Poster

From capture to catalysis: Insights from atomistic simulations into MOF and COF host-guest interactions and guest dynamics

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A key feature of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) is their ability to capture, convert, and release guest molecules. This capability is governed by multiple factors such as pore volume and surface area, chemical environment, and the nature of the host-guest intermolecular interactions. X-ray diffraction (XRD) experiments are essential to resolve the atomic structures of the frameworks and, ideally, also the guests. However, while XRD provides irreplaceable structural information, it does not offer insights into the dynamic behaviour of guest molecules or the detailed electronic structure of the host-guest interactions. To bridge this gap, we employ various atomistic simulations: molecular docking to determine adsorption sites, DFT simulations to compute interaction energies, electron density and energy decomposition schemes to characterize the host-guest interactions, and ab initio molecular dynamics to simultaneously capture the precise electronic structure and the dynamics of the investigated processes.

First, we will discuss the correlation between simulated guest positions and those observed via XRD [1]. We will also show the characterization of host-guest interactions [2] and compare these interaction characteristics to experimental observations from drug release studies. This will highlight the promise of MOFs and COFs in drug delivery while also demonstrating the potential of simulations to predict effective drug delivery materials [3].

Following this, we will discuss COFs as catalysts. Catalysis within confined spaces often outperforms that in solution or on the surfaces of conventional heterogeneous catalysts, which can be attributed to the unique molecular interactions and reaction dynamics introduced by the spatial constraints. Results from AIMD calculations will be presented, illustrating the effect of confinement in a COF pore on a specific organic reaction, namely the Diels-Alder reaction (Fig. 1).

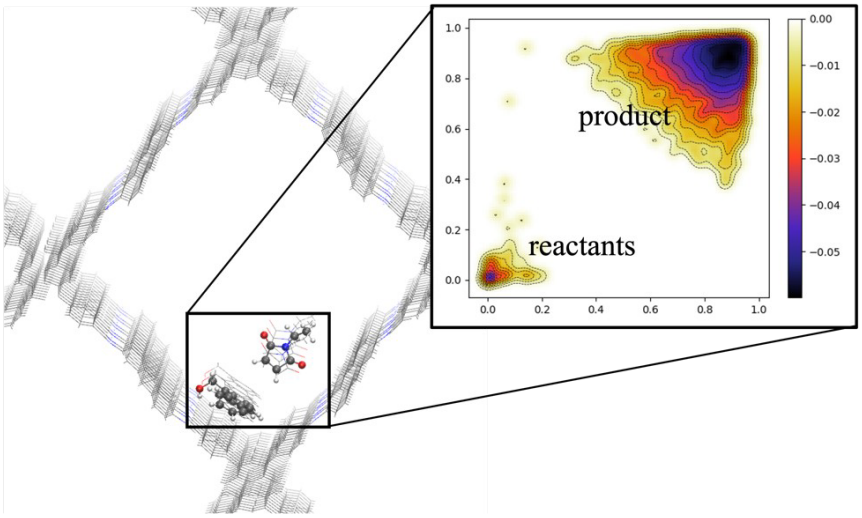

Figure 1. Diels-Alder reactants in COF pore and corresponding simulated free energy surface (Hartree).

[1] Ernst, M., Poręba, T., Gnägi, L. & Gryn'ova, G. (2023). *J. Phys. Chem. C,* **127**, 523-531.

[2] Ernst, M. & Gryn'ova, G. (2022). *ChemPhysChem,* **23**, e202200098.

[3] Ernst, M. & Gryn'ova, G. (2023). *Helv. Chim. Acta*, **106**, e202300013.