Contrasting Ligand Chemistry and Pore Engineering in Zr-MOFs for Environmental Remediation

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Abstract:

Zirconium-based metal-organic frameworks (Zr-MOFs) are emerging adsorbents for environmental remediation due to their tunable porosity, high surface area, and chemical stability. Structural characterization via FTIR, XRD, BET, and SEM confirmed the materials microporous nature, thermal stability, and morphology-dependent adsorption behavior [1]. Two independent studies comprehensively evaluated three Zr-MOFs—MOF-801, MIP-202, and Muc-Zr MOF—for distinct applications: anionic dye removal and gas capture. The adsorption efficiency of these Zr-MOFs was tested for eliminating an anionic dye, from aqueous solutions. MIP-202 exhibited the highest adsorption capacity, outperforming MOF-801 and Muc-Zr MOF. The second study focused on gas-phase adsorption, comparing the same Zr-MOFs for CO_2 and ethanol vapor capture. MIP-202 demonstrated the highest affinity for CO_2 due to amino groups and extra-framework Cl^- ions, which facilitated strong acid-base interactions. Ethanol adsorption highlighted MIP-202's enhanced performance, driven by van der Waals interactions and hydrogen bonding with Cl^-. Monte Carlo simulations corroborated experimental findings, revealing distinct sorption mechanisms. Muc-Zr MOF, with larger pores, showed weaker confinement effects, while MOF-801's mesoporosity contributed to higher CO_2 uptake despite lower interaction strength [2].

Both studies underscore the critical role of ligand functionalization and textural properties in adsorption performance. MIP-202 consistently emerged as the most effective adsorbent, leveraging its amino groups and structural defects for enhanced interactions with both aqueous dyes and gaseous pollutants. These findings highlight the potential of Zr-MOFs, particularly MIP-202, in addressing diverse environmental challenges, from wastewater treatment to greenhouse gas mitigation.