Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A Combined Experimental-Computational Investigation of Water Adsorption in Various ZIFs with SOD and RHO Topology

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Section S1: Details of clusters and partial atomic charges for each ZIF

ZIF-8

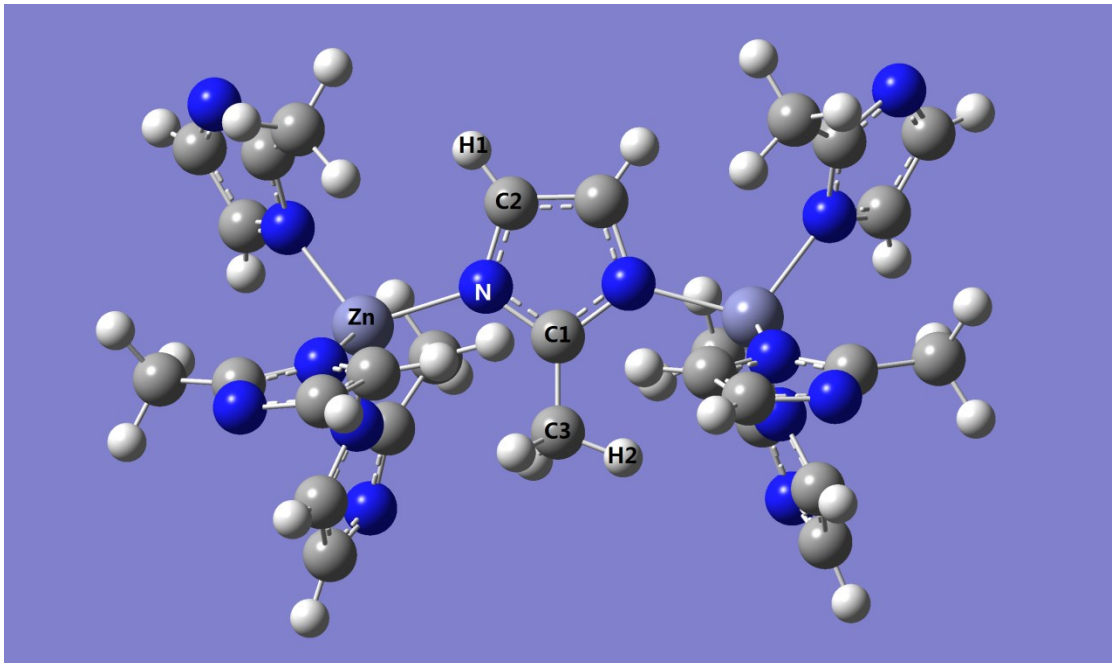

Figure S1. Cluster used for deriving partial charges on ZIF-8 atoms.

Table S1. Partial atomic charges for ZIF-8 atoms.

Atom	Zn	N	C1	C2	C3	H1	H2
Charge(e)	0.884	-0.3985	0.484	-0.124	-0.585	0.1342	0.1452

ZIF-90

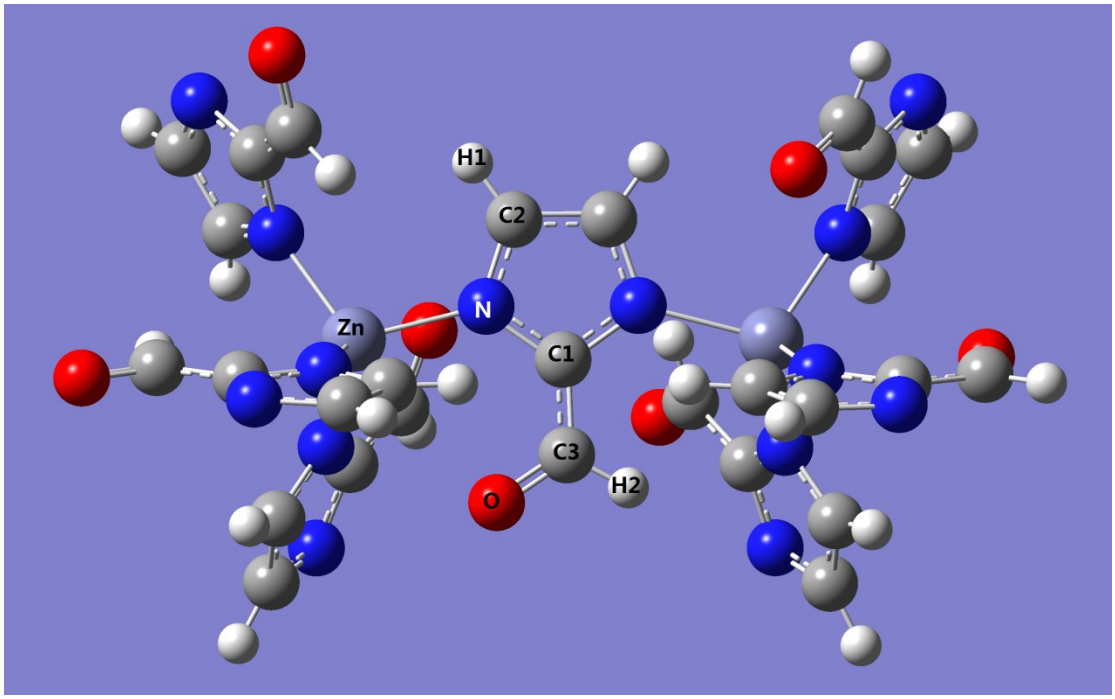

Figure S2. Cluster used for deriving partial charges on ZIF-90 atoms.

Table S2. Partial atomic charges for ZIF-90 atoms.

Atom	Zn	N	C1	C2	C3	H1	H2	O
Charge(e)	0.762	-0.3165	0.253	-0.0171	0.206	0.116	0.0408	-0.4456

SIM-1

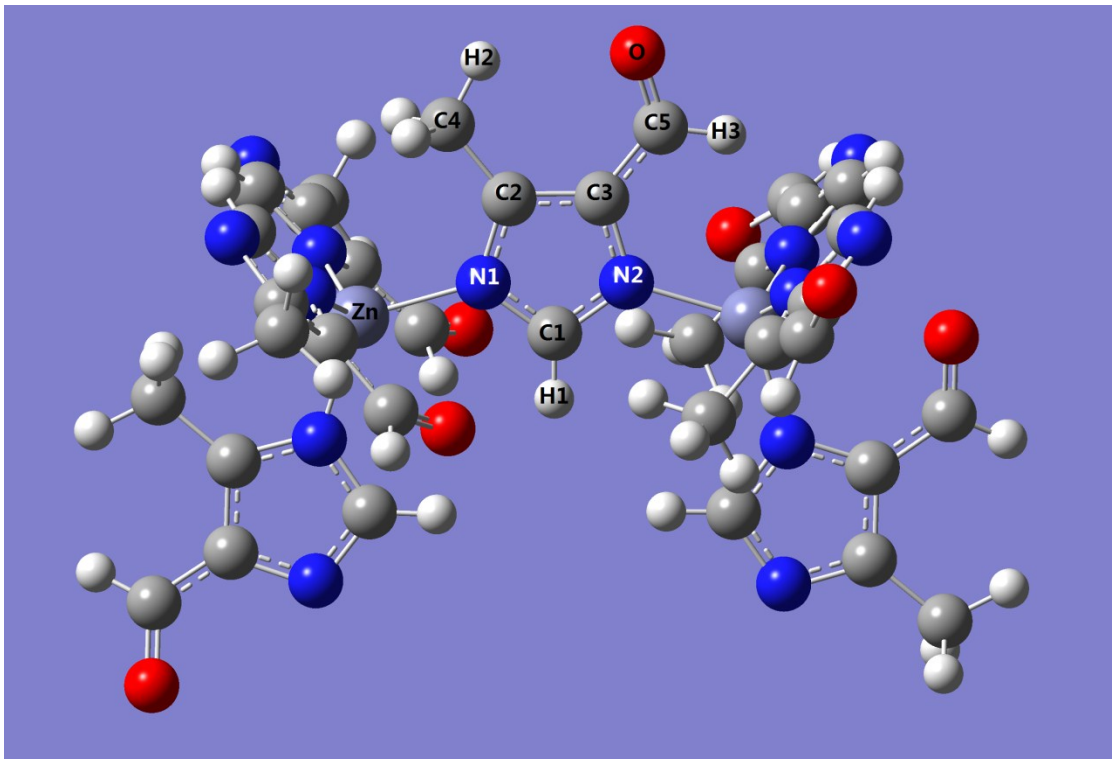

Figure S3. Cluster used for deriving partial charges on SIM-1 atoms.

Table S3. Partial atomic charges for SIM-1 atoms.

Atom	Zn	N1	N2	C1	C2	C3
Charge(e)	0.756	-0.25	-0.389	0.114	0.393	-0.161
Atom	**C4**	**C5**	**H1**	**H2**	**H3**	**O**
Charge(e)	-0.495	0.492	0.087	0.137	-0.075	-0.505

MAF-6

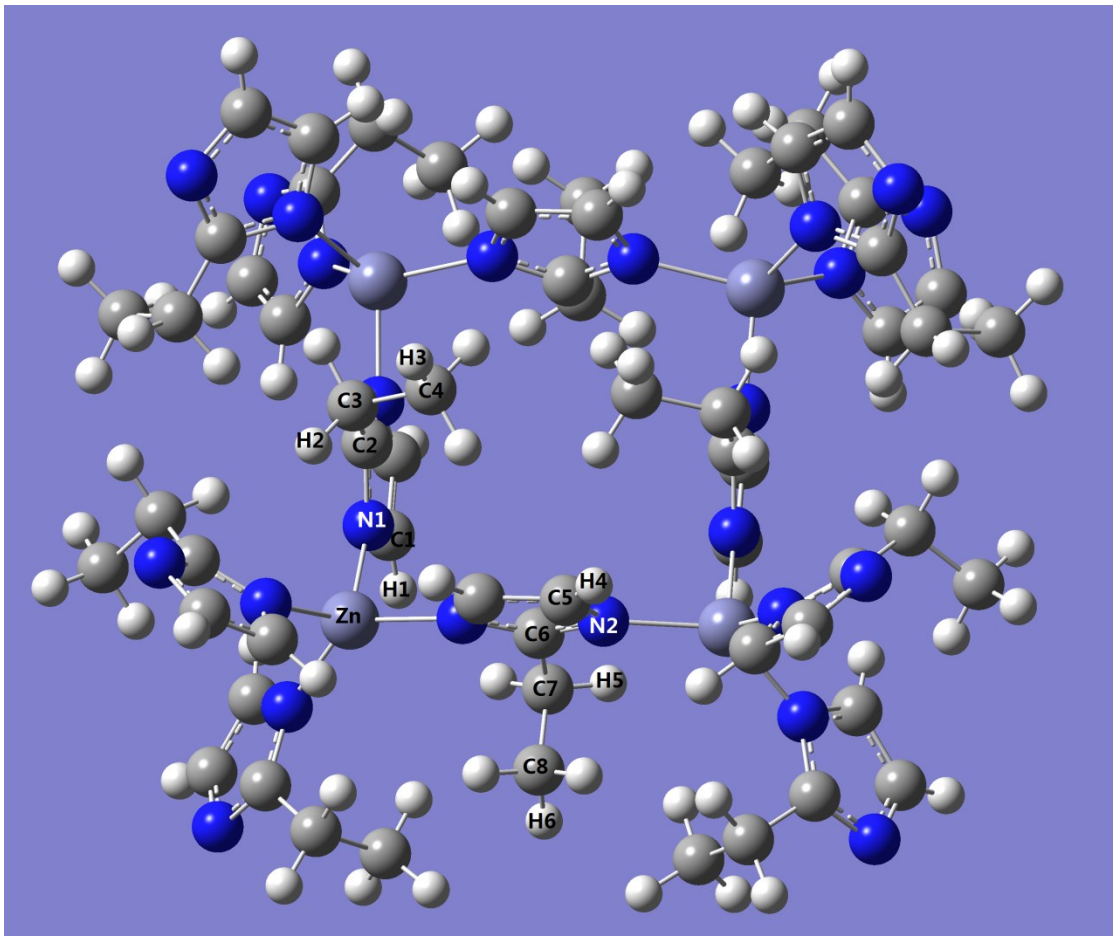

Figure S4. Cluster used for deriving partial charges on MAF-6 atoms.

Table S4. Partial atomic charges for MAF-6 atoms.

Atom	**Zn**	**C1**	**C2**	**C3**	**C4**
Charge(e)	0.757	-0.124	0.018	-0.049	-0.12
Atom		**N1**	**H1**	**H2**	**H3**
Charge(e)		-0.187	0.101	0.0343	0.042
Atom		**C5**	**C6**	**C7**	**C8**
Charge(e)		-0.1918	0.004	-0.428	0.307
Atom		**N2**	**H4**	**H5**	**H6**
Charge(e)		-0.121	0.1345	0.1185	-0.048

ZIF-25

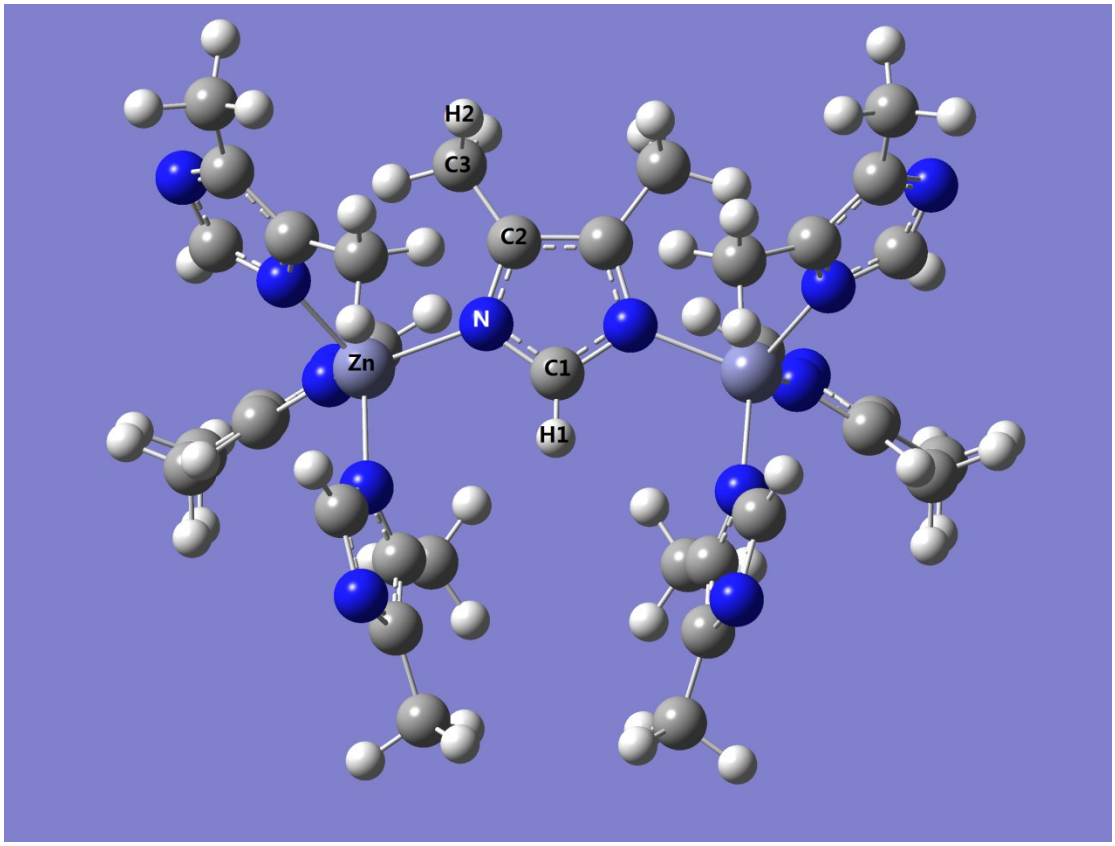

Figure S5. Cluster used for deriving partial charges on ZIF-25 atoms.

Table S5. Partial atomic charges for ZIF-25 atoms.

Atom	Zn	C1	H1	N	C2	C3	H2
Charge(e)	1.006	-0.154	0.128	-0.371	0.166	-0.197	0.0545

ZIF-93

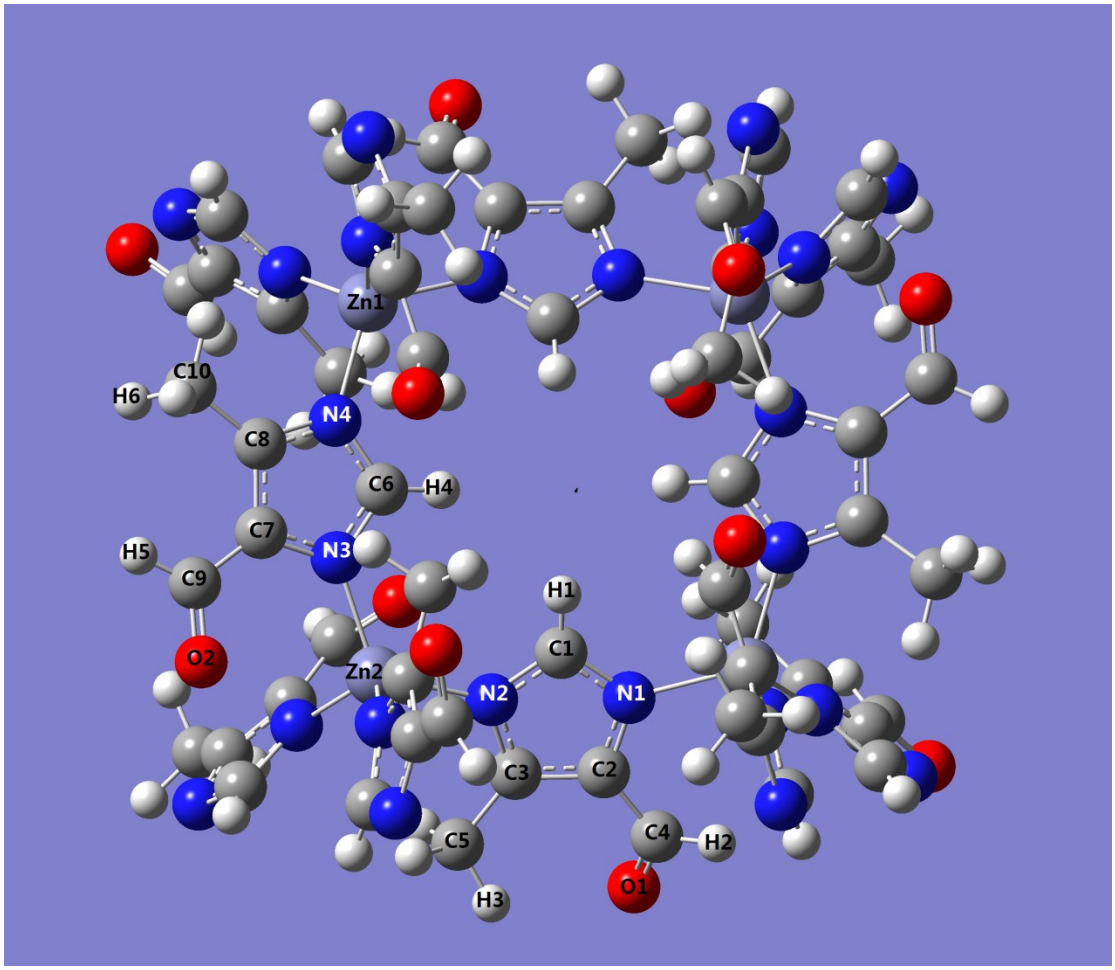

Figure S6. Cluster used for deriving partial charges on ZIF-93 atoms.

Table S6. Partial atomic charges for ZIF-93 atoms.

Atom	**Zn1**	**C1**	**H1**	**N1**	**N2**	**C2**
Charge(e)	0.806	-0.1	**0.119**	-0.26	-0.241	-0.2275
Atom	**C3**	**C4**	**O1**	**H2**	**C5**	**H3**
Charge(e)	0.326	0.55	-0.532	-0.052	-0.432	0.1184
Atom	**Zn2**	**C6**	**H4**	**N3**	**N4**	**C7**
Charge(e)	0.78	-0.083	0.15	-0.0321	-0.202	-0.2
Atom	**C8**	**C9**	**O2**	**H5**	**C10**	**H6**
Charge(e)	0.132	0.405	-0.526	0.0462	-0.2	0.0704

ZIF-97

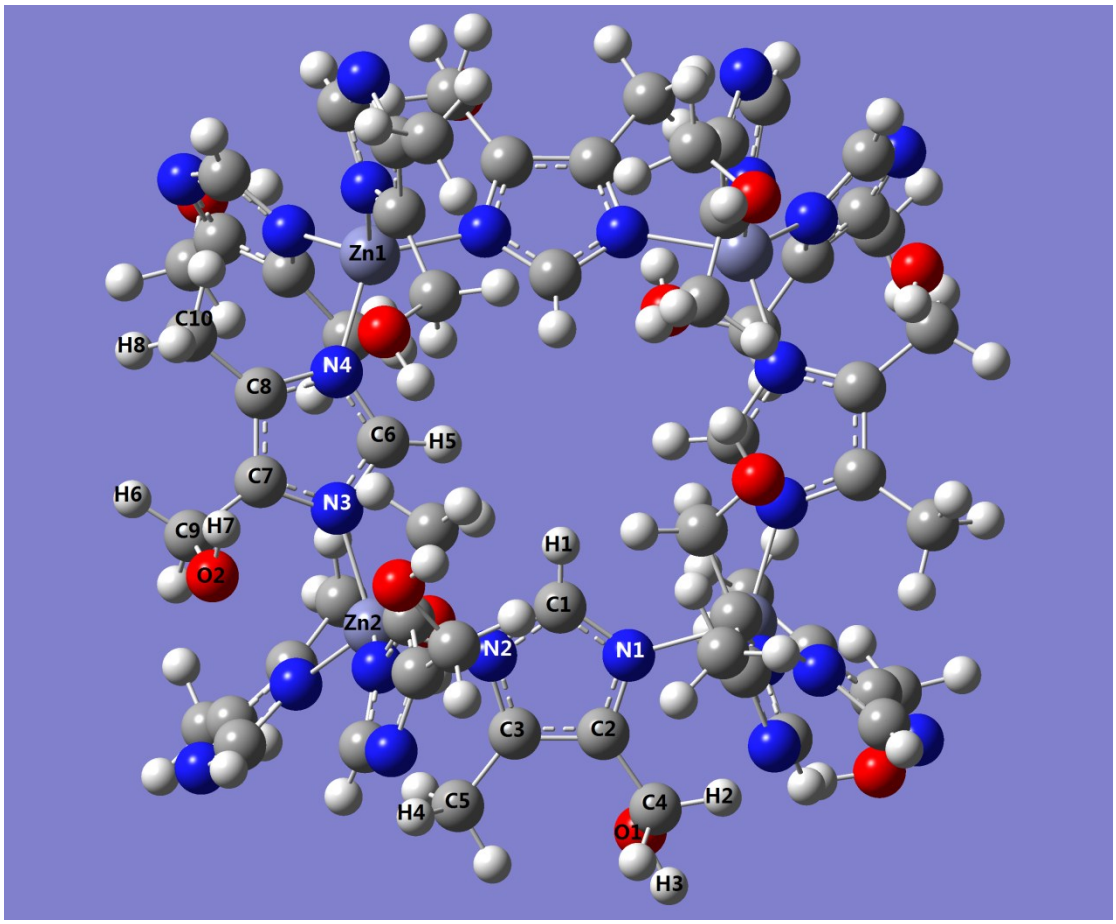

Figure S7. Cluster used for deriving partial charges on ZIF-97 atoms.

Table S7. Partial atomic charges for ZIF-97 atoms.

Atom	**Zn1**	**C1**	**H1**	**N1**	**N2**	**C2**	**C3**
Charge(e)	0.828	-0.066	0.123	-0.31	-0.353	-0.174	0.355
Atom	**C4**	**H2**	**O1**	**H3**	**C5**	**H4**	
Charge(e)	0.548	-0.091	-0.68	0.355	-0.44	0.102	
Atom	**Zn2**	**C6**	**H5**	**N3**	**N4**	**C7**	**C8**
Charge(e)	0.932	-0.022	0.11	-0.187	-0.25	-0.137	0.112
Atom	**C9**	**H6**	**O2**	**H7**	**C10**	**H8**	
Charge(e)	0.24	0.017	-0.615	0.35	-0.156	0.053	

Section S2: DREIDING force field parameters of ZIF atoms

Table S8. DREIDING parameters of ZIF atoms.

Atom	σ (Å)	ε/k_B(K)
Zn	4.045	27.676
C	3.473	47.854
N	3.263	38.948
O	3.033	48.156
H	2.846	7.649

Section S3: Lennard-Jones (LJ) parameters of water and CO_2

Table S9. TIP3P parameters of water and EPM2 parameters of CO_2.

	LJ parameters and charges				bond stretching	bond bending	Ref.
	site	σ (Å)	ε/k_B(K)	charge(e)			
H_2O	O	3.151	76.42	-0.834	$r_{O\text{-}H}$=0.9572 Å	$\theta^0{}_{\angle H\text{-}O\text{-}H}$ = 104.52°	1
	H	0	0	0.417			
CO_2	C	2.76	28.13	0.6512	$r_{O\text{-}H}$=1.149 Å	$\theta^0{}_{\angle O\text{-}C\text{-}O}$ = 180°	2
	O	3.03	80.51	-0.3256			

Section S4: Low and high magnification SEM images of ZIF-90

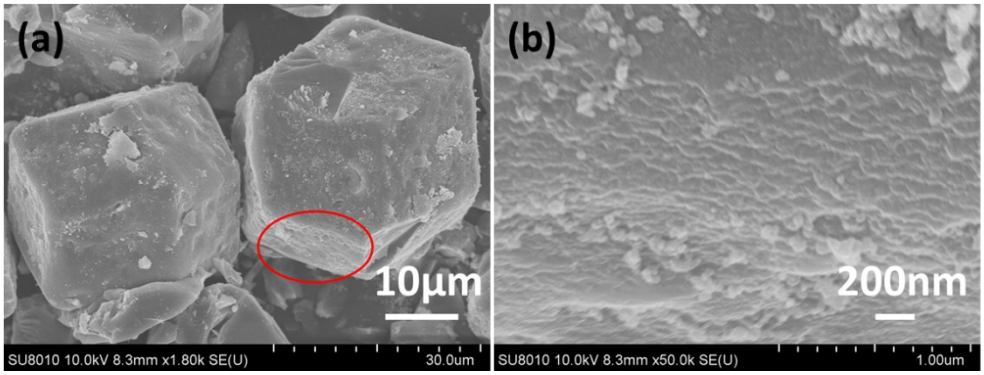

Figure S8. Low (a) and high (b) magnification SEM images of ZIF-90.

Section S5: Simulation water adsorption heat data

Table S10. The specific values of simulated water adsorption heat of ZIFs at infinite dilution.

ZIFs	ZIF-8	ZIF-90	SIM-1	MAF-6	ZIF-25	ZIF-93	ZIF-97
Q^a (kJ/mol)	10.73	31.35	60.25	9.91	17.24	52.18	46.05
Q^b (kJ/mol)	13.60	41.70	—	—	—	55.29	50.14

[a]Simulated water adsorption heat of this work. [b]Simulated water adsorption heat of ref. 3

Section S6: Simulation CO_2 adsorption isotherms

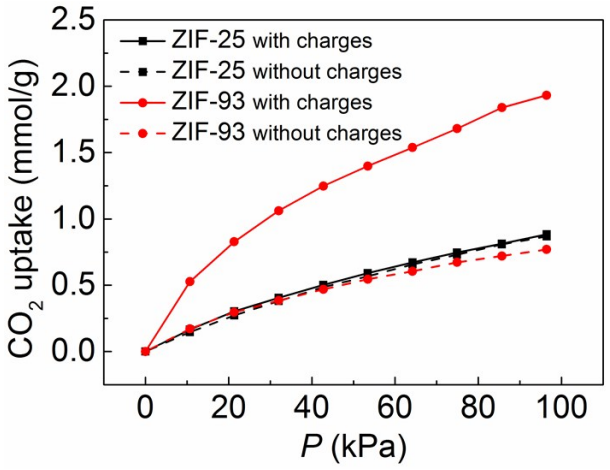

Figure S9. Simulated the CO_2 adsorption isotherms at 298K of ZIF-25 and ZIF-93.

Section S7: Effect of particle size

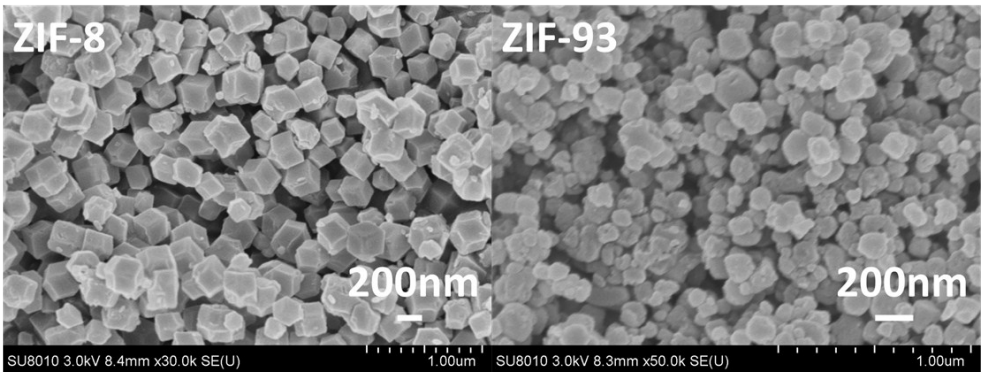

Figure S10. SEM images of ZIF-8 (0.2 μm) and ZIF-90 (0.1 μm).

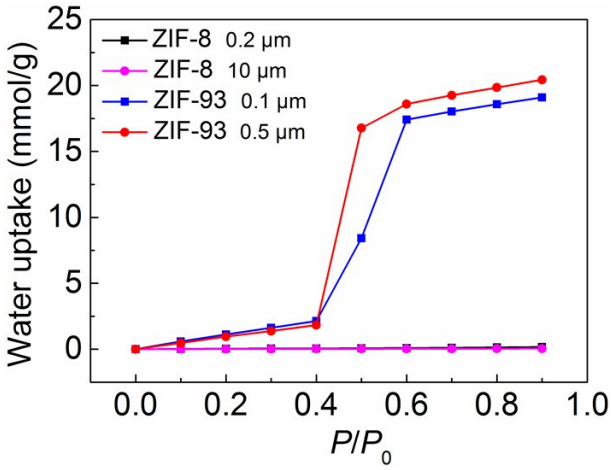

Figure S11. Experimental water adsorption isotherms at 298 K of ZIF-8 (0.2 μm), ZIF-8 (10 μm), ZIF-93 (0.1 μm), and ZIF-93 (0.5 μm).

References

1 P. Mark and L. Nilsson, *Journal of Physical Chemistry A*, 2001, **105**, 9954-9960.

2 J. G. Harris and K. H. Yung, *Journal of Physical Chemistry*, 1995, **99**, 12021-12024.

3 H. Amrouche, B. Creton, F. Siperstein and C. Nieto-Draghi, *RSC Advances*, 2012, **2**, 6028.