Electronic Supplementary Information

Tuning the adsorption and separation properties of noble gases and N_2 in CuBTC by ligand functionalization

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Supplementary table

Table S1. Charge for atoms of CuBTCs.

MOF	Atom type	Charge	MOF	Atom type	Charge
CuBTC	C1	0.7780	3F-CuBTC	C1	0.8656
	C2	-0.0920		C2	-0.3312
	C3	-0.0140		C3	0.3722
	O1	-0.6650		O1	-0.6616
	Cu1	1.0980		Cu1	1.0790
	H1	0.1090		F	-0.1229
3OH-CuBTC	C1	0.8643	$3NH_2$-CuBTC	C1	0.9330
	C2	-0.5219		C2	-0.6699
	C3	0.5569		C3	0.7118
	O1	-0.7932		O1	-0.7676
	O2	-0.6196		Cu1	1.1998
	O3	-0.5691		H1	0.4436
	Cu1	1.2069		N	-0.9267
	H1	0.4791			

Table S2. Force field parameters for adsorbates and adsorbents.

molecules	atom	σ(Å)	ε/k_b(K)
Ar	Ar	3.405	120
Kr	Kr	3.690	170
Xe	Xe	4.100	211
N_2(2-site)	N	3.31	36
	COM	0	0
MOFs	C	3.431	52.84
	H	2.42	15.1
	N	3.261	34.724
	O	3.118	30.19
	F	2.997	25.16
	Cu	3.114	2.516

Table S3. The lattice parameters of all MOFs

MOFs	Cell angle (deg)	Unit cell (nm)
CuBTC	α=β=γ=90	a=b=c=2.634
3F-CuBTC	α=β=γ=90	a=b=c=2.631
3OH-CuBTC	α=β=γ=90	a=b=c=2.638
$3NH_2$-CuBTC	α=β=γ=90	a=b=c=2.613