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The Applicability of Different Quantum Mechanical Methods to Transition Metal Oxides ORKID COSKUNER, EMILY JARVIS, THOMAS ALLISON, CARLOS GONZALEZ, ANNE CHAKA, National Institute of Standards and Technology, Physical and Chemical Properties, Gaithersburg, MD 20889, NIST, COMPUTATIONAL CHEMISTRY GROUP TEAM — Numerous quantum mechanical methods and basis sets have been applied extensively to organic molecules. However, the performance of these is not well understood for transition metal oxides. We employed different methods along with several basis sets for optimizing the geometries in the gas phase and calculating the IR spectra as well as thermodynamic properties including Gibbs free energy and enthalpy of linear, trigonal and tetrahedral metal oxides. The MCSCF and DFT methods generally give the most accurate results for organic and inorganic molecules. Surprisingly, our studies showed that the results obtained for iron(III) oxides at the GVB and MP2 levels gave more accurate results than the MCSCF and hybrid methods. Similarly, for aluminum and chromium oxides, the calculations with MP2 and PBE yielded thermodynamic properties, which are closer to experimental values.

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