Surface-Coordination Functionalization of Metal-Organic Framework for Selective Carbon Dioxide Capture and Reversible Hydrogenation to Formic Acid

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Conventional functionalization techniques for Metal-Organic Frameworks (MOFs) compromise the simultaneous optimization of structural integrity, CO2 absorption, and catalytic selectivity, diminishing overall performance and restricting new functionalities. Surface functionalizations, although promising, are often hindered by complex, costly processes or weak, unstable interactions. Herein, MOF nanoparticles (NPs) with charged functional groups, UiO-66-NH2, are utilized as surface capping agents for the defective MOF-808 structure through a novel, facile, cost-effective approach, enabling a unified framework for selective CO2 absorption and reversible hydrogenation to formic acid, for the first time. The controlled hydrogen storage and generation are achieved through a directed spatial activation by in situ functionalizing photocatalytic and electrocatalytic reagents, tin oxide NPs and nickel NPs, within the two distinct structures. Detailed characterization, performance evaluations, and computational analysis demonstrated successful attachments through secondary functional coordination sites, which introduced additional active sites, enhanced structural stability, and enabled high CO2 selectivity through positive charge modulation of the surface charge while retaining the high CO2 absorption capacity, surpassing most reported structures. The controlled sequential reactions exhibited selective activation through controlled diffusion of reactants and the synergistic effect with minimal undesired byproducts while attaining high formation rates under ambient conditions, avoiding precious metals requiring challenging controlled environments. This functionalization enables new capabilities to address numerous challenges, such as achieving a low-carbon circular economy.

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