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Quantum Monte Carlo study of spin-orbit interaction effects in Tungsten atomic and molecular systems CODY MELTON, M. CHANDLER BENNETT, LUBOS MITAS, North Carolina State Univ — We study the electronic properties of selected Tungsten molecular systems using averaged and explicit spin-orbit interactions using many-body methods. In particular, we apply recently developed quantum Monte Carlo methods that can treat spin-orbit and other types of spin-dependent interactions explicitly. Our fixed-phase spin-orbital diffusion Monte Carlo (FPSODMC) method is based on a two-component spinor formalism along with a generalization of the fixed-phase approximation and projection of the non-local operators with appropriate spinor-based and Jastrow-factor correlated trial wave functions. The determinantal parts of trial wave functions are generated at several levels of accuracy such as single configuration, multi-configuration within the open-shells and large CI expansions. The corresponding impacts on the accuracy of projections and fixed-phase biases are studied on Tungsten molecular systems and the results are compared with the spin-averaged calculations. The binding energies require consistent treatment of spin-orbit and correlations in both atomic and molecular systems. The low symmetry of spinor wave functions increases the multi-reference character of the states and therefore demand appropriate sizes of determinantal expansions.

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