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Quantum Monte Carlo study of 4d vs 5d atomic and molecular systems. MICHAEL BENNETT, North Carolina State University, ADEM KULAHLIOGLU, Meliksah University, CODY MELTON, LUBOS MITAS, North Carolina State University — We investigate the electronic properties of Mo and W atomic and molecular systems by quantum Monte Carlo (QMC) methods. One area of interest in these systems are the systematic changes in the fixed-node errors from 4d to 5d elements and corresponding changes in the correlation effects. We find that similarly to first and second-row systems the fixed-node biases grow with increasing degree of charge localization for similarly complex wave functions and bonding patterns. The second area of interest is the impact of relativistic effects on the electronic structure, in particular, to which extent they affect the bonding properties. We use scalar-relativistic energy-consistent pseudopotentials with averaged spin-orbit effects and we contrast these calculations with the explicit inclusion of the spin-orbit in the two-component framework.

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