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Study of pseudopotential errors in transition metal molecules:implications for quantum Monte Carlo MINYI ZHU, LUBOS MITAS, North Carolina State University — We investigate pseudopotential errors for the electron structure in transition-metal molecules with strong electron correlation. We compare high spin-low spin state energy differences within Density Functional Theory (DFT), Hartree-Fock and hybrid functionals. In particular, we compare results from small-core Dirac-Fock pseudopotentials and both relativistic and non-relativistic all-electron calculations. The presence of exact exchange affects these errors and points towards the importance of exact exchange in this context. Since the accuracy of quantum Monte Carlo (QMC) results depends on pseudopotential in a crucial manner, we study the implications for QMC calculations.

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