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.

We use *in silico* tools to study and characterize these interactions: 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 to characterize them. Based on several different examples and application cases, we show how to identify, quantify, and describe these host-guest interactions and how to relate our results to experimental data.

Eventually, these insights pave the way towards a set of design guidelines to tune the host-guest interactions for future targeted applications.