Strength and nature of host-guest interactions in metal-organic frameworks from a quantum chemical perspective

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A key feature of metal-organic frameworks (MOFs) is their ability to capture, transport, and release guest molecules. The nature, quality, and quantity of the associated absorption depends on pore size and volume, surface area, solvent, and in particular the host-guest intermolecular interactions.

Various methods for the analysis of intermolecular interactions have been described in the literature and were applied to study e.g. chemical reactivity, catalysis, biomolecular interactions, or organic electronics. However, the application of such methods to host-guest interactions in MOFs is still scarce. For this reason, we computed periodic and finite wavefunctions for well-chosen MOF-guest systems and tested these tools [1]. This includes the interaction energy, its decomposition with different energy decomposition schemes, investigation of the electron density with Bader's quantum theory of atoms in molecules, the non-covalent interaction index [2], or the density overlap regions indicator [3]. This analysis contributes to the understanding of host-guest interactions, with the ultimate goal of rationally designing MOFs for targeted applications.

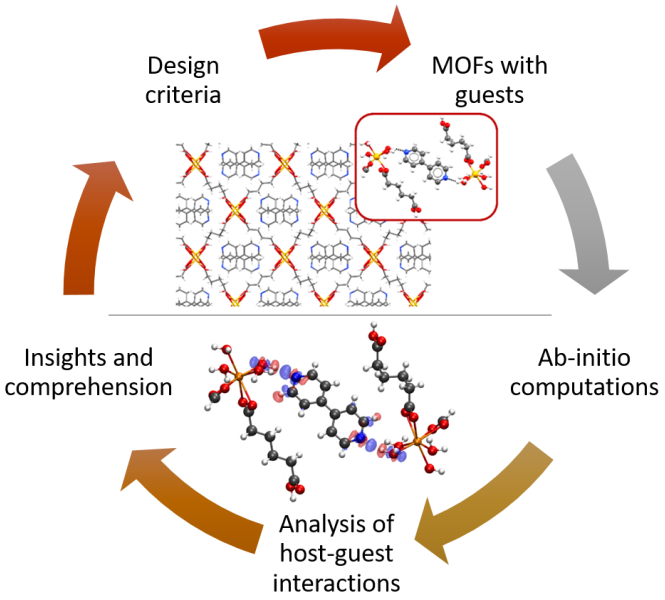

Figure 1. Our research focuses on the identification, visualization, analysis, and quantification of host-guest interactions in order to provide a fundamental molecular-level insight into the adsorption behaviour of MOFs.

[1] Ernst, Michelle; Gryn'ova, Ganna (2021): Strength and Nature of Host-Guest Interactions in Metal-Organic Frameworks from a Quantum-Chemical Perspective. ChemRxiv. Preprint. https://doi.org/10.26434/chemrxiv.14363024.v1

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