Supporting Information

Design of tetraphenyl silsesquioxane based covalent-organic frameworks as hydrogen storage materials

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The supporting information provides the space group symmetries and coordinates of four designed sil-COF frameworks (Table S1-S4) and the entire heat of adsorption at all the adsorption points simulated (Table S5).

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Table S1 The space group symmetries and coordinates of four designed sil-COF-1.

Name: sil-COF-1			
Space group symmetry: I-43m			
a = b = c = 33.466597			
alpha = betha = gamma = 90º			
Atom	x	y	z
O1	0.45339	0.28026	0.62504
Si2	0.46185	0.24191	0.65258
B3	0.42832	0.48890	0.46797
O4	0.43498	0.45560	0.49465
C5	0.51415	0.33692	0.53916
C6	0.50860	0.36974	0.51348
C7	0.48510	0.32720	0.56826
C8	0.47409	0.39386	0.51643
C9	0.44534	0.38446	0.54587
C10	0.45067	0.35149	0.57141
H11	0.53966	0.32025	0.53606
H12	0.53012	0.37577	0.49262
H13	0.42005	0.40137	0.54896
H14	0.42897	0.34572	0.59217
O15	0.50000	0.25000	0.56946

Table S2 The space group symmetries and coordinates of four designed sil-COF-2.

Name : sil-COF-2			
Space group symmetry : P-43m			
a = b = c = 21.684387			
alpha = betha = gamma = 90º			
Atom	x	y	z
C1	0.14060	0.61381	0.06127
C2	0.17262	0.66021	0.09341
H3	0.15897	0.59802	0.02072
H4	0.21312	0.67630	0.07530
Si5	0.95745	0.54251	0.95745
C6	0.08387	0.59096	0.08387
C7	0.14865	0.68509	0.14865
O8	0.91403	0.50000	0.00000
O9	0.00000	0.58538	0.00000
B10	0.73849	0.82075	0.82075
O11	0.76623	0.76623	0.84723

Table S3 The space group symmetries and coordinates of four designed sil-COF-3.

Name : sil-COF-3			
Space group symmetry : I-43m			
a = b = c = 49.524858			
alpha = betha = gamma = 90º			
Atom	x	y	z
B1	0.37058	0.53350	0.47781
O2	0.38860	0.53391	0.45493
C3	0.58804	0.46560	0.31769
C4	0.56773	0.50957	0.30941
C5	0.55049	0.50578	0.33168
C6	0.55187	0.48190	0.34716
C7	0.57086	0.46190	0.34001
H8	0.60147	0.45055	0.31317
H9	0.57234	0.44442	0.35093
H10	0.56614	0.52720	0.29869
H11	0.53695	0.52065	0.33644
O12	0.37888	0.51230	0.49597
C13	0.43811	0.46927	0.47668
C14	0.44553	0.48405	0.45280
C15	0.40054	0.50097	0.48391
C16	0.40642	0.51387	0.45982
C17	0.42848	0.50573	0.44425
C18	0.41606	0.47907	0.49255
H19	0.43130	0.51609	0.42676
H20	0.41060	0.47086	0.51056
C21	0.58664	0.48947	0.30206
Si22	0.49427	0.27571	0.60635
O23	0.46829	0.27009	0.62498
O24	0.50000	0.25000	0.66256

Table S4 The space group symmetries and coordinates of four designed sil-COF-4.

Name: sil-COF-4			
Space group symmetry: P-43m			
a = b = c = 32.215251			
alpha = betha = gamma = 90º			
Atom	x	y	z
O1	0.32517	0.16221	0.88929
C2	0.17108	0.20270	0.76587
C3	0.16927	0.29500	0.86107
C4	0.20109	0.26562	0.86026
H5	0.22210	0.26824	0.88358
H6	0.14531	0.61608	0.05260
H7	0.10731	0.56549	0.01422
C8	0.11775	0.60556	0.06438
C9	0.09527	0.57564	0.04185
C10	0.10216	0.62132	0.10216
C11	0.05677	0.56071	0.05677
Si12	0.97138	0.52867	0.97138
B13	0.34484	0.12439	0.87561
O14	0.94220	0.50000	0.00000
O15	0.00000	0.55760	0.00000

Table S5 The isosteric heat of adsorption (kJ/mol) in four sil-COFs under pressure from 0.1–100 bar at both 77 K and 298 K.

Pressure	sil-COF-1		sil-COF-2		sil-COF-3		sil-COF-4	
(bar)	77	298	77	298	77	298	77	298
0.1	3.68	4.14	3.64	4.03	3.21	3.37	4.15	2.97
0.5	3.61	3.59	4.76	3.90	2.84	3.85	4.15	3.48
1	4.11	3.71	4.68	4.98	3.53	2.70	3.14	3.07
2.5	3.69	3.96	4.82	4.15	2.77	3.86	2.97	3.27
5	3.78	4.48	2.93	4.27	1.99	2.93	2.44	3.00
7.5	3.50	4.10	2.95	3.79	3.26	3.04	2.57	3.33
10	3.01	4.19	3.00	3.78	2.09	3.16	2.60	3.85
20	3.10	4.86	2.63	3.81	2.57	3.31	3.22	2.47
30	3.47	4.05	3.15	4.18	1.95	4.45	2.45	3.38
40	3.93	4.24	2.78	4.83	2.64	3.96	2.46	3.51
50	3.14	4.68	3.93	3.97	2.94	3.85	2.03	3.53
60	5.20	3.88	2.89	3.77	3.04	3.52	2.20	3.10
70	4.39	4.47	4.19	4.72	2.62	3.67	2.25	3.95
80	3.39	4.98	3.48	3.94	2.47	2.77	2.29	3.51
90	3.39	4.78	4.46	4.67	2.28	3.63	2.17	3.50
100	4.06	4.45	3.83	4.09	3.18	3.43	2.44	3.30
average	3.72	4.28	3.63	4.18	2.71	3.47	2.72	3.33