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Efficiency and accuracy in transition-metal chemistry: a self-consistent GGA+U approach HEATHER KULIK, MATTEO COCOCCIONI, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — Transition-metal centers are the active sites for a broad variety of biological and inorganic chemical reactions. Notwithstanding this central importance, density-functional theory calculations based on local-density or generalized gradient approximations often fail qualitatively and quantitatively in describing energetics, multiplet structures, reaction barriers, and geometries around the active sites. We suggest here an alternative approach, mutuated from the Hubbard U correction to solid-state problems, that provides an excellent agreement with accurate, correlated-electron quantum chemistry calculations in paradigmatic test cases that range from the ground state of the Fe_2 dimer to the potential energy surfaces for the addition-elimination of molecular hydrogen on FeO^+. The Hubbard U is determined with a novel self-consistent procedure based on a linear-response approach.

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