Computational Design of a Photoresponsive Metal-Organic Framework for Post Combustion Carbon Capture

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A Mg-IRMOF-74-Ⅲ structure with azopyridine molecules attached to its unsaturated metal sites is proposed as a new photoresponsive metal-organic framework (MOF) for CO_2 capture. Computational simulations indicate that the photochemically induced trans-to-cis transition of the material leads to significant alteration in the CO_2 capacity. Specifically, the grand canonical Monte Carlo simulation showed a CO_2 adsorption capacity of 89.6 cm^3/g at the trans phase, which is higher than any other photoresponsive MOF reported thus far. Moreover, a large desorption capacity of 82.7% can be explained from significant alteration of the pore size distribution that comes from the trans-to-cis transition. Our work is anticipated to provide a blueprint for computational designing of the new photoresponsive MOF prior to the actual experimental synthesis.