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Effect of open metal sites on carbon capture by metal-organic framework (MOF-16); a DFT approach

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Rising CO2 concentrations, reported at 414 ppm in 2021, largely driven by fossil fuel combustion and deforestation, have intensified global efforts to combat climate change. Among various strategies, carbon capture and storage (CCS) has emerged as the most promising. Metal-Organic Frameworks (MOFs), known for their porosity and chemical tunability, have shown significant potential as effective adsorbents for CO2.
MOF-16, in particular, exhibits enhanced CO2 capture capabilities due to the role of open metal site (OMS) defects. These defects create active sites that facilitate CO2 adsorption, but their impact on framework porosity, geometry, and CO2 diffusion remains underexplored. Comprehensive studies are essential to understand these aspects and maximize the potential of OMS defects.
Since their discovery in the late 1990s, MOFs have been evaluated for carbon capture based on parameters like CO2 selectivity, storage capacity, adsorption/desorption kinetics, stability through cycles, and enthalpy of CO2 adsorption. MOFs can be customized with features like OMS, polar functional groups, tunable pore sizes, framework flexibility, and Lewis basic sites. These properties enable multiple interactions with CO2, leading to high adsorption capacity while suppressing competing gases such as N2, CH4, and H2O.
This study aims to use Density Functional Theory (DFT) simulations to examine the formation energies of OMS defects in MOF-16. Preliminary findings suggest that introducing OMS defects improves CO2 adsorption capacity. The study will further analyze the effects of OMS on framework structure, CO2 diffusion, and porosity, offering insights to optimize MOF-16 for carbon capture.
This exploration highlights the importance of MOFs and OMS defects in advancing carbon capture technologies to address rising atmospheric CO2 levels and mitigate climate change.

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