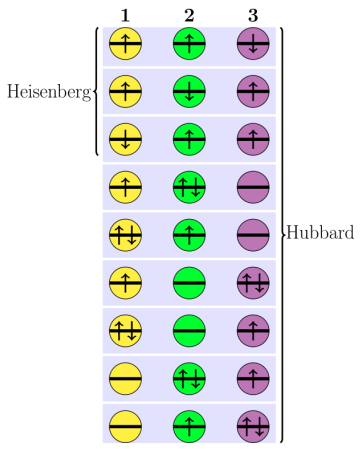
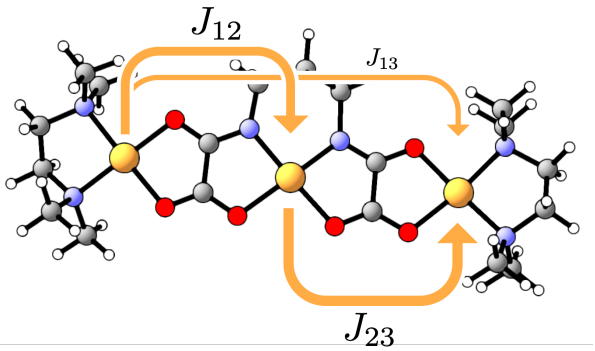
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

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.





- Useful and intuitive physical insights into magnetic couplings;
- 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.

Request a free trial at www.q-chem.com