Title:	Polar Sulfone-Functionalized Oxygen-Rich Metal–Organic Frameworks for Highly Selective CO2 Capture and Sensitive Detection of Acetylacetone at ppb Level
Authors:	Chakraborty, G. (/jspui/browse?type=author&value=Chakraborty%2C+G.) Das, Prasenjit (/jspui/browse?type=author&value=Das%2C+Prasenjit) Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.)
Keywords:	Polar sulfone-functionalized Metal−organic frameworks Selective CO2 capture Luminescent acetylacetone sensing at ppb level Computational studies
Issue Date:	2020
Publisher:	American Chemical Society
Citation:	ACS Applied Materials and Interfaces 12(10), pp. 11724-11736
Abstract:	A rational combination of an oxygen-rich pyridyl substituted tetrapodal ligand, tetrakis(4-pyridyloxymethylene)methane (TPOM), and a polar sulfone-functionalized conjugated bent dicarboxylate linker, dibenzothiophene-5,5′-dioxide-3,7-dicarboxylic acid (H2(3,7-DBTDC)), with d10 metal centers, Zn(II) and Cd(II), has led to the construction of two new three-dimensional (3D) metal–organic frameworks,{[Zn2(TPOM)(3,7-DBTDC)2]·7H2O·DMA}n (1) and {[Cd2(TPOM)(3,7-DBTDC)2]·6H2O·3DMF}n (2). Single-crystal X-ray analysis indicates that 1 is a 3D framework with a dinuclear repeating unit having two different Zn(II) centers (tetrahedral and square pyramidal) and 2 is a 3D framework comprised of a dinuclear repeating unit with one crystallographically independent distorted pentagonal bipyramidal Cd(II) coordinated to chelating/bridging carboxylates and nitrogen atoms of the TPOM ligand. In both cases, the pores are aligned with oxygen atoms of the TPOM ligand and decorated with polar sulfone moieties. On the basis of the stability established by thermogravimetric analysis and powder X-ray diffraction (PXRD) and the presence of large solvent accessible voids (25.4% for 1 and 40.6% for 2), gas sorption studies of different gases (N2, CO2, and CH4) and water vapor have been explored for both 1 and 2. The CO2 sorption isotherm depicts type I isotherm with an uptake of 93.6 cm3 g–1 (for 1) and 100.6 cm3 g–1 (for 2) at 195 K. Additionally, sorption of CO2 is highly selective over that of N2 and CH4 for both 1 and 2 due to the strong quadrupolar interactions between sulfone moieties and CO2 molecules. Configurational bias Monte Carlo (CBMC) molecular simulation has further justified the highly selective CO2 capture. On the other hand, the luminescence nature of 1 and 2 has been employed for highly selective detection of acetylacetone in aqueous methanol with a limit of 59 ppb in 1 and 66 ppb in 2, which are among the best reported values so far in the literature. The Stern–Volmer plots, spectral overlap, density functional theory calculations, CBMC simulation, and time-resolved lifetime measurements have been utilized for an extensive mechanistic study. The exclusive selectivity for acetylacetone in 1 and 2 have been confirmed by competitive selectivity test. Both exhibited good recyclability and stability after sensing experiments analyzed by fluorescence, PXRD, and field emission scanning electron microscopy studies.
URI:	https://pubs.acs.org/doi/10.1021/acsami.9b22658 (https://pubs.acs.org/doi/10.1021/acsami.9b22658) http://hdl.handle.net/123456789/3369 (http://hdl.handle.net/123456789/3369)

Appears in Collections: Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/3369/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/3369?mode=full)

(/jspui/handle/123456789/3369/statistics)