Insights into the nature of host-guest interactions in emergent framework materials

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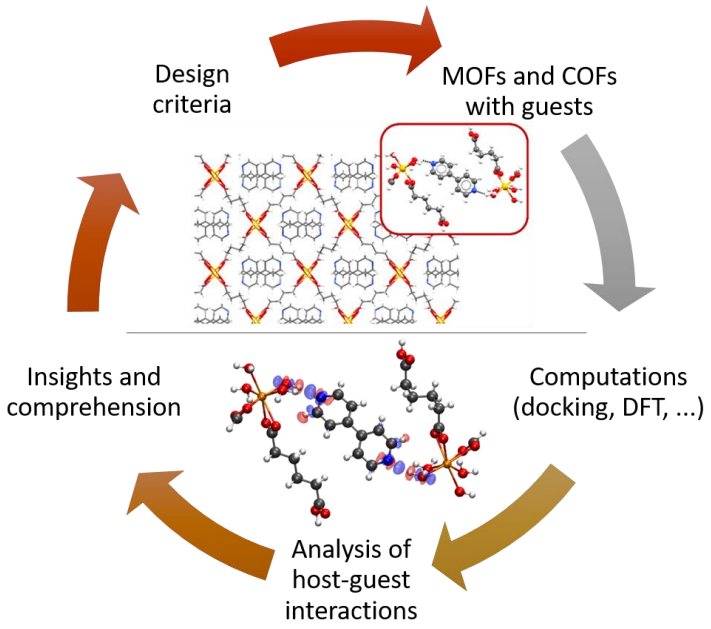
A key feature of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) is their ability to capture, transport, and release guest molecules. The nature, quality, and quantity of the associated absorption depend on pore size and volume, surface area, chemical environment, and in particular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

But how does the functionalization of a MOF influence the release of a given drug from its pores? And by which mechanism does a COF catalyze a reaction?

To answer these and related questions, we use computational methods: molecular docking to identify adsorption sites, periodic and finite DFT simulations to compute interaction energies, and in-depth analyses of the non-covalent interactions between host frameworks and guests. Based on several different examples and application cases, we show how to identify, characterize, and quantify host-guest interactions using for example the quantum theory of atoms in molecules, the non-covalent interaction index, and various energy decomposition schemes.



We intend to establish a set of design guidelines to tune the host-guest interactions for future targeted applications.

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