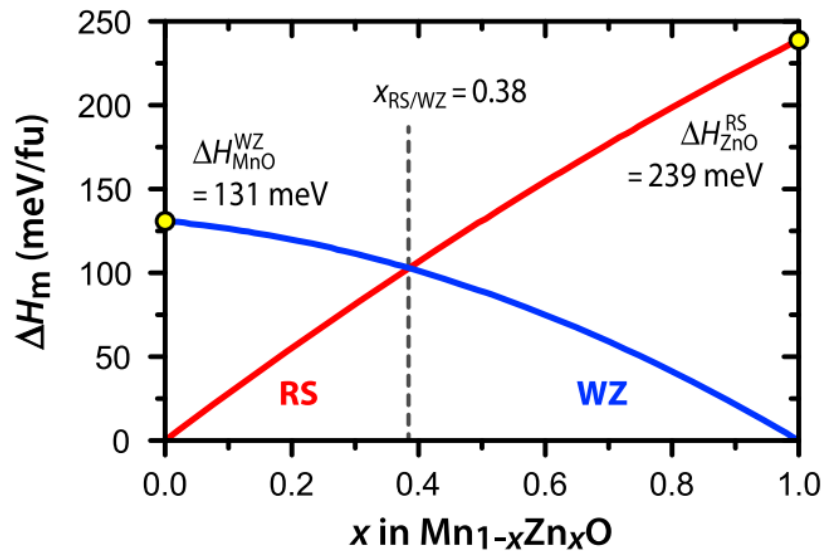
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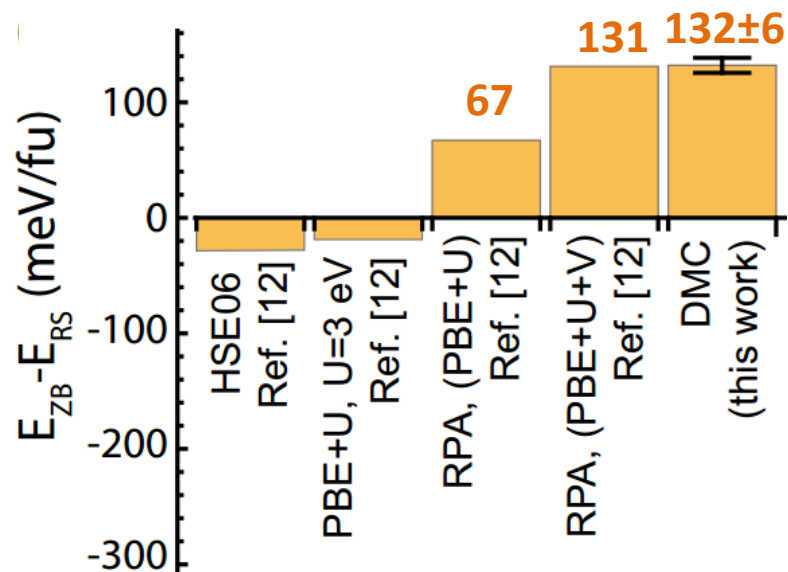
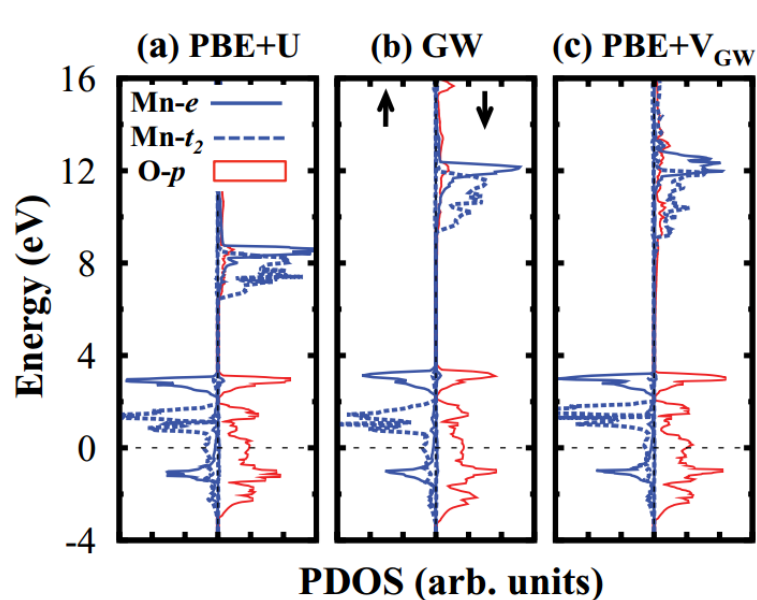
Metastable Functional Materials



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GGA, HSE, RPA and QMC for MnO



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Synergy of vdW & SIC

