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Quantum Monte Carlo of atomic and molecular systems with heavy elements LUBOS MITAS, ADEM KULAHLIOGLU, CODY MELTON, CHANDLER BENNETT, North Carolina State University — We carry out quantum Monte Carlo calculations of atomic and molecular systems with several heavy atoms such as Mo, W and Bi. In particular, we compare the correlation energies vs their lighter counterparts in the same column of the periodic table in order to reveal trends with regard to the atomic number Z. One of the observations is that the correlation energy for the isoelectronic valence space/states is mildly decreasing with increasing Z. Similar observation applies also to the fixed-node errors, supporting thus our recent observation that the fixed-node error increases with electronic density for the same (or similar) complexity of the wave function and bonding. In addition, for Bi systems we study the impact of the spin-orbit on the electronic structure, in particular, on binding, correlation and excitation energies.

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