Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information for

What Makes Zeolitic Imidazolate Frameworks Hydrophobic or Hydrophilic? Impact of Geometry and Functionalization on Water Adsorption

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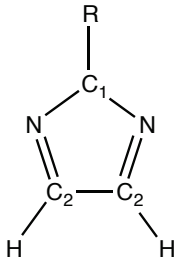

	SALEM-2	ZIF-8	ZIF-Cl	ZIF-90	ZIF-65
Zn	1.10	1.10	0.79	0.85	0.792
N	–0.54	–0.54	–0.17	–0.30	–0.12
C_1	0.64	0.64	0.47	0.48	0.45
C_2	–0.08	–0.08	–0.32	–0.20	–0.30
H	0.144	0.144	0.1725	0.14725	0.172
–R	**–H**	**–CH_3**	**–Cl**	**–HCO**	**–NO_2**
C	—	–0.67	—	0.30	—
O	—	—	—	–0.52	–0.53
H	–0.238*	0.144	—	–0.03	—
N	—	—	—	—	0.71
Cl	—	—	–0.23	—	—

Table S1. Atomic point charges used to model the various ZIFs studied in this work.

** Since SALEM-2 was not studied by Amrouche et al. (ref. 44), we approximated the charge of the H atom by the total charge of the CH_3 group in closely related ZIF-8. We checked that this approximation does not impact the resulting adsorption isotherm and heat of adsorption, because the water–ZIF interactions are dominated by dispersive interactions in this hydrophobic material.*

	ZIF-7
Zn	1.10
N	–0.465
C_1	0.39
C_2	0.00
C_3	–0.120
H	0.094

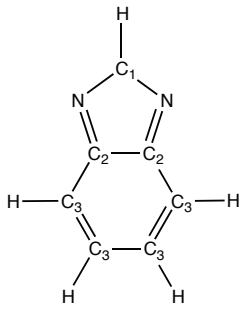

Table S2. Atomic point charges used to model ZIF-7.

Atom	ε (K)	σ (Å)
Zn	43.084	2.338
N	23.974	3.997
O	20.847	3.118
Cl	78.872	3.516
C	36.483	3.259
H	15.288	2.440

Table S3. Van der Waals parameters used for ZIF atoms.

	ε (K)	σ (Å)
H_2O	78.03	3.1536

$r_{O\text{-}H}$	$\widehat{HOH}$	q (O)	q (H)	q (M)	$r_{O\text{-}M}$
0.9572 Å	104.52°	0	0.52	–1.04	0.15 Å

Table S4. Parameters of the water TIP4P model.

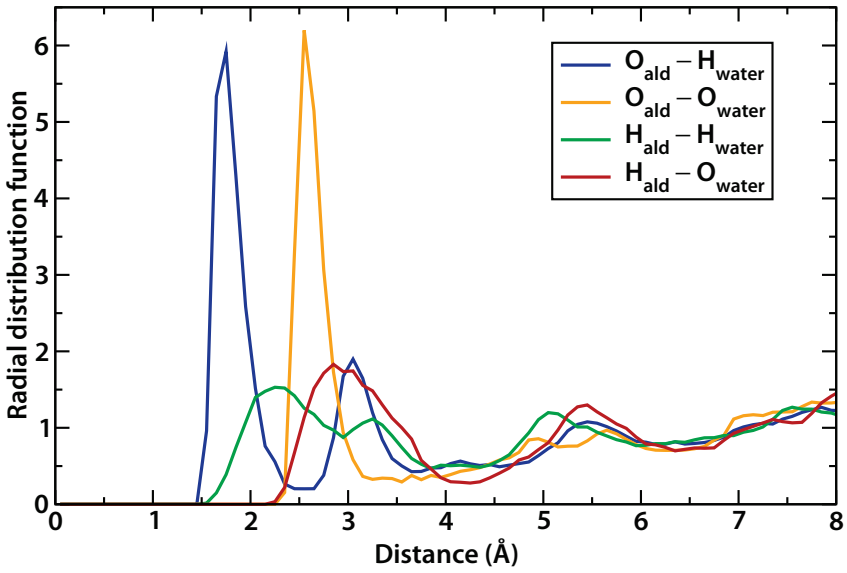

Figure S1. Aldehyde–water radial distribution functions for water adsorbed in ZIF-90 at $P = 0.2$ kPa.