Simulation of MOFs with classical MD

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Metallorganic frameworks (MOFs) have proven to be effective catalysts for the electroreduction of CO2 in aqueous media. However, the factors responsible for such enhancements remain unknown.

Reactivity in side MOF pores has been studied with discrete DFT in cluster models. These models describe MOFs well locally but fail to capture the effects of interfaces, counterions, electric fields, and defects. In our group, we are developing a reactive forcefield for MOFs based on classical mechanics and empirical valence bonds. We believe that it will open a window into overlooked effects in MOF-mediated reactions.

Semi-empirical π-electron theory – a blast from the past

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Some of the first practically useful quantum-chemical theories were based on a treatment of the π-electrons in conjugated organic molecules. Hückel theory had extensive influence on organic chemistry, and served as the foundation for perturbation theory treatments which are still taught today.

To progress beyond Hückel theory, we need to add electron correlation, which was accomplished independently by Pople and Parr and Pariser in what became known as the Pariser-Parr-Pople (PPP) method. Due to its relatively good accuracy for predicting electronic excitation energies, PPP theory was thoroughly developed in the 50's–70's and remained in use in the dye industry at least until the 80's.

While much more accurate methods are available today, semi-empirical methods like Hückel and PPP theory have gained in popularity due to their speed and application in for high-throughput screening and machine learning. Due to their simplicity and use of a minimal basis set, they are also very interpretable.

In this talk, I will show applications of simple π-electron methods to (1) screen for the next generation of OLED materials, (2) perform parameter tuning and alchemical optimization using differentiable Hückel theory, and (3) quantify the aromatic properties of polycyclic aromatic hydrocarbons in the ground and excited states. We have implemented these methods in the open-source Python package Coulson, that is freely available to the community and integrates with PySCF.