Modeling spin-orbit coupling using a localized active space approach

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Multi-metallic transition metal complexes have applications as single molecule magnets and molecular qubits. Obtaining quantitatively accurate spin state couplings and energetics of these complexes often require performing multiconfigurational calculations. However, these calculations can be unfeasible for larger systems due to the poor scaling of multiconfigurational methods. A method recently developed by our group, localized active space self-consistent field (LASSCF), addresses this issue, whereby the active space is decomposed into subspaces localized on different areas of the system. With state interaction (SI)-LASSCF explicit electron correlation between LAS subspaces is introduced, allowing us to model properties such as the J-coupling between spin centers.

Building on the SI-LASSCF framework, in this presentation we introduce an approach to calculate spin-orbit coupling between different LAS states using an effective one-electron spin-orbit Hamiltonian. With this method we will be able to obtain accurate descriptions of the electronic structure and magnetic properties of multi-metallic complexes.