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Reaction Energies of Oxides using Random Phase Approximation JUN YAN, JENS HUMMELSHOEJ, JENS NØRSKOV, Stanford University — Oxides are widely used in industrial heterogeneous catalysis, photo catalysis, electrochemistry and in making batteries and fuel cells. To facilitate the computational engineer and design of novel materials in these fields, it is vital important to quantitatively predict the formation and reactions energies of the oxides. LDA/GGA, the success of which has largely relied on the mysterious error cancellation in the exchange-correlation term, generally failed for these oxides, showing systematic and non-canceling errors. Recently, the use of exact exchange (EXX), plus correlation energy from Random Phase Approximation (RPA) emerges as a promising approach to obtain non-empirical exchange-correlation terms. Exact exchange energy is free of self-interaction error, while RPA correlation energy takes into account dynamic electronic screening and is fully non-local. EXX+RPA has shown to systematically improve lattice constants, atomization energies, adsorption energies, reaction barriers for a wide range of systems that have ironic, covalent and van der Waals interactions. In this talk I will present our results comparing RPA and GGA functional for the formation and reaction energies of oxides.

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