Supporting Information

Acetylene Storage and Separation using Metal-Organic Frameworks with Open Metal Sites

A. Luna-Triguero[a], J. M. Vicent-Luna[a], R. M. Madero-Castro[a], P. Gómez-Álvarez[b]*, and S. Calero[a]*

[a]Department of Physical, Chemical and Natural Systems, Universidad Pablo de Olavide, Ctra. Utrera Km. Seville ES-41013, Spain

[b]Laboratorio de Simulación Molecular y Química Computacional, CIQSO-Centro de Investigación en Química Sostenible and Departamento de Ciencias Integradas, Universidad de Huelva, 21007 Huelva, Spain

Corresponding authors:
Email: paula.gomez@dci.uhu.es
Email: scalero@upo.es

Table S1. Crossed host-guest interaction parameters between acetylene and M-MOF-74, Cu-BTC, and PCN-16. ε/kB in K (top) and σ in Å (bottom).

	MOF-74- C_{C2H2}	Cu-BTC- C_{C2H2}	PCN-16- C_{C2H2}
C	78.9618 3.0548	68.4335 4.0004	73.6977 3.2730
H	31.5690 2.7917	27.3598 3.6557	29.4644 2.9911
O	79.2335 2.8701	68.6691 3.7584	73.9513 3.0751
Co	40.4134 2.9889	-	-
Fe	38.9246 2.8775	-	-
Cu	-	12.0744 2.7658	30.1861 3.1115

Table S2. Point charges of M-MOF-74, PCN-16, and ZJNU-30.

	Co-MOF-74	Fe-MOF-74	PCN-16	ZJNU-30
C1	0.486	0.356	0.527	0.006
C2	-0.207	-0.148	-0.13	0.033
C3	0.2401	0.172	0.055	-0.045
C4	-0.124	-0.088	-0.018	0.013
C5	-	-	0.015	-0.035
C6	-	-	-0.013	0.155
C7	-	-	-	-0.05
C8	-	-	-	0.025
C9	-	-	-	-0.032
C10	-	-	-	-0.006
C11	-	-	-	-0.017
C12	-	-	-	-0.017
C13	-	-	-	-0.005
C14	-	-	-	-0.002
C15	-	-	-	-0.027
C16	-	-	-	0.014
C17	-	-	-	0.027
C18	-	-	-	-0.051
O1	-0.543	-0.601	-0.58	-0.623
O2	-0.611	-0.439	-0.579	-0.237
O3	-0.673	-0.56	-	-0.255

O4	-	-	-	-0.27
H1	0.096	0.0812	-	0.095
H3	-	-	0.07	0.034
H4	-	-	0.08	0.004
H5	-	-	-	0.02
H9	-	-	-	0.012
H10	-	-	-	0.007
H11	-	-	-	0.014
H12	-	-	-	0.016
H15	-	-	-	0.019
H16	-	-	-	0.009
H18	-	-	-	0.028
Co	1.3359	-	-	-
Fe	-	1.2268	-	-
Cu	-	-	1.273	-
Zr1	-	-	-	1.044
Zr2	-	-	-	1.037

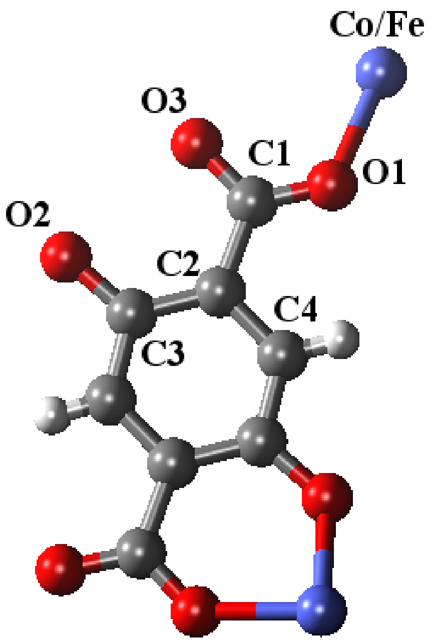

Figure S1. Schematic representation of the M-MOF -74 linker and atom labels.

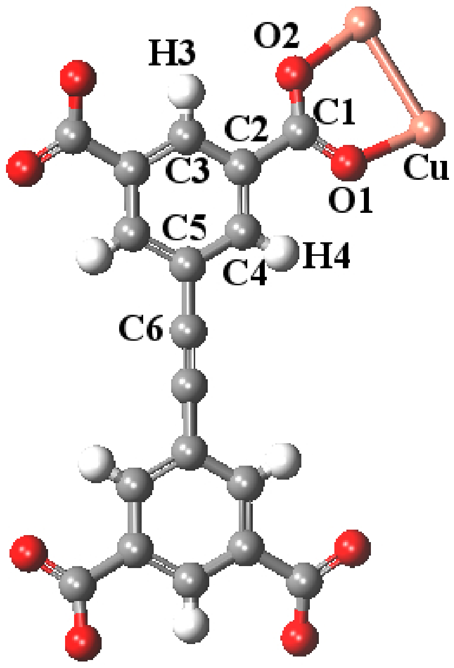

Figure S2. Schematic representation of the PCN-16 linker and atom labels.

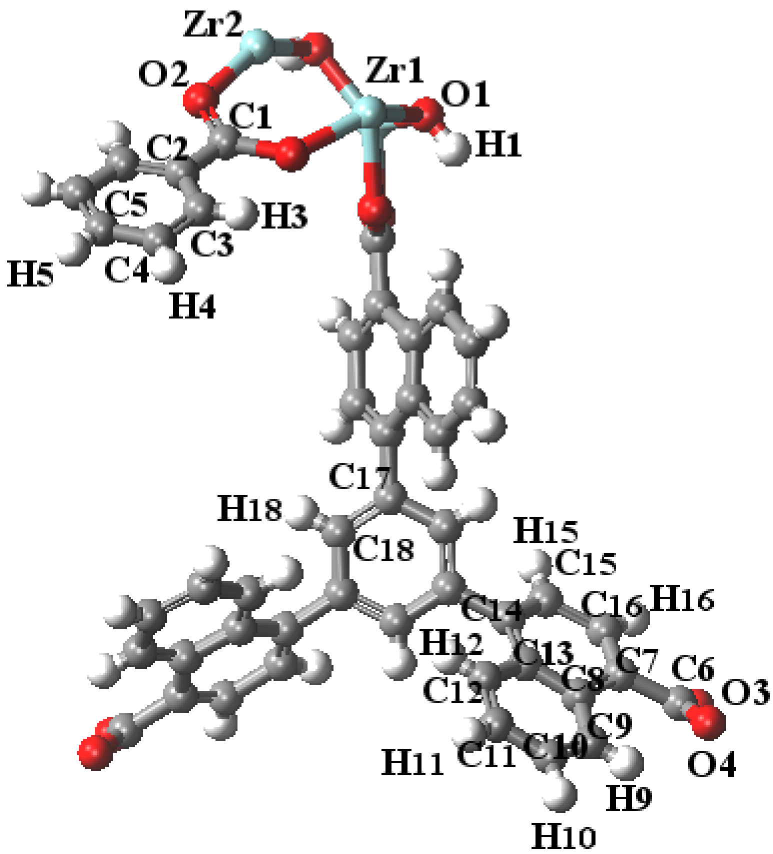

Figure S3. Schematic representation of the ZJNU-30 linker and atom labels.

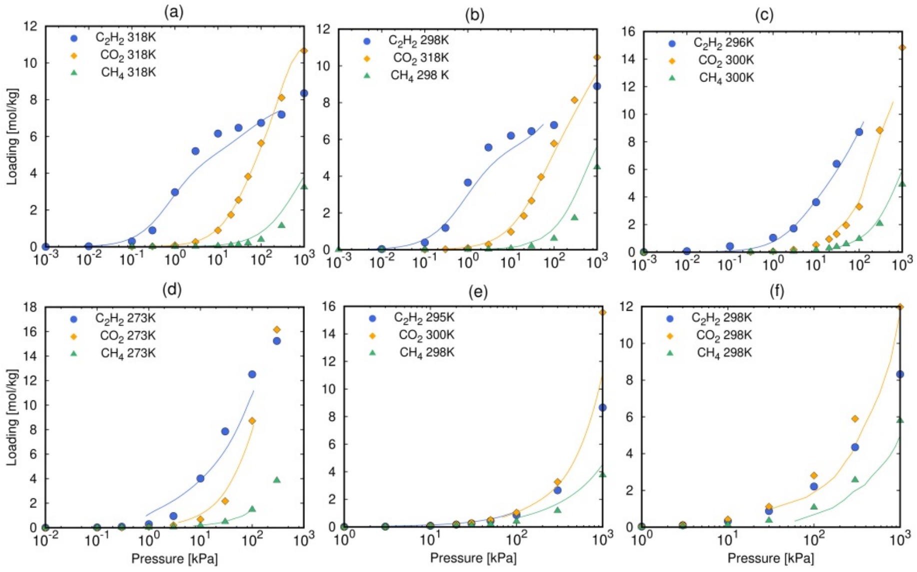

Figure S4. Adsorption isotherms of acetylene, carbon dioxide and methane in (a) Co-MOF-74, (b) Fe-MOF-74, (c) Cu-BTC, (d) PCN-16, (e) IRMOF-1, and (f) ZJNU-30. Comparison of calculated and experimental results from the literature.[1-8]

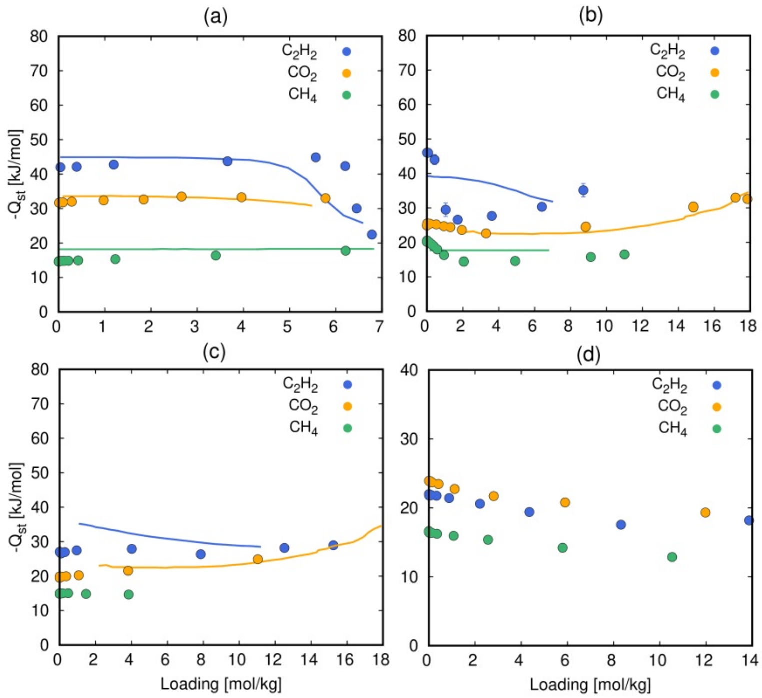

Figure S5. Heats of adsorption as a function of loading in a) Co-MOF-74, b) Cu-BTC c) PCN-16, and d) ZJNU-30. Comparison of computed and experimental data from literature.[1-6, 8]

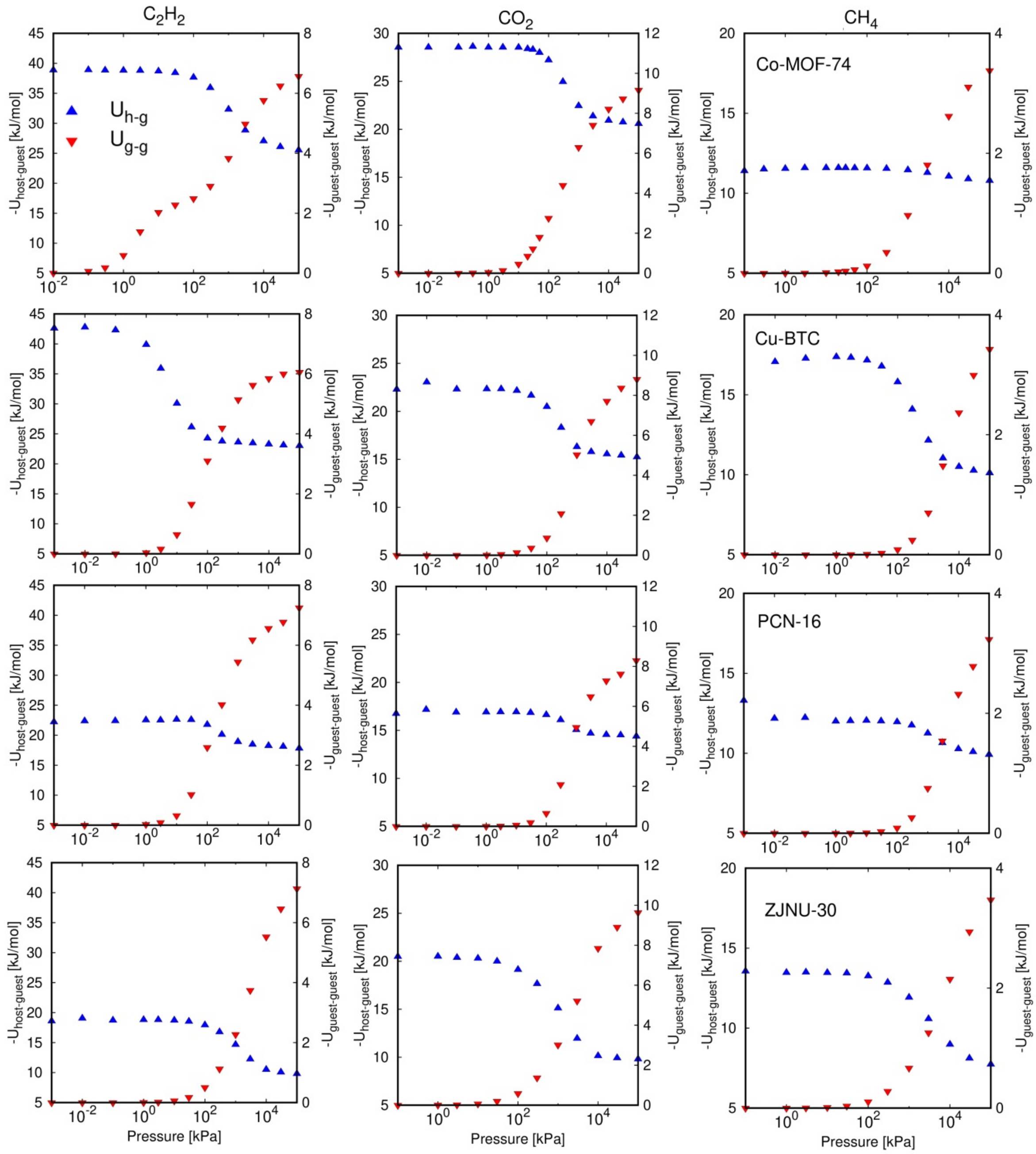

Figure S6. Potential energy of host-guest (blue) and guest-guest (red) interactions as a function of pressure for acetylene, carbon dioxide, and methane in Co-MOF-74, Cu-BTC, PCN-16, and ZJNU-30 at 318K.

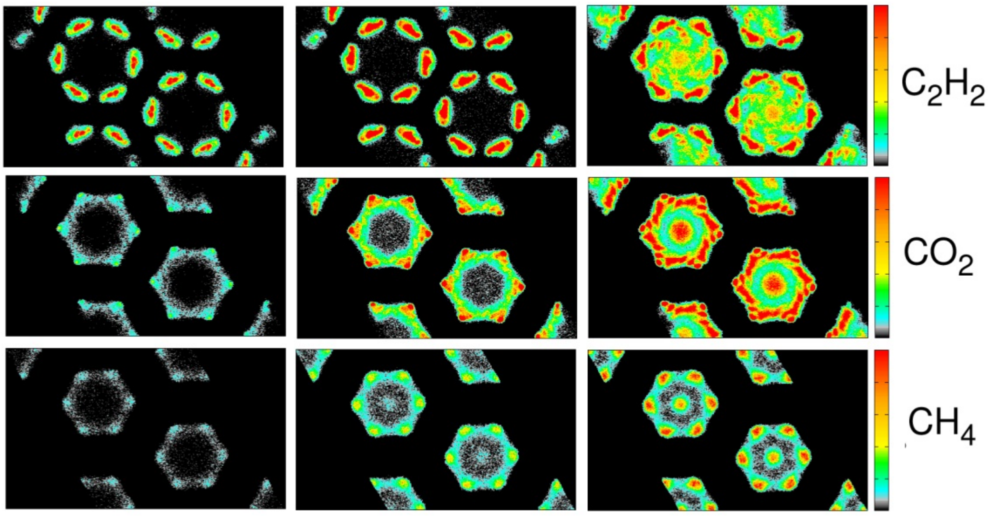

Figure S7. Average occupational profiles of adsorption of acetylene, carbon dioxide, and methane at low, medium, and high loading in Fe-MOF-74.

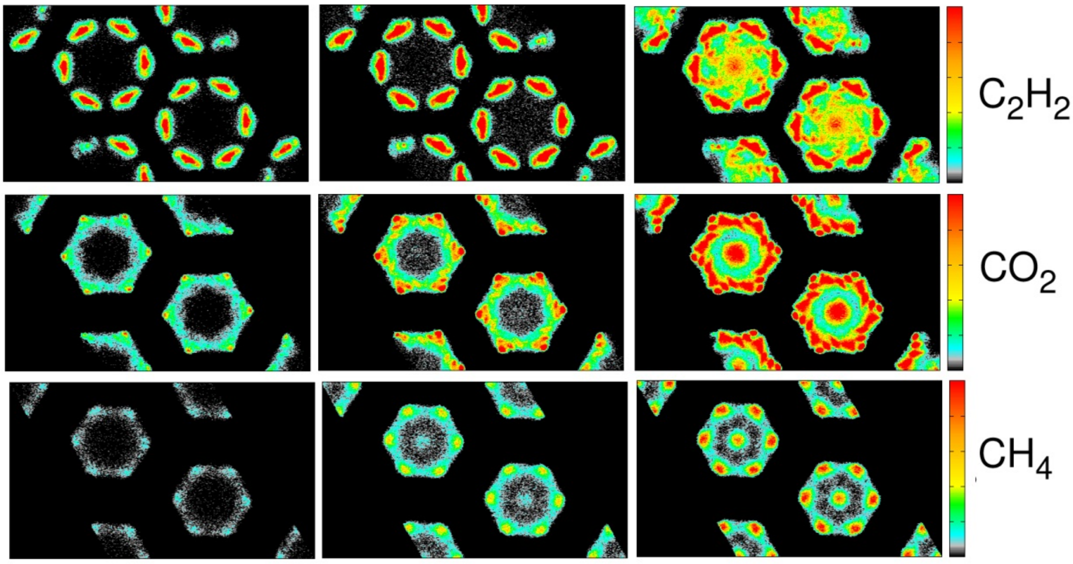

Figure S8. Average occupational profiles of adsorption of acetylene, carbon dioxide, and methane at low, medium, and high loading in Co-MOF-74.

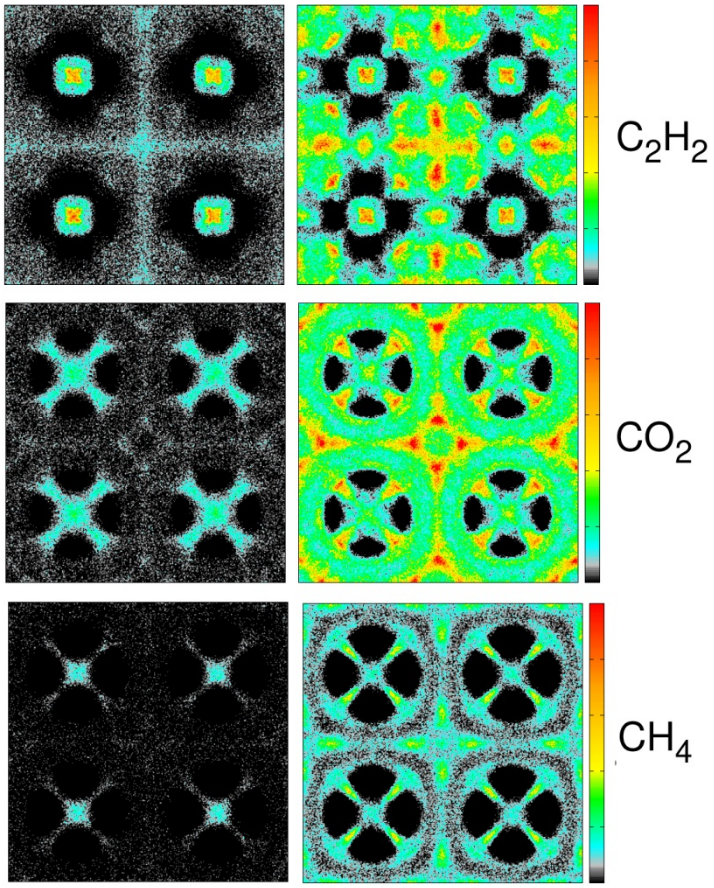

Figure S9. Average occupational profiles of adsorption of acetylene, carbon dioxide, and methane at low and high loading in Cu-BTC.

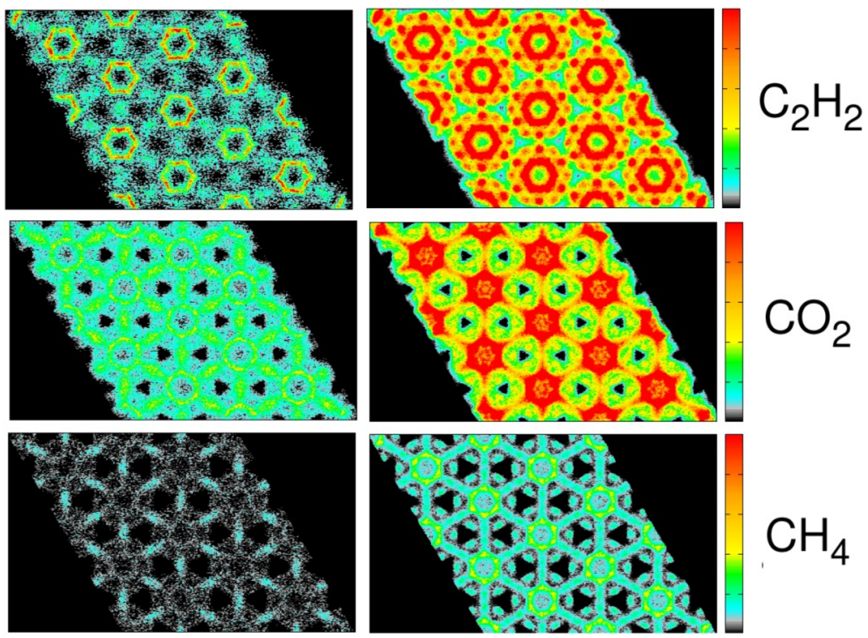

Figure S10. Average occupational profiles of adsorption of acetylene, carbon dioxide, and methane at low and high loading in PCN-16.

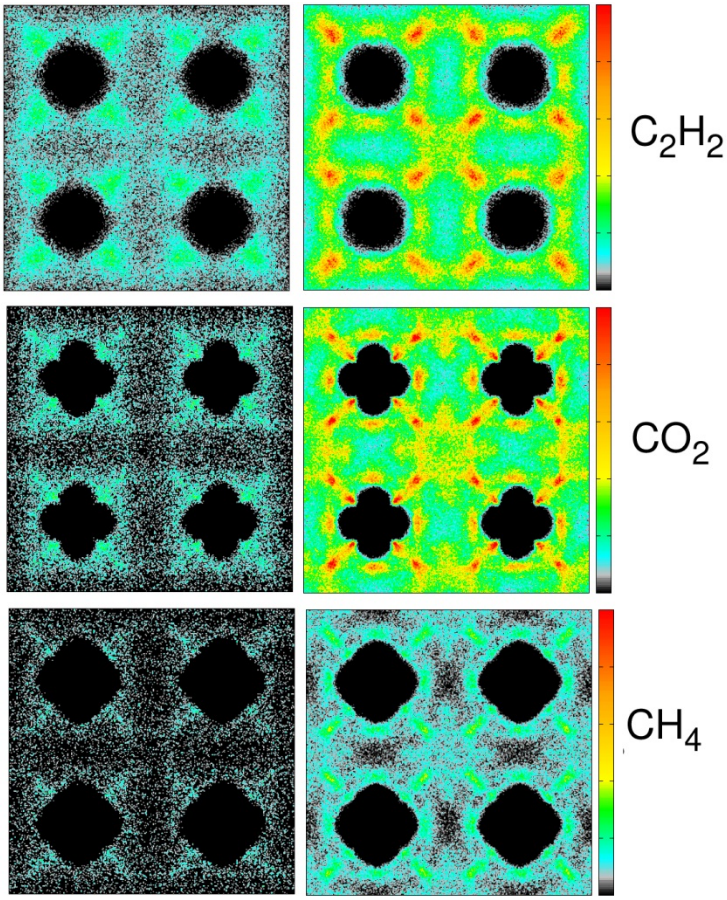

Figure S11. Average occupational profiles of adsorption of acetylene, carbon dioxide, and methane at low and high loading in IRMOF-1.

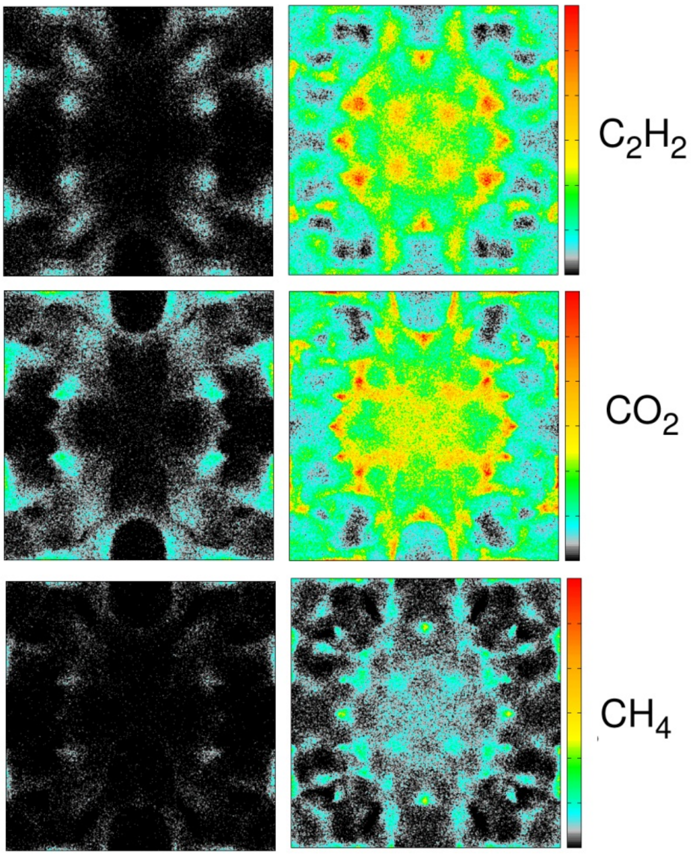

Figure S12. Average occupational profiles of adsorption of acetylene, carbon dioxide, and methane at low and high loading in ZJNU-30.

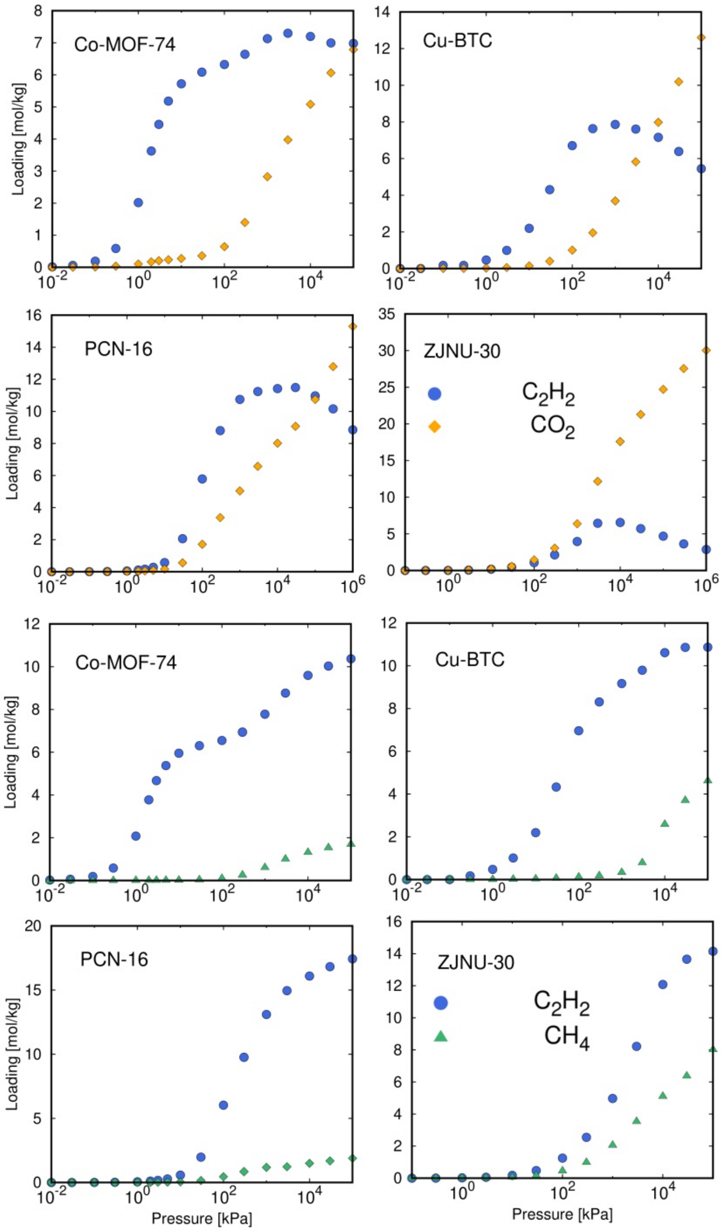

Figure S13. Equimolar adsorption isotherms of acetylene/carbon dioxide and acetylene/methane at 298 K.

References

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