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Supplementary Information

Enhanced water stability and CO_2 gas sorption properties in a methyl functionalized titanium metal-organic framework

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Table S1. The fractional atomic coordinates of TiBDC and m-TiBDC, respectively, both of which belong to a tetragonal space group (No. 139; *I*4/*mmm*) with unit cell parameters, $a = b = 18.6543$ Å, $c = 18.1444$ Å, $\alpha = \beta = \gamma = 90°$.

TiBDC

Atom	x	y	z
TI1	0.20830	0.07400	0.50000
O1	0.31110	0.05800	0.50000
O2	0.18190	0.00000	0.42650
O3	0.10740	0.10740	0.50000
O4	0.22590	0.14420	0.42680
C1	0.19304	0.28408	0.28557
C2	0.46246	0.06475	0.50000
C3	0.34482	0.00000	0.50000
C4	0.42419	0.00000	0.50000
C5	0.19782	0.19782	0.39718
C6	0.22661	0.22661	0.32322
H1	0.31357	1.14618	0.68786
H2	0.11254	0.44128	0.50000

m-TiBDC

Atom	x	y	z
TI1	0.20830	0.07400	0.50000
O1	0.31110	0.05800	0.50000
O2	0.18190	0.00000	0.42650
O3	0.10740	0.10740	0.50000
O4	0.22920	0.14279	0.42039
C1	0.50000	1.08241	1.13719
C2	0.50000	0.96084	1.06643
C3	0.50000	0.92318	1.00000
C4	0.13889	0.13889	0.73967
C5	0.19639	0.19639	0.74599
C6	0.27904	0.27904	0.68392
C7	0.31030	0.31030	0.61386
C8	0.22537	0.22537	0.67991
C9	0.19806	0.19806	0.39270
C10	0.34448	0.00000	0.50000
H1	0.59207	0.33941	0.79083
H2	0.29994	0.36889	0.61187
H3	0.54799	1.06135	1.17080
H4	0.50000	1.13852	1.12377
H5	0.28718	0.28718	0.56316
H6	0.61852	0.38148	0.70712

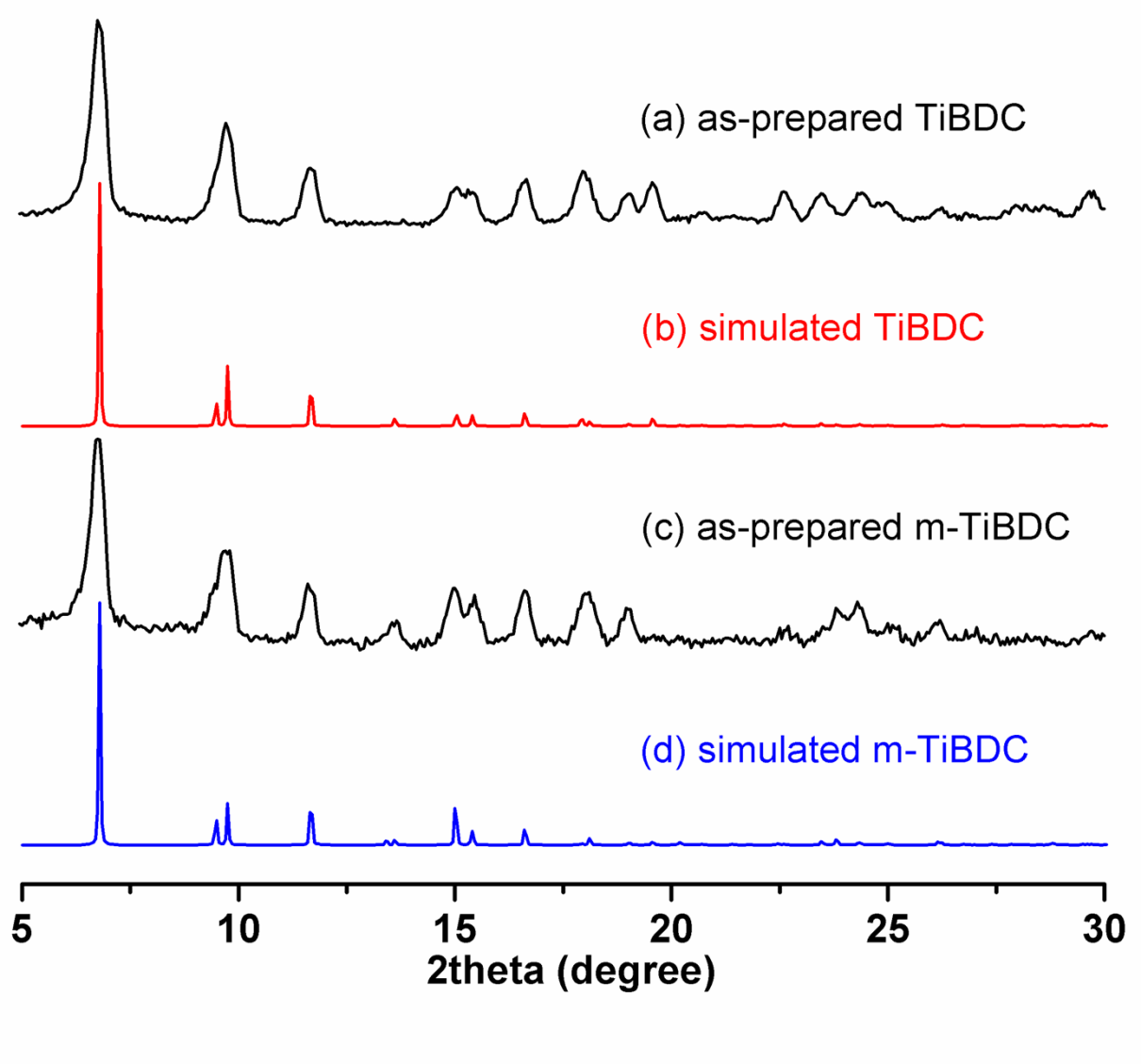

Fig. S1 Powder X-ray diffraction (PXRD) patterns for (a) as-prepared TiBDC, (b) simulated TiBDC derived from the optimized model structure, (c) as-prepared m-TiBDC, and (d) simul ated m-TiBDC derived from the optimized model structure.

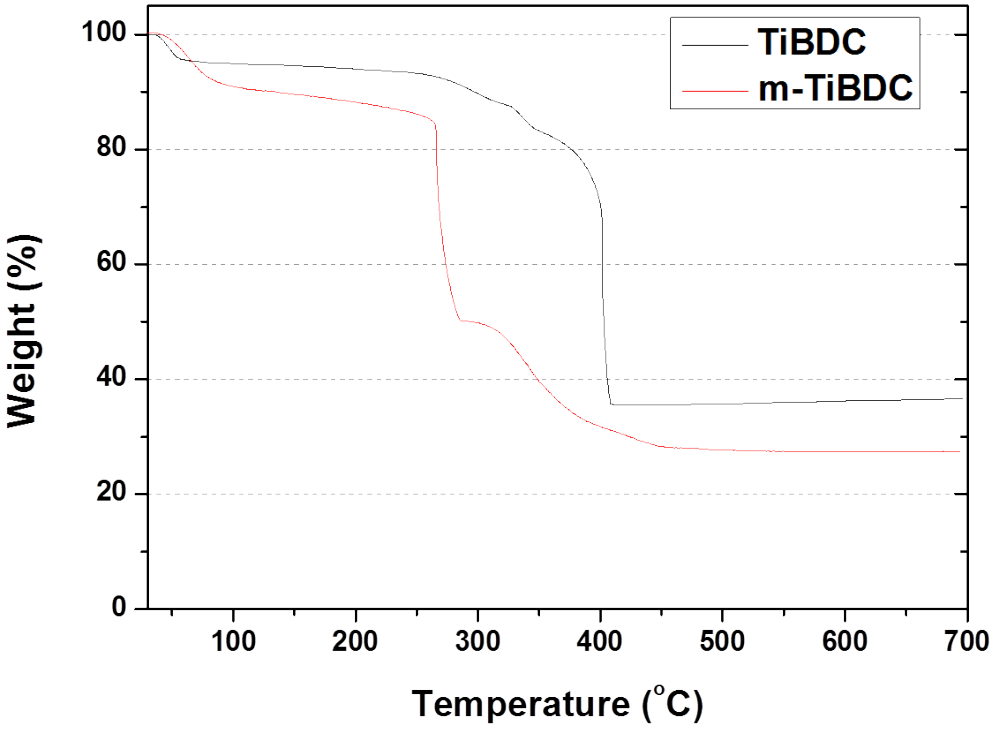

Fig. S2 TGA curves for as-synthesized TiBDC and m-TiBDC.

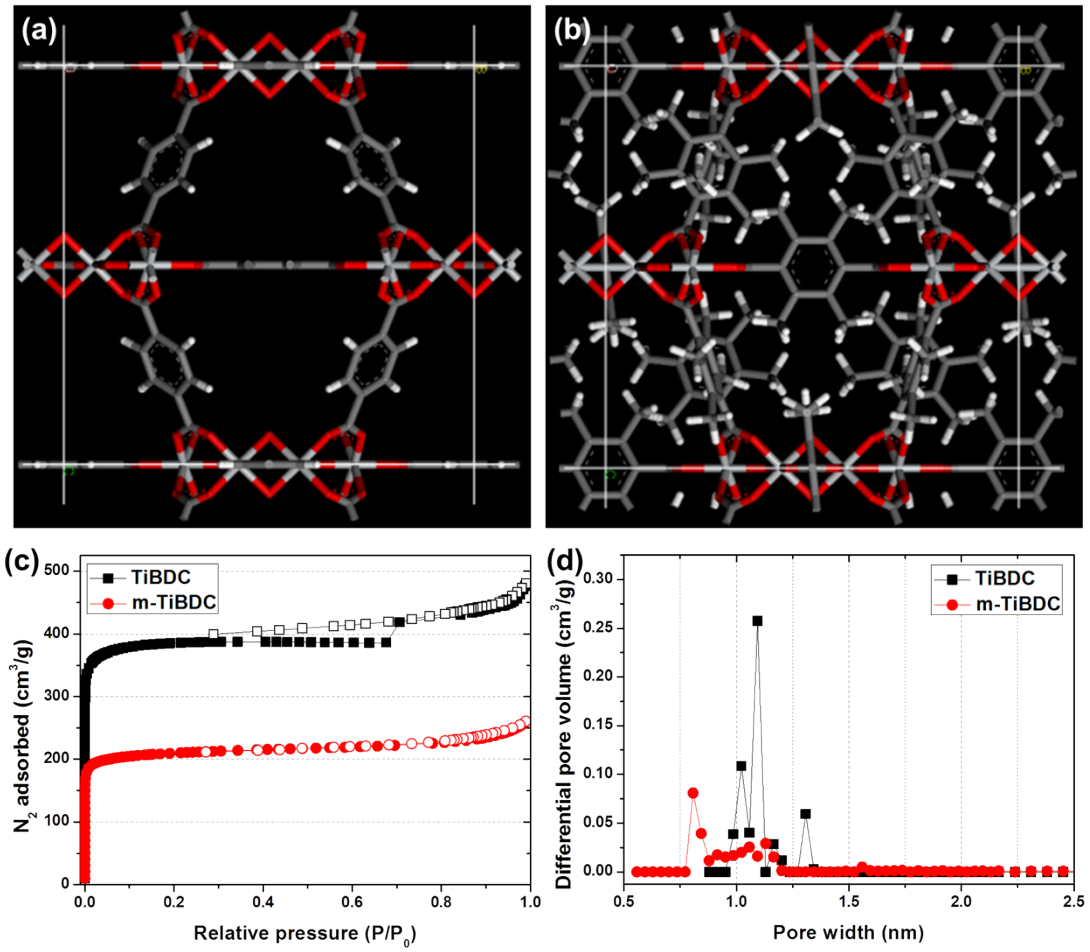

Fig. S3 The simulated structures for (a) TiBDC and (b) m-TiBDC, and (c) nitrogen gas sorpti on isotherms and (d) pore size distributions for TiBDC and m-TiBDC.

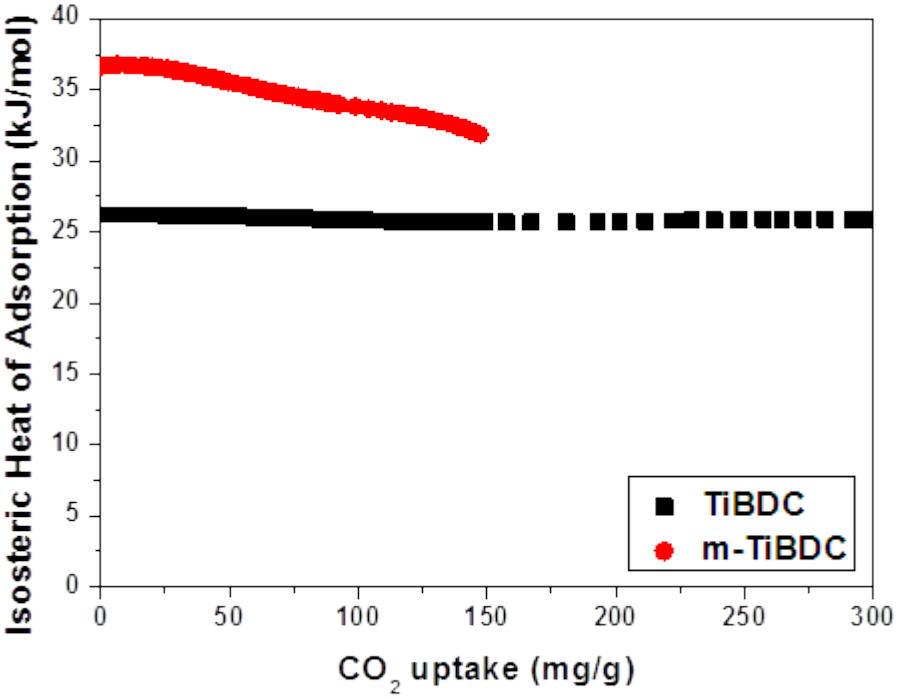

Fig. S4 Isosteric heats of CO_2 adsorption of TiBDC and m-TiBDC.

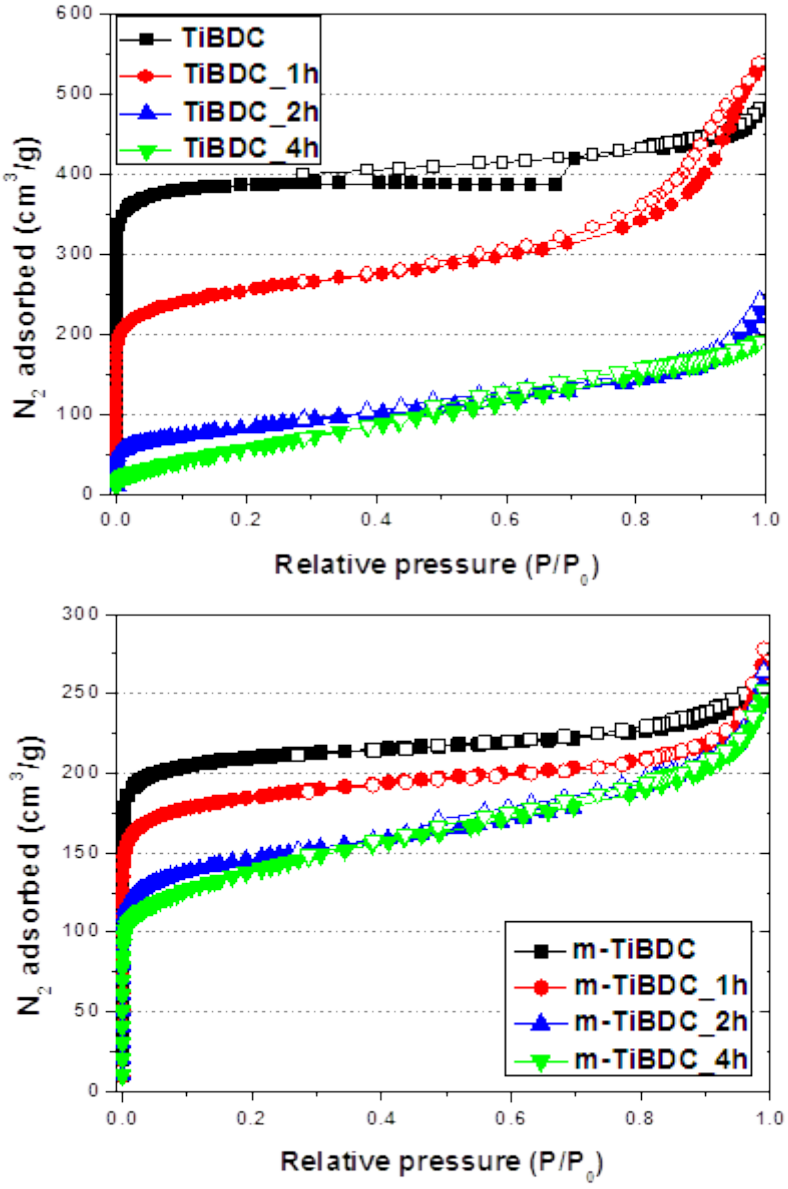

Fig. S5 N_2 gas sorption isotherms of TiBDC_xh and m-TiBDC_xh at 77 K.

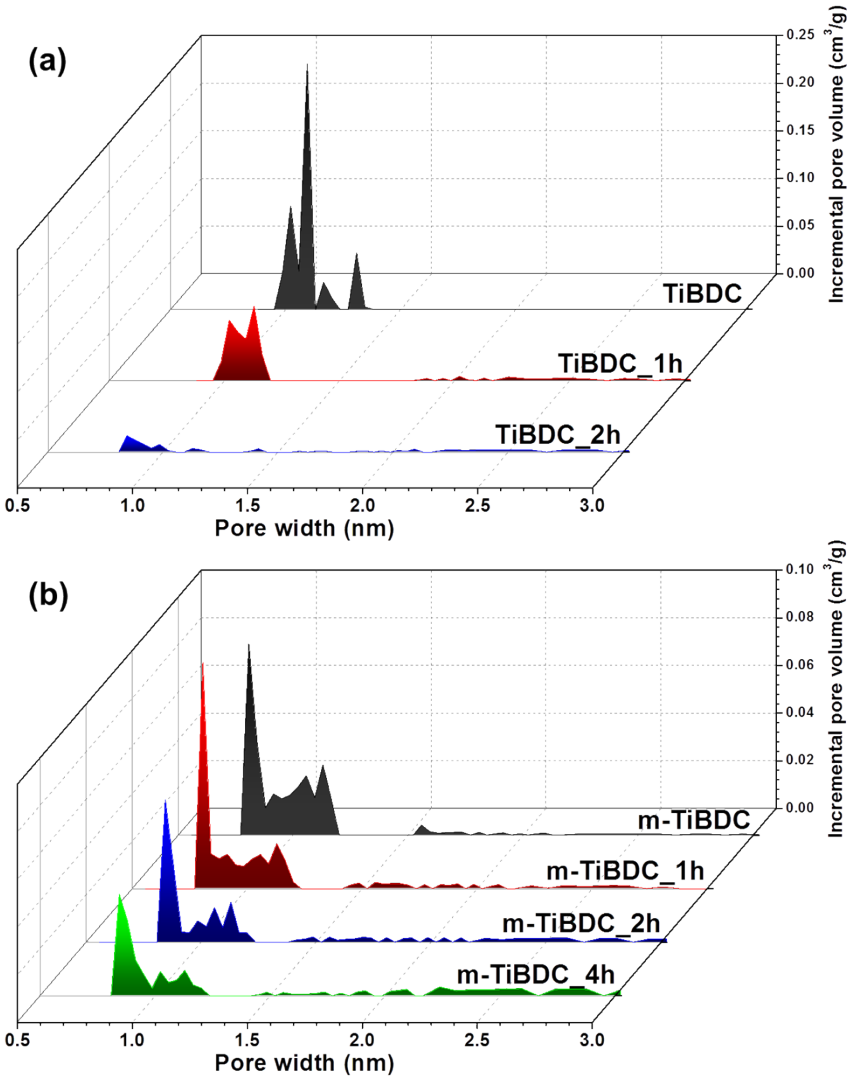

Fig. S6 Pore size distribution for TiBDC_xh and m-TiBDC_xh.