Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

A Computational Screening of Iodine Uptakes in Zeolitic Imidazolate Frameworks in a Water-containing System

Supporting Information

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Table S1. Linker types of ZIFs

name	composition	linker		Reference
ZIF-8	$Zn(mIm)_2$	mIm	2-methylimidazolate	[1]
ZIF-10	$Zn(Im)_2$	Im	imidazolate	[1]
ZIF-60	$Zn_2(Im)_3(mIm)$	Im mIm	imidazolate 2-methylimidazolate	[2]
ZIF-82	Zn(cnIm)(nIm)	cnIm nIm	4-cyanoimidazolate 2-nitroimidazolate	[3]
ZIF-3	$Zn(Im)_2$	Im	imidazolate	[1]
ZIF-80	Zn(dcIm)(nIm)	dcIm nIm	4,5-dichloroimidazolate 2-nitroimidazolate	[3]
ZIF-2	$Zn(Im)_2$	Im	imidazolate	[1]
ZIF-67	$Co(mIm)_2$	mIm	2-methylimidazolate	[2]
ZIF-79	Zn(mbIm)(nIm)	mbIm nIm	5-methylbenzimidazolate 2-nitroimidazolate	[3]
ZIF-96	$Zn(cyamIm)_2$	cyamIm	5-cyanoaminoimidazolate	[4]
ZIF-90	$Zn(Ica)_2$	Ica	imidazolate-2-carboxyaldehyde	[5]
ZIF-93	$Zn(almeIm)_2$	almeIm	4-aldemethylimidazolate	[4]
ZIF-69	Zn(cbIm)(nIm)	cbIm nIm	5-chlorobenzimidazolate 2-nitroimidazolate	[3]
ZIF-97	$Zn(hymeIm)_2$	hymeIm	4-hydroxymethyl-5-methylimidazolate	[4]
ZIF-65	$Co(nIm)_2$	nIm	2-nitroimidazolate	[2]
ZIF-81	Zn(brbIm)(nIm)	brbIm nIm	5-bromobenzimidazolate 2-nitroimidazolate	[3]
ZIF-78	Zn(nbIm)(nIm)	nbIm nIm	5-nitrobenzimidazolate 2-nitroimidazolate	[3]
ZIF-25	$Zn(dmIm)_2$	dmeIm	4,5-dimethylimidazolate	[4]
ZIF-91	$Zn(hmIm)_2$	hmIm	2-hydroxymethylimidazolate	[5]
Y1	$Zn(Im)_2$	Im	imidazolate	[6]
Y3	$Zn(Im)_2$	Im	imidazolate	[6]

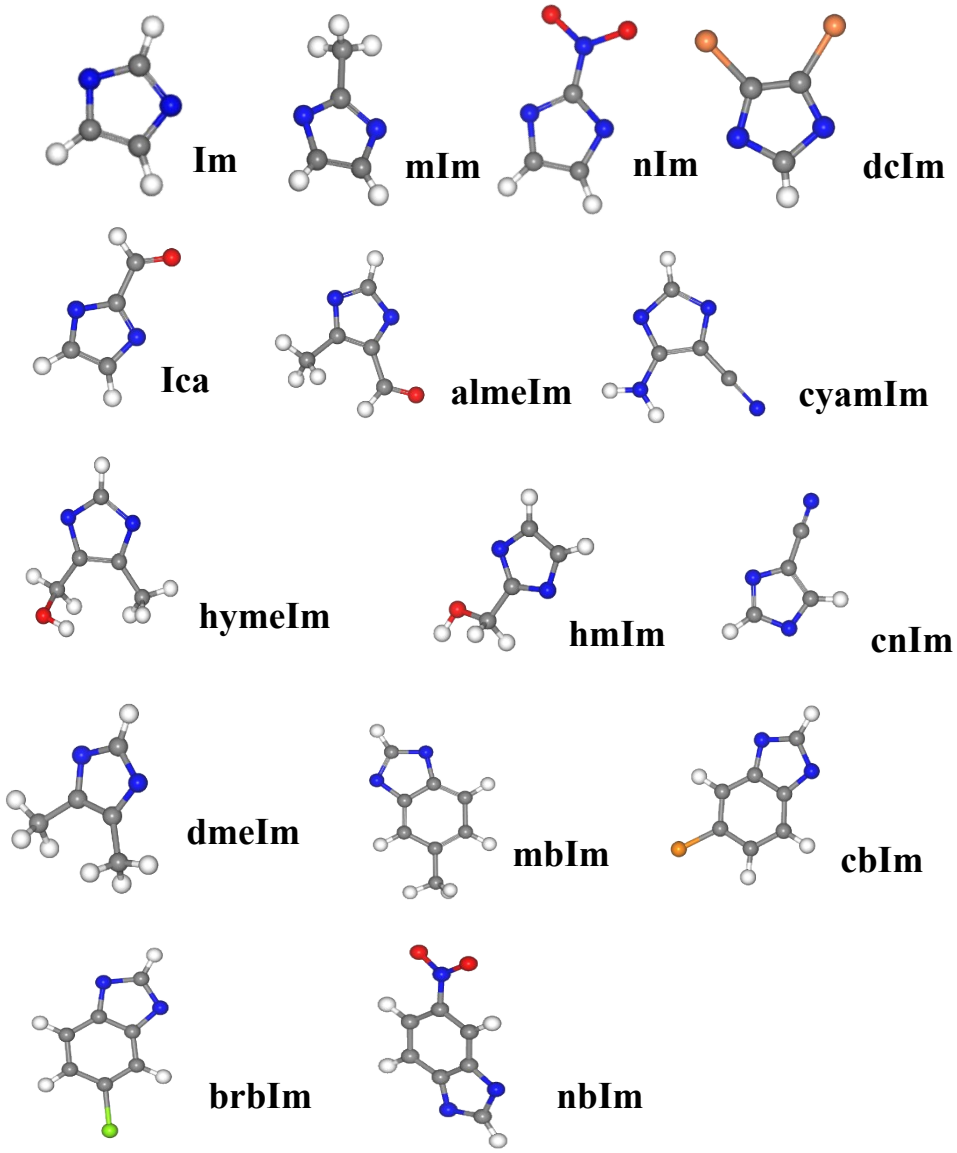

Figure S1. Linker types of ZIFs. Atom colors: C, Gray; H, white; N, blue; O, red; Cl, orange; Br, green.

Table S2. Potential Parameters of ZIFs

site	σ(Å)	ε/k_B(K)
C	3.431	52.79
H	2.571	22.122
N	3.26	34.691
Zn	2.462	62.343
Co	2.559	7.039
O	3.118	30.166
Cl	3.516	114.128
Br	3.732	126.194

Table S3. Atomic charges of ZIF-10

Atom	Charge(e)
Zn	0.7979
N1	-0.3062
N2	-0.2750
C1	0.0290
C2	0.1544
C3	0.0626
C4	-0.0687
H1	0.0565
H2	0.0097
H3	0.0089
H4	0.0546

Table S4. Atomic charges ZIF-60

Atom	Charge(e)
Zn	0.8952
N1	-0.4839
N2	-0.3421
C1	0.2288
C2	0.0900
C3	0.3896
C4	-0.0773
C5	-0.1633
H1	0.0512
H2	0.0070
H3	0.0804
H4	0.0477

Table S5. Atomic charges of ZIF-82

Atom	Charge(e)
Zn	0.7910
N1	-0.2839
N2	-0.5342
N3	-0.4353
N4	0.3770
O	-0.3579
C1	0.1860
C2	0.0102
C3	0.0413
C4	0.4037
C5	0.4533
C6	0.0490
H1	0.0899
H2	0.0429
H3	0.0976

Table S6. Atomic charges of ZIF-96

Atom	Charge(e)
Zn1	0.6342
Zn2	0.9203
N1	-0.4847
N2	-0.7835
N3	-0.5257
N4	-0.3627
C1	0.1640
C2	0.5131
C3	-0.1342
C4	0.4781
H1	0.1706
H2	0.2882

Table S7. Structural parameters of ZIFs

name	unit cell (Å)	cell angle (°)	atom number/unit
ZIF-8	α =16.991 β =16.991 γ =16.991	α = β = γ = 90°	276
ZIF-10	α =27.061 β =27.061 γ =19.406	α = β = γ = 90°	544
ZIF-60	α =27.245 β =27.245 γ =19.225	α = β = γ = 90°	592
ZIF-82	α =26.442 β =22.899 γ =18.970	α = β = 90° γ =120°	480
ZIF-3	α =18.970 β =18.970 γ =16.740	α = β = γ = 90°	272
ZIF-80	α=26.307 β=22.783 γ =19.361	α = β = 90° γ =120°	456
ZIF-96	α=28.356 β=28.356 γ =28.3561	α = β = γ = 90°	1104
ZIF-67	α=16.959 β=16.959 γ =16.959	α = β = γ = 90°	276
ZIF-79	α=25.926 β=22.452 γ =19.653	α = β = 90° γ =120°	672
ZIF-2	α=9.679 β=24.114 γ =24.450	α = β = γ = 90°	272
ZIF-90	α=17.271 β=17.271 γ =17.271	α = β = γ = 90°	252
ZIF-93	α=28.357 β=28.357 γ =28.357	α = β = γ = 90°	1296
ZIF-69	α=26.084 β=22.589 γ =19.408	α = β = 90° γ =120°	600
ZIF-97	α=28.432 β=28.432 γ =28.432	α = β = γ = 90°	1488
ZIF-65	α=17.272 β=17.272 γ =17.272	α = β = γ = 90°	251
ZIF-81	α=25.993 β=22.511 γ =19.700	α = β = 90° γ =120°	600
ZIF-78	α=26.117 β=22.618 γ =19.491	α = β = 90° γ =120°	648
ZIF-25	α=27.788 β=27.788 γ =27.788	α = β = γ = 90°	1392
ZIF-91	α=16.604 β=16.336 γ =16.759	α = β = γ = 90°	300
Y1[b]	α=9.801 β=24.104 γ =24.356	α = β = γ = 90°	272
Y3[c]	α =18.389 β =18.389 γ =19.129	α = β = γ = 90°	272

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