Title:	Efficient and Highly Selective CO2 Capture, Separation, and Chemical Conversion under Ambient Conditions by a Polar-Group-Appended Copper(II) Metal–Organic Framework
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Abstract:	A polar sulfone-appended copper(II) metal–organic framework (MOF; 1) has been synthesized from the dual-ligand approach comprised of tetrakis(4-pyridyloxymethylene)methane and dibenzothiophene-5,5′-dioxide-3,7-dicarboxylic acid under solvothermal conditions. This has been studied by different techniques that included single-crystal X-ray diffractometry, based on which the presence of Lewis acidic open-metal sites as well as polar sulfone groups aligned on the pore walls is identified. MOF 1 displays a high uptake of CO2 over N2 and CH4 with an excellent selectivity (S = 883) for CO2/N2 (15:85) at 298 K under flue gas combustion conditions. Additionally, the presence of Lewis acidic metal centers facilitates an efficient size-selective catalytic performance at ambient conditions for the conversion of CO2 into industrially valuable cyclic carbonates. The experimental investigations for this functional solvent-free heterogeneous catalyst are also found to be in good correlation with the computational studies provided by configurational bias Monte Carlo simulation for both CO2 capture and its conversion.
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