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On the origins of the deficiencies of density functional theory exchange-correlation functionals for transition metal oxides ANN E. MATTSSON, Sandia National Laboratories, RICKARD ARMIENTO, MIT, FENG HAO, Sandia National Laboratories — The transition metal oxides (TMO) are a class of compounds that are difficult to treat in density functional theory (DFT) with simple local and semi-local functionals. Especially for CuO, they failed to give the correct equilibrium monoclinic structure. The major source of the deficiency is attributed to the imperfect cancellation of the electronic self-interaction (SI) in the approximated exchange energy. Previous studies [1] show that a large part of the SI error is connected to the confinement error that can be modeled by harmonic-oscillator (HO) systems. We discuss recent advances towards a simple methodology to quantify the confinement errors in real TMO systems. Our results show that these confinement errors may account for the deficiencies of DFT functionals in obtaining the correct equilibrium structure of the TMO. 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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