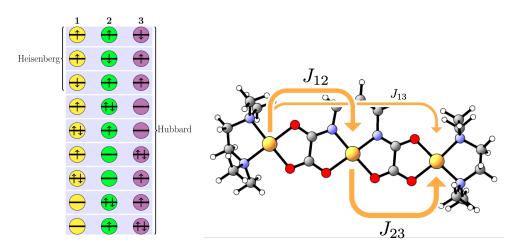


Effective Hamiltonians From Correlated Wavefunctions

Effective Hamiltonians deliver physical insights from the complicated many-body Hamiltonians. Q-Chem's effective Hamiltonian implementations offer a straightforward and rigorous way to extract model Hamiltonian parameters from high-level correlated wavefunctions, enabling studies of magnetic properties in large systems.



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- Straightforward extraction of model Hamiltonian parameters for multi-site systems;
- Direct comparison between ab initio and experimental coupling parameters;
- Model Hamiltonians enable calculations of an entire low-energy manifold of states in large strongly correlated systems from just one inexpensive single spin-flip calculation;
- Q-Chem offers effective Hamiltonian extractions for two types of correlated wavefunctions:
 - EOM-SF-CCSD Effective Hamiltonian
 - * Based on highly accurate coupled-cluster wavefunctions;
 - Parameter extraction for Heisenberg and Hubbard model Hamiltonians;
 - * Available in Hermitian (Bloch) and non-Hermitian (des Cloizeaux) formulations.
 - RAS(h,p)-1SF Effective Hamiltonian
 - * Parameter extraction for Heisenberg Hamiltonian;
 - Enables studies on large high-spin systems with multiple orbitals per site.

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