Supporting Information

"Metal Organic Frameworks Provide Large Negative Thermal Expansion Behavior"

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Table S1. Temperature-dependent lattice parameters (Å) of MOFs averaged from 100 to 200 ps of MD simulation. These values correspond to one crystal cell dimension.

Temp. (K)	MOF-C6	MOF-C10	MOF-C16	MOF-C22	MOF-C30
10	25.291	29.645	33.793	38.122	42.309
50	25.267	29.642	33.785	38.113	42.291
100	25.256	29.632	33.757	38.085	42.251
150	25.243	29.592	33.737	38.050	42.237
200	25.228	29.573	33.729	38.017	42.227
250	25.218	29.553	33.716	38.006	42.200
300	25.208	29.547	33.701	37.983	42.191
350	25.202	29.525	33.683	37.966	42.157
400	25.196	29.508	33.679	37.924	42.133
500	25.177	29.493	33.656	37.917	42.113
600	25.166	29.469	33.632	37.887	42.054

Table S2. Temperature-dependent volume ($Å^3$) of MOFs averaged from 100 to 200 ps of MD simulation. These values correspond to one crystal cell dimension.

Temp. (K)	MOF-C6	MOF-C10	MOF-C16	MOF-C22	MOF-C30
10	16177.001	26052.798	38590.486	55402.203	75735.288
50	16130.991	26044.889	38563.085	55362.973	75638.666
100	16109.932	26018.538	38467.285	55241.044	75424.246
150	16085.068	25913.314	38398.953	55088.885	75349.295
200	16056.411	25863.432	38371.643	54945.677	75295.788
250	16037.325	25810.993	38327.292	54897.996	75151.448
300	16018.254	25795.276	38276.160	54798.389	75103.376
350	16006.819	25737.699	38214.862	54724.844	74921.954
400	15995.389	25693.267	38201.249	54543.426	74794.067
500	15959.230	25654.104	38123.038	54513.229	74687.606
600	15938.321	25591.527	38041.539	54383.938	74374.136

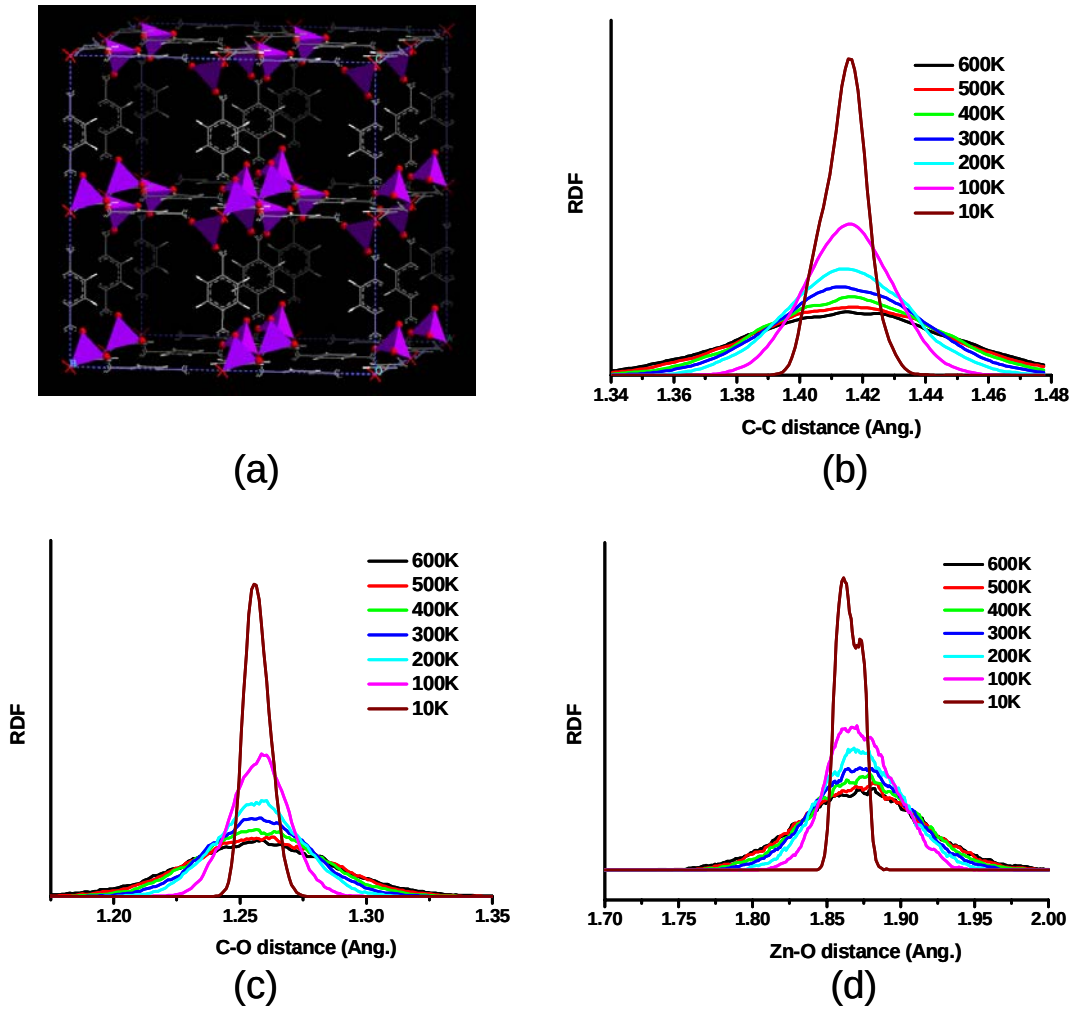

Figure S1. Atomistic crystal structure of MOF-C6 (a) and radial distribution functions (RDFs) for C-C (b), C-O (c), and Zn-O (d) bonds in the MOF-C6 with temperature.

Table S3. Temperature-dependent bulk modulus, B (GPa) of MOFs calculated from MD simulations.

Temp. (K)	MOF-C6	MOF-C10	MOF-C16	MOF-C22	MOF-C30
10	19.37	14.81	13.83	9.22	6.16
100	19.18	13.36	12.95	7.33	5.34
200	18.18	11.33	12.17	7.01	4.61
300	16.66	11.28	10.05	6.88	4.11
400	16.63	10.11	8.23	6.64	4.29
500	16.02	9.29	7.20	5.75	4.00
600	15.31	6.74	6.35	5.29	3.27

Table S4. Temperature-dependent shear modulus, C′ (GPa) of MOFs calculated from MD simulations.

Temp. (K)	MOF-C6	MOF-C10	MOF-C16	MOF-C22	MOF-C30
10	18.87	13.98	12.88	8.17	6.03
100	17.11	12.18	10.37	7.33	5.75
200	14.53	10.70	9.65	6.67	5.57
300	13.10	9.70	7.84	6.08	5.12
400	12.04	8.57	6.81	6.09	5.46
500	10.34	8.01	6.51	6.11	4.76
600	8.22	6.83	6.09	5.48	4.24

Table S5. Temperature-dependent elastic constant C_{11} (GPa) of MOFs calculated from MD simulations.

Temp. (K)	MOF-C6	MOF-C10	MOF-C16	MOF-C22	MOF-C30
10	44.53	33.45	31.00	20.11	14.20
100	41.99	29.60	26.78	17.10	13.01
200	37.55	25.60	25.04	15.90	12.04
300	34.13	24.21	20.50	14.99	10.94
400	32.68	21.54	17.31	14.76	11.57
500	29.81	19.97	15.88	13.90	10.35
600	26.27	15.85	14.47	12.60	8.92

Table S6. Temperature-dependent elastic constant C_{44} (GPa) of MOFs calculated from MD simulations.

Temp. (K)	MOF-C6	MOF-C10	MOF-C16	MOF-C22	MOF-C30
10	1.82	1.59	1.58	0.62	1.17
100	1.73	1.45	1.38	0.58	1.01
200	1.72	1.22	1.07	0.56	0.74
300	1.36	0.97	0.80	0.53	0.46
400	1.09	0.72	0.81	0.38	0.46
500	1.22	0.58	0.52	0.32	0.49
600	1.04	0.32	0.34	0.13	0.34