Supporting Information

Melting Point Depression and Phase Identification of Sugar Alcohols Encapsulated in ZIF Nanopores

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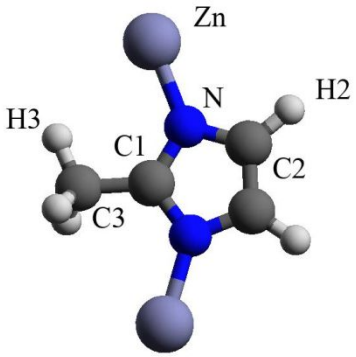
Table S1. Force field parameters for ZIF-8 framework.



atoms	σ (Å)	ε(kcal/mol)	partial charge (e)
Zn	1.960	0.0125	0.6326
N	3.250	0.1700	-0.3591
C1	3.400	0.0860	0.3961
C2	3.400	0.0860	-0.0854
C3	3.400	0.1094	-0.5759
H2	2.511	0.0150	0.1109
H3	2.471	0.0157	0.1769

bonds	r_0 (Å)	K_r (kcal/mol Å^2)
C1-C3	1.490	346.543
C1-N	1.335	488.000
C2-C2	1.350	540.249
C2-N	1.370	440.210
C2-H2	1.080	367.000
C3-H3	1.090	340.000
Zn-N	2.011	78.500

angles	θ_0 (deg)	K_θ (kcal/mol rad^2)
C1-C3-H3	109.32	48.088
C1-N-C2	105.27	71.254
C1-N-Zn	128.33	48.680
C2-C2-N	108.65	73.750
C2-C2-H2	125.67	49.451
C2-N-Zn	126.40	32.477
C3-C1-N	123.92	66.015
H3-C3-H3	109.50	35.000
N-C1-N	112.16	75.484
N-C2-H2	125.68	49.954
N-Zn-N	109.48	35.240

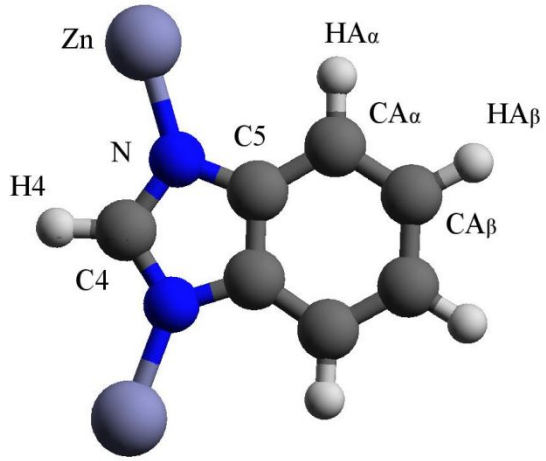
torsions [a]	γ_0 (deg)	K_φ (kcal/mol)	n
X-C1-N-X	180	5.000	2
X-C2-N-X	180	2.325	2
X-C2-C2-X	180	5.150	2

improper	ψ_0 (deg)	K_ψ (kcal/mol rad^2)
N-C3-C1-N	180	2
C2-H2-C2-N	180	2
C2-Zn-N-C1	180	2

The force field for ZIF-8 cites the results from Ref. S1.

[a] X denotes wildcard atoms. i.e., X-A-B-X means any dihedral combination having A-B as central atoms. Unmentioned combinations are assumed as negligible torsional potential.

Table S2. Force field parameters for ZIF-11 framework.



atoms [c]	σ (Å)	ε(kcal/mol)	partial charge (e)
Zn	1.960	0.0125	0.6342
N	3.250	0.1700	-0.3584
C4	3.400	0.0860	0.1712
C5	3.400	0.0860	0.1434
CAα	3.400	0.0860	-0.1730
CAβ	3.400	0.0860	-0.0953
H4	2.420	0.0150	0.0847
HAα	2.511	0.0150	0.1004
HAβ	2.511	0.0150	0.0964

bonds	r_0 (Å)	K_r (kcal/mol Å^2)
C4-H4	1.080	367.00
C4-N	1.335	488.00
C5-C5	1.350	540.25
C5-CA [b]	1.404	469.00
C5-N	1.370	440.21
CA-CA [b]	1.400	469.00
CA-HA [b]	1.080	367.00
Zn-N	2.011	78.50

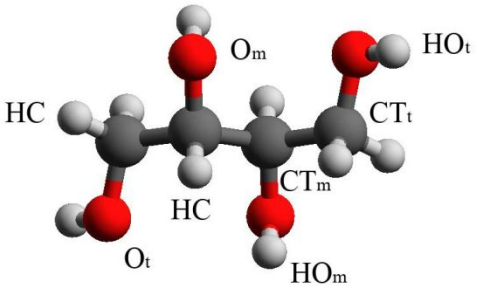
angles	θ_0 (deg)	K_θ (kcal/mol rad^2)
C4-N-C5	105.33	71.254
C4-N-Zn	128.33	48.680
C5-C5-CA [b]	120.00	63.000
C5-C5-N	108.65	73.750
C5-CA-CA [b]	120.00	63.000
C5-CA-HA [b]	120.00	50.000
CA-C5-N [b]	132.40	70.000
CA-CA-CA [b]	120.00	63.000
CA-CA-HA [b]	120.00	50.000
N-C4-H4 [b]	120.00	50.000
N-C4-N	112.16	75.484
N-Zn-N	109.48	35.240
Zn-N-C5	126.40	32.477

torsions [a]	γ_0 (deg)	K_φ (kcal/mol)	n
X-C4-N-X	180	5.000	2
X-C5-N-X	180	2.325	2
X-C5-C5-X	180	5.150	2
X-C5-CA-X [b]	180	14.000	4
X-CA-CA-X [b]	180	14.500	4

improper	ψ_0 (deg)	K_ψ (kcal/mol rad^2)
C4-Zn-N-C5	180	2
C5-CA-C5-N	180	2
C5-HA-CA-CA	180	2
CA-CA-HA-CA	180	2
N-H4-C4-N	180	2

[a] X denotes wildcard atoms. i.e., X-A-B-X means any dihedral combination having A-B as central atoms. Unmentioned combinations are assumed as negligible torsional potential.
[b] The force field for ZIF-11 except for b marked terms cites the results from Ref. S1. The b marked terms cite the general AMBER force field.
[c] Subscripts α and β correspond to the description for CA, HA in a benzene ring, which is expressed in the inset structure schema.

Table S3. Force field parameters for erythritol.



atoms [c]	σ (Å)	ε (kcal/mol)	partial charge (e)
CT_t	3.400	0.0125	0.145
CT_m	3.400	0.1700	0.205
O_t	3.066	0.2104	-0.683
O_m	3.066	0.2104	-0.700
HO_t	0.000	0.0000	0.418
HO_m	0.000	0.0000	0.435
HC	2.471	0.0157	0.060

bonds	r_0 (Å)	K_r (kcal/mol Å^2)
CT-CT	1.410	320.0
CT-CT	1.526	310.0
CT-HC	1.090	- [d]
O-HO	0.960	- [d]

angles	θ_0 (deg)	K_θ (kcal/mol rad^2)
HC-CT-HC	109.5	35.0
O-CT-HC	109.5	50.0
CT-O-HO	108.5	55.0
CT-CT-HC	109.5	50.0
CT-CT-O	109.5	50.0
CT-CT-CT	109.5	40.0

torsions [a]	γ_0 (deg)	K_φ (kcal/mol)	n
X-CT-CT-X	0	0.156	3
X-CT-O-X	0	0.167	3

The force field for erythritol cites the results from Ref. S2.

[a] X denotes wildcard atoms. i.e., X-A-B-X means any dihedral combination having A-B as central atoms.

[c] Subscripts *t* and *m* correspond to the terminal and mid CT, T, HO units in a carbon backbone.

[d] The CT-HC and O-HO bonds are held rigid by the SHAKE method.

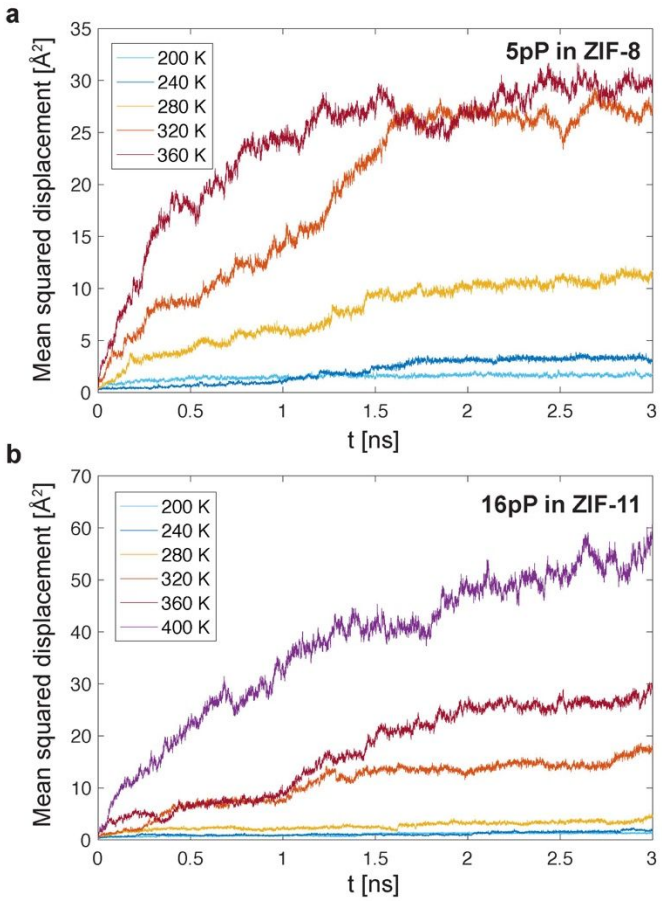


Figure S1. Mean squared displacement of erythritol molecules inside ZIF pores. (a) 5pP in ZIF-8. (b) 16pP in ZIF-11. The saturated trend of MSD at long times shows that erythritol molecules cannot diffuse between the ZIF pores, consistent with confined liquid behavior as depicted in Fig. 4a.

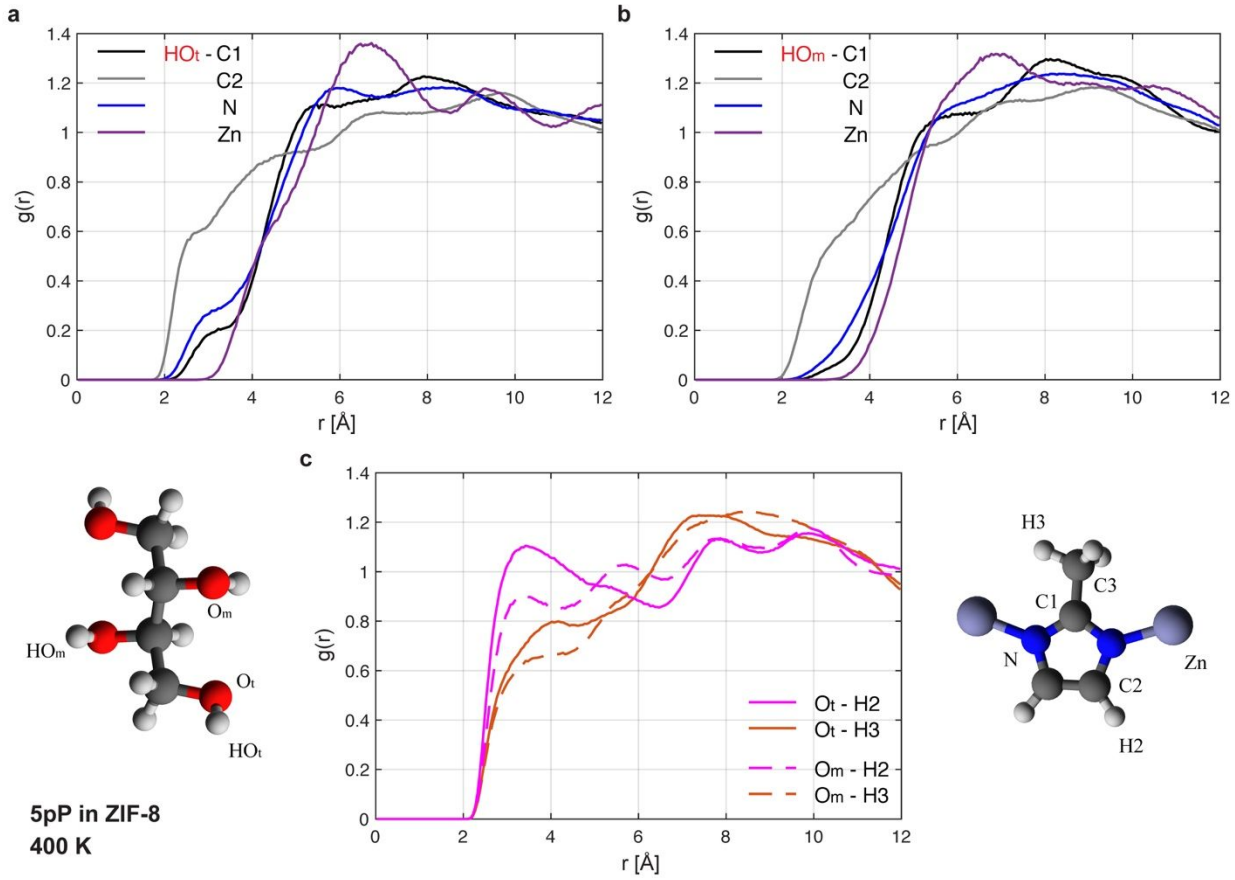


Figure S2. Radial distribution function at possible hydrogen bonding pairs between SAs and ZIF-8. If hydrogen bonds were present, a strong first peak would show up around 2 Å. (a) Pairs between HO_t atom in erythritol and four types of non-hydrogen atoms in ZIF-8. (b) Pairs between HO_m atom in erythritol and four types of non-hydrogen atoms in ZIF-8. (c) Pairs between oxygen atoms in erythritol and hydrogen atoms in ZIF-8. In all cases no hydrogen-bonding peaks are seen.

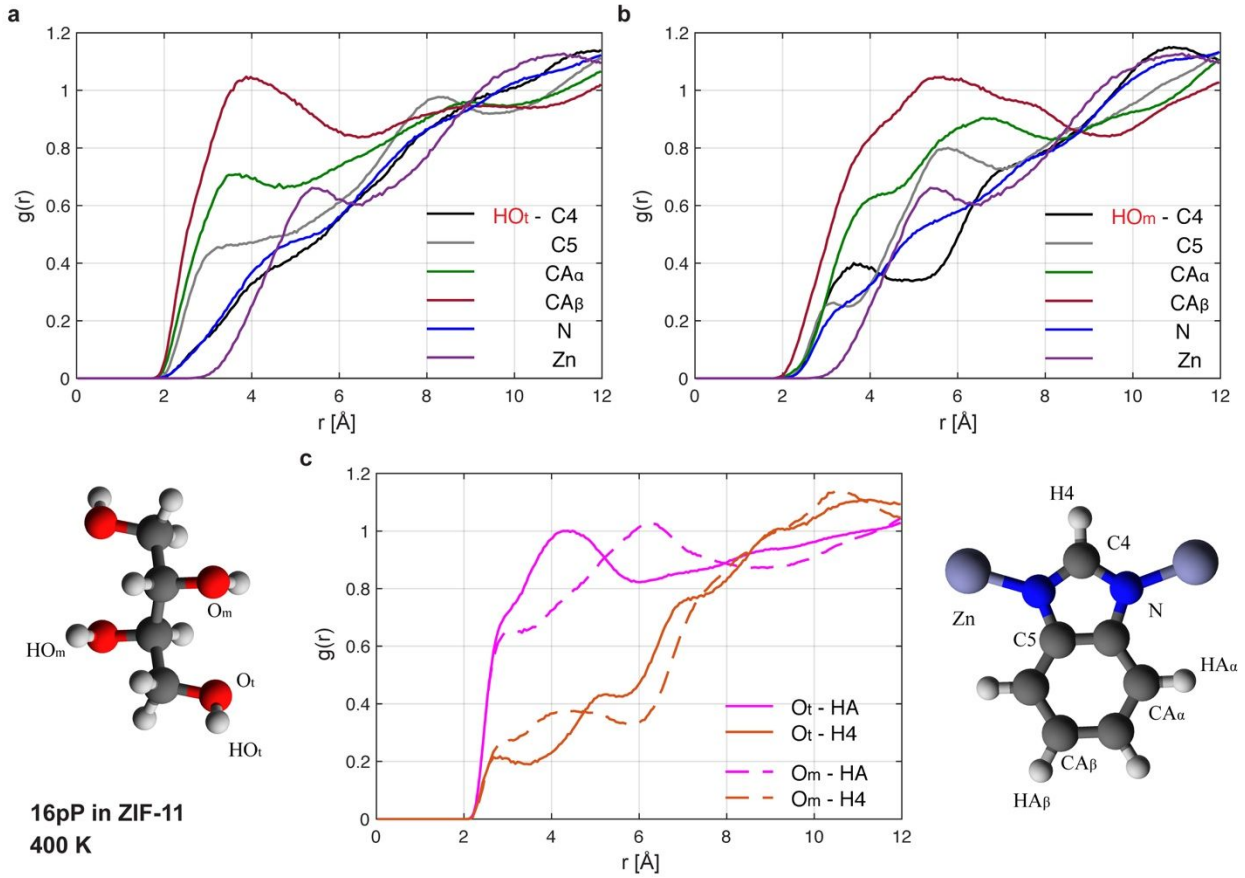


Figure S3. (Like Fig. S2 but here for ZIF-11). Radial distribution function at possible hydrogen bonding pairs between SAs and ZIF-11. If hydrogen bonds were present, a strong first peak would show up around 2 Å. (a) Pairs between HO_t atom in erythritol and six types of non-hydrogen atoms in ZIF-11. (b) Pairs between HO_m atom in erythritol and six types of non-hydrogen atoms in ZIF-11. (c) Pairs between oxygen atoms in erythritol and hydrogen atoms in ZIF-11. In all cases no hydrogen-bonding peaks are seen.

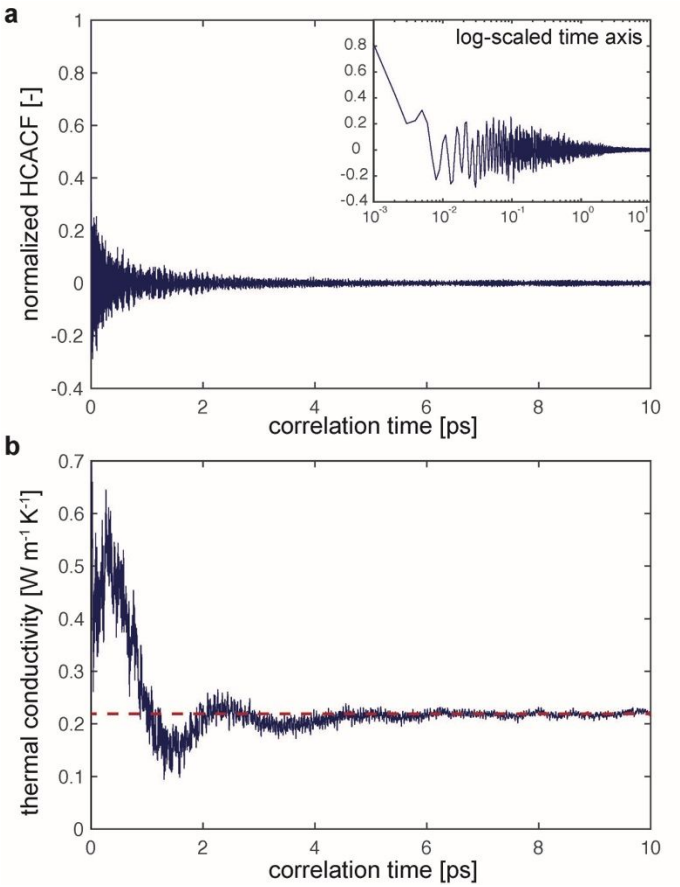


Figure S4. (a) Normalized heat current autocorrelation function and (b) thermal conductivity by using the Green-Kubo method as a function of correlation time, both for the pristine ZIF-8 at 400 K.

Supplementary references

S1. Zheng, B.; Sant, M.; Demontis, P.; Suffritti, G. B., Force field for molecular dynamics computations in flexible ZIF-8 framework. *The Journal of Physical Chemistry C* **2012,** *116* (1), 933-938.

S2. Inagaki, T.; Ishida, T., Computational analysis of sugar alcohols as phase-change material: insight into the molecular mechanism of thermal energy storage. *The Journal of Physical Chemistry C* **2016,** *120* (15), 7903-7915.