Contribution ID : **162** Type : **Oral Presentation**

Functionalization of NU-1000 MOFs with Phosphonate Ligands: An Ab-Initio DFT and NMR Study

Metal-organic frameworks (**MOFs**) have emerged as a revolutionary class of materials characterized by remarkable versatility and extensive applications across various scientific disciplines. MOFs, composed of metal nodes interconnected by organic linkers, exhibit exceptional tunability, high surface areas, and intriguing porosity. These distinctive attributes confer upon MOFs extraordinary properties, making them highly sought after for diverse applications encompassing gas storage and separation, catalysis, sensing, and drug delivery systems.

Within the diverse range of MOFs, the **NU-1000** structure has attracted significant attention due to its remarkable properties and potential applications across various disciplines. NU-1000 is an exceptionally robust and highly stable MOF characterized by a meticulously defined structure composed of 558 atoms (264 carbon, 180 hydrogen, 96 oxygen, and 18 zirconium) within its unit cell. The deliberate design and synthesis of NU-1000 serve as a platform for investigating the fundamental principles governing MOF behaviour and provide a roadmap for advancing sophisticated functional materials.

In this study, ab-initio density functional theory (**DFT**) calculations were used to investigate the functionalization of the Zr6 cluster-nodes, particularly focusing on their catalytic and reactive properties with phosphonate molecules. The adsorption energies and structural parameters of the NU-1000 structure were examined in the presence of five distinct phosphonate molecules, Fig 1. Nuclear magnetic resonance (**NMR**) spectra simulations are conducted to elucidate the diverse chemical shift ranges that the various atomic reconstructions can exhibit, contingent upon their atomic adsorption (coordination) within each type of 31P NMR. This comprehensive analysis aims to provide an exhaustive overview of each type of Phosphonate molecule. A comparison between the simulated and experimentally measured spectra establishes the reliability of the DFT calculations. This work, conducted as part of the PHOSPORE project, advances the understanding of MOFs and facilitates the tailored design of MOFs for a wide range of applications in catalysis and functional materials.

Figure 1. NU-1000 components and functionalizing molecules: (a) Zr6 node, (b) organic linker. Phosphonate molecules studied: (c) Phenylphosphonic acid, (d) Phenyl di-phosphonic acid, (e) Phenylphosphinic acid, (f) Phenyl di-phosphinic acid, (g) Propylphosphonic acid.

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