MS35-P2 Using PIXEL to investigate as adsorption in metal-organic frameworks

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Over the last decade, the study of metal-organic frameworks (MOFs) has become a very popular avenue of research, with particular focus on their potential uses for gas storage and separation. Structurally, MOFs are made up of metal-ligand nodes that are connected by organic bridging ligands to form 3-dimensional porous frameworks. Synthesis of such frameworks can be achieved by combinations of these nodes and linkers to give a variety of structures with different pore sizes, topologies and chemical functionalities.[1] This so-called "modular synthesis" means that it is theoretically possible to create a vast catalogue of metal-organic frameworks for specific applications that is not possible for other porous materials such as zeolites.[2]

To date, there are over 10,000 MOF structures recorded in the Cambridge Structural Database (CSD).[3] However, comparatively little work has been done to investigate the precise locations of adsorption sites in these structures since such experiments can be difficult to carry out and require specialist equipment.[4] Additionally, the time taken to determine these positions for such a large number of structures experimentally renders such experimental methods impractical. Consequently, computational modelling of gas adsorption in metal-organic frameworks is a very appealing alternative, as calculations can be performed under a range of different simulated conditions, and additionally theoretical MOFs can be tested for suitability before any synthetic work is undertaken.

This presentation, timed to coincide with the 50th anniversary of the Cambridge Structural Database, demonstrates how geometric analysis and PIXEL[5] energy calculations have been used to investigate adsorbate-adsorbent interactions in a range of metal-organic frameworks and gas molecules. Results are reported for adsorption between MOF-5 and Ar, MOF-5 and N_2, and HKUST-1 and CO_2. The locations of the adsorption sites and the calculated energies, which show differences in the Coulombic or dispersion characteristic of the interaction, are compared to experimental data and literature energy values calculated using standard computational methods of analysis for adsorption in metal-organic frameworks.

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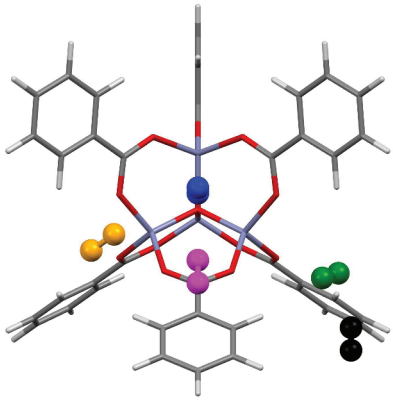

Figure 1. Nitrogen adsorption sites in MOF-5 calculated using PIXEL

Keywords: Gas adsorption, metal-organic frameworks, PIXEL