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Pseudopotentials for quantum Monte Carlo calculations of transition metal oxides[1] JARON KROGEL, JUAN SANTANA, PAUL KENT, FERNANDO REBOREDO, Oak Ridge National Laboratory — Quantum Monte Carlo calculations of transition metal oxides are partially limited by the availability of high quality pseudopotentials that are both accurate in QMC and compatible with major electronic structure codes, e.g. by not being overly hard in the standard planewave basis. Following insight gained from recent GW calculations, a set of neon core pseudopotentials with small cutoff radii have been created for the early transition metal elements Sc to Zn within the local density approximation of DFT. The pseudopotentials have been tested for energy consistency within QMC by calculating the first through fourth ionization potentials of the isolated transition metal (TM) atoms and the binding curve of each TM-O dimer. The vast majority of the ionization potentials fall within 0.3 eV of the experimental values, with exceptions occurring mainly for atoms with multiple unpaired d electrons where multireference effects are the strongest. The equilibrium bond lengths of the dimers are within 1% of experimental values and the binding energy errors are typically less than 0.3 eV. Given the uniform treatment of the core, the larger deviations occasionally observed may primarily reflect the limitations of a Slater-Jastrow trial wavefunction.

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