Quantum Chemical Modeling
Structure & Reactivity of Ground & Excited States
Coordination Chemistry and Catalysis

Key features of modeling strategies:
- Balanced treatment of strong and weak bonding interactions
- Long-range electrostatics
- Excited states

Innovations:
- Validation of models connecting clusters and periodic systems
- Multiscale models for characterization of reaction paths

Scope of Effort:
- Catalysis in MOFs
- Response to photostimuli

\[
H_{ia,jb}^{\text{VEM}}(k) = \delta_{ij}\delta_{ab}[\varepsilon_a - \varepsilon_i] - ( ja \parallel ib ) \\
+ \delta_{ij}\langle \psi_a | \Delta\Phi(k) | \psi_b \rangle - \delta_{ab}\langle \psi_i | \Delta\Phi(k) | \psi_j \rangle
\]