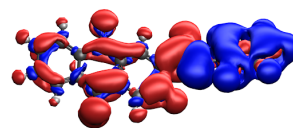
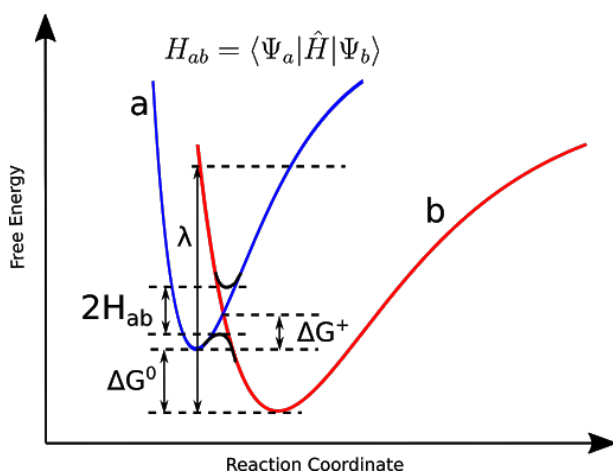


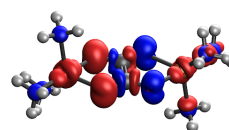
Constrained Density Functional Theory (CDFT)

CDFT adds additional potentials to the Kohn-Sham Hamiltonian in DFT calculations in order to obtain charge-localized states, which can be used to approximate diabatic states in electron-transfer reactions.

- CDFT is a powerful tool to construct diabatic states, which may not be accessible with standard SCF calculations, and to calculate the corresponding electronic coupling and other electron transfer parameters;
- Q-Chem offers two types of constraints: total charge or spin charge constraints on different molecular fragments.



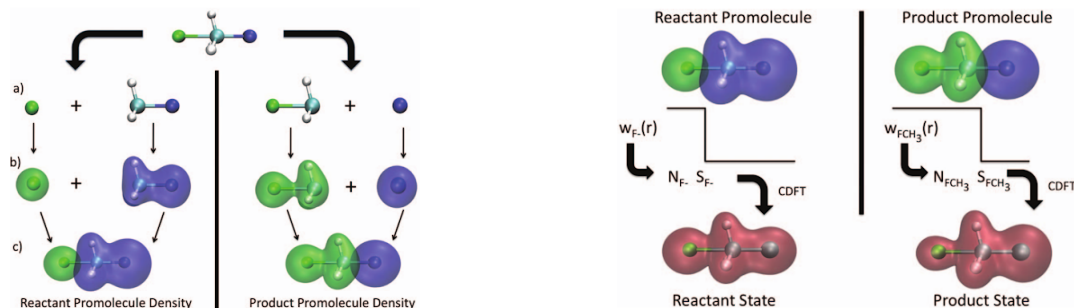
(a) Total charge difference of the charge-localized state of the FAAQ molecule



(b) Spin charge of the charge-localized state of the Cu-Ox molecule

Predicting Reaction Barrier Heights with Constrained DFT Configuration Interaction (CDFT-CI):

- Transition-state energies are searched in the configuration space spanned by two diabatic-like configurations: reactant and product;
- The reactant and product configurations are obtained by applying charge- and spin-density constraints in DFT calculations, to maximally retain the reactant and product electronic character;
- CDFT-CI significantly improves the calculated reaction barrier heights compared to traditional DFT.



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