Capturing both weak and strong correlations in transition metal chemistry using classical and quantum methods

James Shee[1]

[1] Rice University; Norman Hackerman-Welch Investigator, Assistant Professor of Chemistry

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Reliable computational modeling of transition metal compounds requires electronic structure theories that can accurately describe both weak and strong correlations in a scalable manner. Weak (dynamical) correlations include dispersion and screening effects, which are crucial in many types of organometallic bonding. Strong (static) correlations can arise due to the presence of nearly-degenerate electronic states, leading to low-spin states of open-shell character encountered, e.g., in polynuclear transition metal complexes. I will introduce two *ab initio* methods which capture these essential features in a systematically improvable way - phaseless auxiliary-field quantum Monte Carlo, and variational cluster Jastrow wavefunctions inspired by Hubbard physics. These approaches can yield near-exact ground-state energies with tractable computational costs, and can be implemented on both classical and quantum computers.