Title:	Unprecedented High Temperature CO2 Selectivity and Effective Chemical Fixation by a Copper-Based Undulated Metal–Organic Framework
Authors:	Das, Prasenjit (/jspui/browse?type=author&value=Das%2C+Prasenjit) Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.)
Keywords:	Metal organic frameworks Mixtures Ethers Selectivity Gases
Issue Date:	2020
Publisher:	American Chemical Society
Citation:	ACS Applied Materials and Interfaces, 12(33), pp.37137-37146.
Abstract:	Post- and precombustion CO2 capture and separation are the vital challenges from industrial viewpoint, as the accessible technologies are not cost-effective and cumbersome. Thus, the development of functional metal–organic frameworks (MOFs) that are found to be promising materials for selective CO2 capture, separation, and conversion is gaining an importance in the scientific world. Based on the strategic design, a new functionalized triazine-based undulated paddle-wheel Cu-MOF (1), {[Cu(MTABA)(H2O)]·4H2O·2EtOH·DMF}n (where, H2MTABA = 4,4′-((6-methoxy-1,3,5-triazine-2,4-diyl)bis(azanediyl))dibenzoic acid), has been synthesized under solvothermal conditions and fully characterized. MOF 1 contains a one-dimensional channel along the a-axis with pore walls decorated with open metal sites, and multifunctional groups (amine, triazine, and methoxy). Unlike other porous materials, activated 1 (1′) possesses exceptional increment in CO2/N2 and CO2/CH4 selectivity with increased temperature calculated by the ideal adsorbed solution theory. With an increase in temperature from 298 to 313 K, the selectivity of CO2 rises from 350.3 to 909.5 at zero coverage, which is unprecedented till date. Moreover, 1′ behaves as a bifunctional heterogeneous catalyst through Lewis acid (open metal) and Brönsted acid sites to facilitate the chemical fixation of CO2 to cyclic carbonates under ambient conditions. The high selectivity for CO2 by 1′ even at higher temperature was further corroborated with configurational bias Monte Carlo molecular simulation that ascertains the multiple CO2-philic sites and epoxide binding sites in 1′ to further decipher the mechanistic pathway.
URI:	https://pubs.acs.org/doi/10.1021/acsami.0c09024 (https://pubs.acs.org/doi/10.1021/acsami.0c09024) http://hdl.handle.net/123456789/3187 (http://hdl.handle.net/123456789/3187)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/3187/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/3187?mode=full)

(/jspui/handle/123456789/3187/statistics)