

Abstract Submitted
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The confinement error corrections for the exchange energy in transition metal oxides FENG HAO, Sandia National Laboratories, RICKARD ARMIENTO, MIT, ANN E. MATTSSON, Sandia National Laboratories — We present some recent advances towards a straightforward scheme to correct for the confinement errors of the exchange energy of the transition metal oxides (TMO). This approach includes two steps: (i) identifying the spatial regions where the confinement errors exist, using local density and kinetic energy density information, and (ii) mapping these spatial regions to harmonic-oscillator (HO) models [1], and quantifying and correcting the relative confinement errors based on the model system. The scheme has been applied to calculations with several local and semi-local functionals, and a trend of improvement for the equilibrium structure is obtained after applying these confinement error corrections. Sandia is a multiprogram laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

[1] Hao et al, PRB **82**, 115103 (2010).

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