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Carbon Dioxide Capture in Microporous Metal-Organic Frameworks

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Metal-organic frameworks represent a new class of materials exhibiting high internal surface areas, tunable pore dimensions, and tailorable surface functionality. Research in our laboratory has focused on the development of metal-organic frameworks with surfaces bearing open metal coordination sites for high-enthalpy hydrogen adsorption. Recently, we have initiated efforts to utilize such materials for the selective capture of CO_2 from flue gas. Here, open metal coordination sites can deliver a high CO_2 loading capacity at low pressures. However, additional criteria, such as water stability and the selective binding of CO_2 over N₂, must also be taken into consideration. Towards that end, we have targeted air- and water-stable frameworks bearing surfaces coated with amine groups. For example, the use of 1,3,5-benzenetristriazolate (BTTri³⁻) as a bridging ligand has led to sodalite-type frameworks such as HCu[(Cu₄Cl)₃(BTTri)₈], possessing open Cu^{2+} coordination sites and exhibiting good chemical and thermal stability. Attachment of ethylenediamine to the Cu^{2+} sites within this structure generates a material that selectively binds small amounts of CO_2 over N₂. Details of the characterization of this and related materials will be presented.