Computational simulations on the metal-organic framework: UiO-66

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Metal-organic frameworks (MOFs) constitute a new generation of porous crystals. They can be described as crystalline hybrid inorganic/organic solids with structures which are composed of clusters of a few metallic atoms held together in a three-dimensional structure by organic linkers. This class of compounds has the remarkable advantage of combining both organic and inorganic fragments as part of the same structure. The remarkable crystallinity of MOF structures defines pores and cavities on the nanometric scale. The possibility for guest molecules to enter the internal voids of MOFs, frequently of high volume, causes these materials in many respects to resemble the behavior of zeolites. However, MOFs are attractive not only because of the structural diversity that they provide, but also because of their remarkable physico-chemical properties. Currently, MOFs are considered as important materials of academic interests and with possible industrial applications within catalysis, petrochemistry, gas adsorption and storage (e.g., H_2, CH_4, CO_2, etc.), selective separation, sensing, molecular recognition, and so on.

However, MOFs have applications limited to the gas adsorption and seperation due to the weakness and lack of fundamental understanding and detailed knowledge of the relationship between structure and properties from experiments.

On the other hand, computational chemistry and physics have made dramatic advances in the past two decades, enabling the prediction of novel molecules and exotic extended structures that often contradict the chemical and physical intuitions. Many theoretical chemists and physicists have participated in this endeavor by proposing myriads of unusual molecules and bulk solid structures. The computational simulations are powerful tool to predict new materials as well as their properties and get insight into the prerequisite experimental aspects. Most of the publications relating to MOFs are experimental in nature owing to the fact that the number of atoms involved in simulations is much greater than that in many other materials. Thousands of different MOFs have been synthesized so far. However, the enormous number of different possible MOFs means that purely experimental means for screening or designing optimal MOFs for targeted applications is inefficient. Atomic-level simulations provide a means to complement experimental methods for identifying potential MOFs.

This presentation will demonstrate how the computational simulations correct the experimental MOF structures and provide detailed knowledge of electric structure, chemical bonding, optical properties. This may shed insight into the potential synthesis and application of novel and stable MOFs.