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Near-Exact Wave Functions: Pushing Towards Accurate Transition Metal Simulations

In this modern area of computation, the core methods of quantum chemistry are continuously applied to a vast range of chemistries. Despite the usefulness of these approaches, however, well-known deficiencies reduce their utility for some of the most interesting electronic states being studied in the laboratory. This is especially the case when unpaired electrons are in play, for example, in transition metal complexes where so-called “strong correlation” impedes the accuracy of commonplace electronic structure techniques. This correlation problem can in principle be treated with benchmark-level electronic structure techniques—notably the full configuration interaction wave function, which is exact—but intractable costs have so far precluded this possibility. This presentation will discuss our group’s pathway towards computationally tractable, polynomial scaling approximations of electronic states in molecules. Using a specific many-body expansion of the electronic energy, near-exact results can be achieved for polyatomic molecules and transition metal complexes. Introduction of this technique, which we call iFCI, will be followed by studies of strongly correlated transition metal complexes with complicated spin states.

Suggested Reading:

Hosted by Professor Anna Krylov

*The scientific community is invited*