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Supplementary Materials

Effect of Modulation and Functionalization of UiO-66 Type MOFs on Their Surface Thermodynamic Properties and Lewis Acid–Base Behavior

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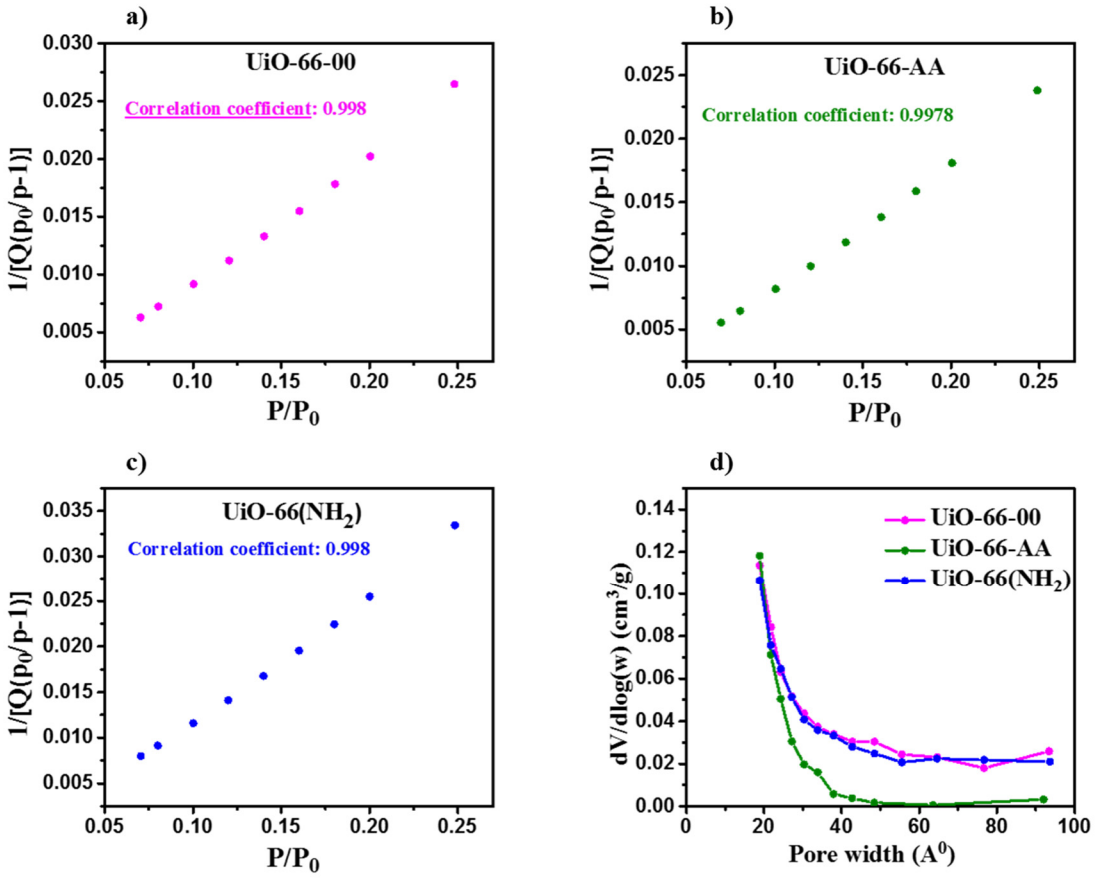

Figure S1. BET surface area plot and correlation coefficient: (a) for UiO-66-00, (b) for UiO-66-AA, (c) for UiO-66(NH_2) and (d) the plot of pore size distribution of MOFs.

Table S1. Values of the dispersive component of the surface energy γ_s^d (mJ/m^2) of UiO-66-00 material as a function of the temperature.

γ_s^d (mJ/m^2) (UiO-66-00)								
Temperature (K)	**313.15**	**323.15**	**333.15**	**343.15**	**353.15**	**363.15**	**373.15**	**383.15**
Cylindrical	22.40	21.89	21.34	20.75	20.10	19.39	18.59	17.70
Redlich-Kwong	34.90	33.85	32.74	31.55	30.28	28.90	27.41	25.77
VDW	21.41	20.77	20.09	19.36	18.58	17.73	16.82	15.81
Geometric	17.35	17.15	16.94	16.70	16.42	16.10	15.73	15.29
Spherical	60.44	57.69	54.85	51.92	48.87	45.70	42.39	38.90
Kiselev	22.23	21.58	20.90	20.17	19.38	18.53	17.60	16.57
Hamieh model	34.99	32.34	29.73	27.17	24.67	22.21	19.79	17.43
Dorris-Gray	40.10	38.94	37.77	36.60	35.44	34.27	33.11	31.94
Dorris-Gray-Hamieh	38.35	36.75	35.15	33.55	31.95	30.35	28.75	27.16

Table S2. Values of the dispersive component of the surface energy γ_s^d (mJ/m^2) of UiO-66-AA material as a function of the temperature.

γ_s^d (mJ/m^2) (UiO-66-AA)								
Temperature (K)	**313.15**	**323.15**	**333.15**	**343.15**	**353.15**	**363.15**	**373.15**	**383.15**
Cylindrical	33.58	31.95	30.32	28.69	27.06	25.43	23.81	22.17
Redlich-Kwong	52.57	49.71	46.86	43.99	41.13	38.27	35.42	32.55
VDW	32.34	30.59	28.84	27.1	25.34	23.59	21.84	20.09
Geometric	26.02	25.04	24.06	23.08	22.10	21.12	20.14	19.16
Spherical	91.02	85.01	79.00	72.99	66.98	60.97	54.96	48.95
Kiselev	33.6	31.803	30.00	28.203	26.403	24.603	22.803	21.00
Hamieh model	51.82	47.38	42.94	38.5	34.06	28.90	25.18	20.74
Dorris-Gray	43.15	41.76	40.37	38.98	37.59	36.20	34.8	33.42
Dorris-Gray-Hamieh	52.07	50.155	48.23	46.31	44.39	42.47	40.55	38.63

Table S3. Values of the dispersive component of the surface energy γ_s^d (mJ/m^2) of UiO-66-FA material as a function of the temperature.

γ_s^d (mJ/m^2) (UiO-66-FA)								
Temperature (K)	**313.15**	**323.15**	**333.15**	**343.15**	**353.15**	**363.15**	**373.15**	**383.15**
Cylindrical	47.31	45.42	43.48	41.48	39.40	37.24	34.97	32.57
Redlich-Kwong	73.64	70.20	66.69	63.08	59.38	55.56	51.61	47.48
VDW	45.16	42.98	40.90	38.69	36.42	34.08	31.65	29.13
Geometric	36.57	35.52	34.43	33.29	32.10	30.84	29.49	28.02
Spherical	128.64	120.67	112.70	104.69	96.65	88.57	80.44	72.23
Kiselev	47.33	45.14	42.91	40.62	38.26	35.83	33.31	30.68
Hamieh model	74.20	67.39	60.85	54.59	48.60	42.88	37.43	32.24
Dorris-Gray	63.13	61.27	59.41	57.56	55.70	53.84	51.99	50.13
Dorris-Gray-Hamieh	59.87	57.37	54.87	52.37	49.87	47.37	44.87	42.37

Table S4. Values of the dispersive component of the surface energy γ_s^d (mJ/m^2) of UiO-66(NH$_2$) material as a function of the temperature.

γ_s^d (mJ/m^2) (UiO-66(NH$_2$))								
Temperature (K)	**313.15**	**323.15**	**333.15**	**343.15**	**353.15**	**363.15**	**373.15**	**383.15**
Cylindrical	124.6	121.00	117.34	113.68	110.02	106.36	102.69	99.03
Redlich-Kwong	196.55	189.29	182.04	174.79	167.54	160.28	153.03	145.78
VDW	120.38	115.95	111.52	107.08	102.65	98.21	93.78	89.35
Geometric	96.17	94.53	92.90	91.26	89.62	87.98	86.34	84.71
Spherical	340.95	323.86	306.77	289.68	272.59	255.5	238.41	221.32
Kiselev	124.22	119.80	115.38	110.96	106.54	102.12	97.70	93.27
Hamieh model	193.54	179.65	165.75	151.85	137.96	124.06	110.17	96.27
Dorris-Gray	69.44	67.39	65.351	63.316	61.27	59.224	57.189	55.143
Dorris-Gray-Hamieh	200.77	192.70	184.63	176.56	168.49	160.42	152.35	144.28

Table S5. Values (in kJ/mol) of the specific free energy ($-\Delta G_a^{sp}(T)$) of the various polar solvents adsorbed on UiO-66-00 material surface for different temperatures by using the various IGC models and methods.

Kiselev							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	1.36	1.41	27.56	0.53	7.70	6.74	2.15
498.15	1.50	1.54	28.37	1.02	8.18	6.90	2.19
503.15	1.64	1.67	29.18	1.51	8.65	7.05	2.23
508.15	1.78	1.80	29.99	2.00	9.13	7.21	2.27
513.15	1.92	1.94	30.80	2.49	9.60	7.36	2.31
518.15	2.06	2.07	31.61	2.98	10.08	7.52	2.35
523.15	2.20	2.20	32.42	3.47	10.55	7.67	2.39
528.15	2.34	2.33	33.23	3.96	11.03	7.83	2.43
533.15	2.48	2.47	34.04	4.45	11.50	7.98	2.47
538.15	2.62	2.60	34.85	4.94	11.98	8.14	2.51
543.15	2.75	2.73	35.66	5.43	12.45	8.29	2.55

Spherical							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	30.90	23.51	22.74	6.09	3.98	2.90	0.97
498.15	31.48	23.88	33.08	6.69	4.48	2.97	0.99
503.15	32.06	24.25	32.86	7.29	4.98	3.04	1.01
508.15	32.64	24.62	32.64	7.89	5.48	3.11	1.03
513.15	33.22	24.99	32.42	8.49	5.98	3.18	1.05
518.15	33.80	25.36	32.20	9.09	6.48	3.25	1.07
523.15	34.38	25.73	31.98	9.69	6.98	3.32	1.09
528.15	34.95	26.11	31.76	10.29	7.48	3.39	1.11
533.15	35.53	26.48	31.54	10.89	7.98	3.46	1.13
538.15	36.11	26.85	31.32	11.49	8.48	3.53	1.15
543.15	36.69	27.22	31.10	12.09	8.98	3.60	1.17

Geometric							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	2.14	1.86	2.98	1.03	7.68	1.99	0.58
498.15	2.47	2.16	3.45	1.32	8.00	2.08	0.59

503.15	2.79	2.45	3.93	1.61	8.32	2.16	0.60
508.15	3.12	2.75	4.40	1.90	8.64	2.25	0.61
513.15	3.45	3.04	4.88	2.19	8.96	2.33	0.62
518.15	3.78	3.34	5.35	2.48	9.28	2.41	0.63
523.15	4.11	3.63	5.83	2.77	9.60	2.50	0.64
528.15	4.43	3.93	6.30	3.06	9.92	2.58	0.65
533.15	4.76	4.22	6.78	3.35	10.24	2.66	0.66
538.15	5.09	4.52	7.25	3.64	10.56	2.75	0.67
543.15	5.42	4.81	7.73	3.93	10.87	2.83	0.67

VDW							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	18.70	25.55	6.40	14.24	2.16	5.02	0.20
498.15	19.14	25.97	7.40	14.73	2.40	5.35	0.24
503.15	19.58	26.39	8.40	15.22	2.65	5.68	0.27
508.15	20.01	26.82	9.40	15.70	2.89	6.02	0.31
513.15	20.45	27.24	10.40	16.19	3.13	6.35	0.34
518.15	20.89	27.66	11.40	16.68	3.37	6.68	0.38
523.15	21.32	28.09	12.40	17.17	3.61	7.01	0.41
528.15	21.76	28.51	13.40	17.65	3.85	7.35	0.45
533.15	22.19	28.93	14.40	18.14	4.09	7.68	0.49
538.15	22.63	29.36	15.40	18.63	4.33	8.01	0.52
543.15	23.07	29.78	16.40	19.12	4.57	8.34	0.56

Redlich-Kwong							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	5.15	6.28	35.66	1.71	13.88	3.05	4.01
498.15	5.45	6.51	36.71	2.29	14.24	3.23	4.08
503.15	5.75	6.74	37.76	2.86	14.60	3.42	4.14
508.15	6.05	6.97	38.81	3.44	14.96	3.60	4.21
513.15	6.35	7.20	39.86	4.01	15.32	3.79	4.27
518.15	6.65	7.43	40.91	4.59	15.68	3.97	4.34
523.15	6.95	7.66	41.96	5.16	16.04	4.16	4.40
528.15	7.25	7.88	43.01	5.74	16.40	4.34	4.47
533.15	7.55	8.11	44.06	6.31	16.76	4.53	4.53
538.15	7.85	8.34	45.11	6.89	17.12	4.71	4.60
543.15	8.15	8.57	46.16	7.46	17.48	4.90	4.66

Cylindrical							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	1.41	1.37	24.17	2.14	4.25	6.44	2.85
498.15	1.53	1.49	24.86	2.60	4.69	6.58	2.89
503.15	1.64	1.60	25.56	3.06	5.13	6.71	2.92
508.15	1.76	1.71	26.25	3.52	5.57	6.85	2.96
513.15	1.88	1.83	26.94	3.98	6.01	6.98	2.99
518.15	2.00	1.94	27.64	4.44	6.45	7.12	3.03
523.15	2.12	2.05	28.33	4.90	6.89	7.25	3.07
528.15	2.23	2.17	29.02	5.36	7.33	7.39	3.10
533.15	2.35	2.28	29.72	5.82	7.77	7.52	3.14
538.15	2.47	2.40	30.41	6.28	8.21	7.66	3.18
543.15	2.59	2.51	31.10	6.74	8.65	7.79	3.21

Hamieh model							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	6.96	4.59	34.97	7.81	11.31	8.27	2.19
498.15	7.17	4.78	35.78	8.15	11.60	8.41	2.24
503.15	7.39	4.96	36.58	8.48	11.88	8.56	2.29
508.15	7.60	5.15	37.39	8.82	12.16	8.70	2.34
513.15	7.82	5.33	38.20	9.15	12.44	8.84	2.39
518.15	8.03	5.52	39.01	9.49	12.72	8.99	2.44
523.15	8.25	5.70	39.81	9.82	13.00	9.13	2.49
528.15	8.46	5.89	40.62	10.16	13.28	9.27	2.54
533.15	8.68	6.07	41.43	10.49	13.57	9.41	2.59
538.15	8.89	6.26	42.24	10.83	13.85	9.56	2.64
543.15	9.11	6.44	43.04	11.16	14.13	9.70	2.69

Topological index							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	9.26	6.45	15.92	3.94	20.76	1.27	2.25
498.15	9.25	6.43	15.72	3.91	20.26	1.20	2.26
503.15	9.25	6.42	15.52	3.87	20.10	1.12	2.27
508.15	9.24	6.40	15.32	3.84	20.20	1.05	2.28
513.15	9.23	6.38	15.12	3.80	19.47	0.97	2.29
518.15	9.22	6.37	14.92	3.77	19.43	0.90	2.30
523.15	9.22	6.35	14.72	3.73	19.14	0.82	2.31
528.15	9.21	6.33	14.52	3.70	19.26	0.75	2.32
533.15	9.20	6.32	14.32	3.66	18.90	0.67	2.33
538.15	9.19	6.30	14.12	3.63	18.82	0.60	2.34
543.15	9.19	6.28	13.92	3.59	18.62	0.52	2.35

Deformation polarizability							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	3.50	1.98	23.21	2.60	21.82	1.25	1.67
498.15	3.49	1.97	23.06	2.53	21.28	1.14	1.67
503.15	3.47	1.96	22.90	2.45	21.14	1.01	1.67
508.15	3.45	1.94	22.75	2.38	21.29	1.05	1.67
513.15	3.43	1.93	22.59	2.30	20.47	0.97	1.66
518.15	3.42	1.91	22.44	2.23	20.44	0.62	1.66
523.15	3.40	1.90	22.28	2.15	20.12	0.67	1.66
528.15	3.38	1.89	22.13	2.08	20.27	0.94	1.66
533.15	3.36	1.87	21.97	2.00	19.90	0.81	1.65
538.15	3.35	1.86	21.82	1.93	19.80	0.52	1.65
543.15	3.33	1.84	21.66	1.85	19.56	0.33	1.65

Vapor pressure							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	2.83	2.11	20.12	20.76	20.46	4.60	0.96
498.15	2.81	2.10	20.01	20.65	20.36	4.58	0.96
503.15	2.79	2.09	19.90	20.54	20.27	4.55	0.96
508.15	2.77	2.08	19.79	20.43	20.18	4.53	0.95
513.15	2.75	2.07	19.68	20.32	20.09	4.51	0.95

518.15	2.73	2.06	19.57	20.21	20.00	4.48	0.95
523.15	2.71	2.05	19.46	20.10	19.91	4.46	0.95
528.15	2.69	2.04	19.35	19.99	19.81	4.43	0.95
533.15	2.67	2.03	19.24	19.88	19.72	4.41	0.95
538.15	2.65	2.02	19.13	19.77	19.63	4.38	0.95
543.15	2.63	2.01	19.02	19.66	19.54	4.36	0.95

Table S6. Values (in kJ/mol) of the specific free energy ($-\Delta G_a^{sp}(T)$) of the various polar solvents adsorbed on UiO-66-AA material surface for different temperatures by using the various IGC models and methods.

Kiselev							
T (K)	**DCM**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	7.053	6.744	11.362	25.750	–0.076	0.042	2.464
498.15	6.938	6.631	11.198	25.429	–0.228	–0.058	2.454
503.15	6.823	6.518	11.034	25.107	–0.379	–0.158	2.443
508.15	6.708	6.405	10.870	24.786	–0.531	–0.258	2.433
513.15	6.593	6.292	10.706	24.464	–0.682	–0.358	2.422
518.15	6.478	6.179	10.542	24.143	–0.834	–0.458	2.412
523.15	6.363	6.066	10.378	23.821	–0.985	–0.558	2.401
528.15	6.248	5.953	10.214	23.500	–1.137	–0.658	2.391
533.15	6.133	5.840	10.050	23.178	–1.288	–0.758	2.380
538.15	6.018	5.727	9.886	22.857	–1.440	–0.858	2.370
543.15	5.903	5.614	9.722	22.535	–1.591	–0.958	2.359

Spherical							
T (K)	**DCM**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	6.471	5.393	10.903	10.903	1.135	–0.669	–1.011
498.15	6.418	5.348	10.654	10.654	0.669	–0.726	–1.067
503.15	6.365	5.303	10.405	10.405	0.203	–0.784	–1.123
508.15	6.312	5.258	10.156	10.156	–0.263	–0.841	–1.179
513.15	6.259	5.213	9.907	9.907	–0.729	–0.899	–1.235
518.15	6.206	5.168	9.658	9.658	–1.195	–0.956	–1.291
523.15	6.153	5.123	9.409	9.409	–1.661	–1.014	–1.347
528.15	6.100	5.078	9.160	9.160	–2.127	–1.071	–1.403
533.15	6.047	5.033	8.911	8.911	–2.593	–1.129	–1.459
538.15	5.994	4.988	8.662	8.662	–3.059	–1.186	–1.515
543.15	5.941	4.943	8.413	8.413	–3.525	–1.244	–1.571

Geometric							
T (K)	**DCM**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	7.364	11.859	11.712	8.173	2.755	–0.366	3.558
498.15	7.303	11.951	11.536	7.858	2.415	–0.383	3.574
503.15	7.243	12.044	11.360	7.543	2.074	–0.400	3.590
508.15	7.182	12.136	11.184	7.228	1.734	–0.417	3.606
513.15	7.122	12.229	11.008	6.913	1.393	–0.434	3.622
518.15	7.061	12.321	10.832	6.598	1.053	–0.451	3.638
523.15	7.001	12.414	10.656	6.283	0.712	–0.468	3.654
528.15	6.940	12.506	10.480	5.968	0.372	–0.485	3.670
533.15	6.880	12.599	10.304	5.653	0.031	–0.502	3.686

538.15	6.819	12.691	10.128	5.338	–0.309	–0.519	3.702
543.15	6.759	12.784	9.952	5.023	–0.650	–0.536	3.718

VDW							
T (K)	**DCM**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	6.607	–1.037	3.661	11.389	2.500	0.030	–0.761
498.15	6.571	–1.355	3.474	11.152	2.218	–0.004	–0.793
503.15	6.535	–1.673	3.287	10.914	1.935	–0.038	–0.824
508.15	6.499	–1.991	3.100	10.677	1.653	–0.072	–0.856
513.15	6.463	–2.309	2.913	10.439	1.370	–0.106	–0.887
518.15	6.427	–2.627	2.726	10.202	1.088	–0.140	–0.919
523.15	6.391	–2.945	2.539	9.964	0.805	–0.174	–0.950
528.15	6.355	–3.263	2.352	9.727	0.523	–0.208	–0.982
533.15	6.319	–3.581	2.165	9.489	0.240	–0.242	–1.013
538.15	6.283	–3.899	1.978	9.252	–0.042	–0.276	–1.045
543.15	6.247	–4.217	1.791	9.014	–0.325	–0.310	–1.076

Redlich-kwong							
T (K)	**DCM**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	6.681	–0.976	3.707	0.412	2.483	0.026	–0.760
498.15	6.647	–1.293	3.520	–0.035	2.200	–0.008	–0.792
503.15	6.612	–1.609	3.334	–0.481	1.917	–0.042	–0.823
508.15	6.578	–1.926	3.147	–0.928	1.634	–0.076	–0.855
513.15	6.543	–2.242	2.961	–1.374	1.351	–0.110	–0.886
518.15	6.509	–2.559	2.774	–1.821	1.068	–0.144	–0.918
523.15	6.474	–2.875	2.588	–2.267	0.785	–0.178	–0.949
528.15	6.440	–3.192	2.401	–2.714	0.502	–0.212	–0.981
533.15	6.405	–3.508	2.215	–3.160	0.219	–0.246	–1.012
538.15	6.371	–3.825	2.028	–3.607	–0.064	–0.280	–1.044
543.15	6.336	–4.141	1.842	–4.053	–0.347	–0.314	–1.075

Table S7. Values (in kJ/mol) of the specific free energy ($-\Delta G_a^{sp}(T)$) of the various polar solvents adsorbed on UiO-66-FA material surface for different temperatures by using the various IGC models and methods.

Cylindrical							
T (K)	**DCM**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	7.705	4.747	3.933	17.496	2.316	1.064	1.394
498.15	7.634	4.581	3.785	17.119	1.955	0.995	1.376
503.15	7.563	4.416	3.636	16.743	1.593	0.925	1.359
508.15	7.492	4.250	3.488	16.366	1.232	0.856	1.341
513.15	7.421	4.085	3.339	15.990	0.870	0.786	1.324
518.15	7.350	3.919	3.191	15.613	0.509	0.717	1.306
523.15	7.279	3.754	3.042	15.237	0.147	0.647	1.289
528.15	7.208	3.588	2.894	14.860	–0.214	0.578	1.271
533.15	7.137	3.423	2.745	14.484	–0.576	0.508	1.254
538.15	7.066	3.257	2.597	14.107	–0.937	0.439	1.236
543.15	6.995	3.092	2.448	13.731	–1.299	0.369	1.219

Hamieh model							
T (K)	**DCM**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	3.105	3.899	24.036	26.241	35.992	1.633	0.574

498.15	3.065	3.879	23.800	26.017	35.959	1.573	0.572
503.15	3.025	3.859	23.565	25.793	35.927	1.512	0.569
508.15	2.985	3.839	23.329	25.569	35.894	1.452	0.567
513.15	2.945	3.819	23.094	25.345	35.862	1.391	0.564
518.15	2.905	3.799	22.858	25.121	35.829	1.331	0.562
523.15	2.865	3.779	22.623	24.897	35.797	1.270	0.559
528.15	2.825	3.759	22.387	24.673	35.764	1.210	0.557
533.15	2.785	3.739	22.152	24.449	35.732	1.149	0.554
538.15	2.745	3.719	21.916	24.225	35.699	1.089	0.552
543.15	2.705	3.699	21.681	24.001	35.667	1.028	0.549

Topological index

T (K)	DCM	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	10.204	9.259	14.186	3.211	6.913	5.564	1.902
498.15	10.144	9.220	13.987	3.023	6.571	5.554	1.897
503.15	10.085	9.180	13.787	2.835	6.229	5.543	1.892
508.15	10.025	9.141	13.588	2.647	5.887	5.533	1.887
513.15	9.966	9.101	13.388	2.459	5.545	5.522	1.882
518.15	9.906	9.062	13.189	2.271	5.203	5.512	1.877
523.15	9.847	9.022	12.989	2.083	4.861	5.501	1.872
528.15	9.787	8.983	12.790	1.895	4.519	5.491	1.867
533.15	9.728	8.943	12.590	1.707	4.177	5.480	1.862
538.15	9.668	8.904	12.391	1.519	3.835	5.470	1.857
543.15	9.609	8.864	12.191	1.331	3.493	5.459	1.852

Deformation polarizability

T (K)	DCM	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	4.503	7.184	15.757	3.848	7.994	3.438	0.324
498.15	4.492	7.179	15.453	3.644	7.569	3.410	0.303
503.15	4.482	7.173	15.149	3.439	7.145	3.382	0.282
508.15	4.471	7.168	14.845	3.235	6.720	3.354	0.261
513.15	4.461	7.162	14.541	3.030	6.296	3.326	0.240
518.15	4.450	7.157	14.237	2.826	5.871	3.298	0.219
523.15	4.440	7.151	13.933	2.621	5.447	3.270	0.198
528.15	4.429	7.146	13.629	2.417	5.022	3.242	0.177
533.15	4.419	7.140	13.325	2.212	4.598	3.214	0.156
538.15	4.408	7.135	13.021	2.008	4.173	3.186	0.135
543.15	4.398	7.129	12.717	1.803	3.749	3.158	0.114

Vapor pressure

T (K)	DCM	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	3.322	1.258	12.262	3.262	1.814	1.144	3.026
498.15	3.282	1.211	12.101	3.080	1.602	1.119	3.025
503.15	3.241	1.164	11.939	2.897	1.390	1.094	3.023
508.15	3.201	1.117	11.778	2.715	1.178	1.069	3.022
513.15	3.160	1.070	11.616	2.532	0.966	1.044	3.020
518.15	3.120	1.023	11.455	2.350	0.754	1.019	3.019
523.15	3.079	0.976	11.293	2.167	0.542	0.994	3.017
528.15	3.039	0.929	11.132	1.985	0.330	0.969	3.016
533.15	2.998	0.882	10.970	1.802	0.118	0.944	3.014
538.15	2.958	0.835	10.809	1.620	–0.094	0.919	3.013

543.15	2.917	0.788	10.647	1.437	–0.306	0.894	3.011

Kiselev

T(K)	Dichloromethane	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	4.54	4.25	0.11	3.81	3.87	3.13	0.41
498.15	4.71	4.40	1.01	4.52	4.30	3.35	0.44
503.15	4.89	4.56	1.91	5.24	4.73	3.57	0.47
508.15	5.06	4.71	2.81	5.95	5.16	3.79	0.50
513.15	5.24	4.87	3.71	6.67	5.59	4.01	0.53
518.15	5.41	5.02	4.61	7.38	6.02	4.23	0.56
523.15	5.59	5.18	5.51	8.10	6.45	4.45	0.59
528.15	5.76	5.33	6.41	8.81	6.88	4.67	0.62
533.15	5.94	5.49	7.31	9.53	7.31	4.89	0.65
538.15	6.11	5.64	8.21	10.24	7.74	5.11	0.68
543.15	6.29	5.80	9.11	10.96	8.17	5.33	0.71

Spherical

T(K)	Dichloromethane	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	4.93	4.80	1.47	1.32	4.51	2.62	0.43
498.15	5.14	4.99	2.47	2.06	4.99	2.85	0.46
503.15	5.34	5.18	3.48	2.80	5.48	3.08	0.49
508.15	5.55	5.37	4.48	3.54	5.96	3.31	0.53
513.15	5.75	5.56	5.49	4.28	6.45	3.54	0.56
518.15	5.96	5.75	6.49	5.02	6.93	3.77	0.59
523.15	6.16	5.94	7.50	5.76	7.42	4.00	0.63
528.15	6.37	6.13	8.50	6.50	7.90	4.23	0.66
533.15	6.57	6.32	9.51	7.24	8.39	4.46	0.69
538.15	6.78	6.51	10.51	7.98	8.87	4.69	0.73
543.15	6.98	6.70	11.52	8.72	9.36	4.92	0.76

Geometric

T(K)	Dichloromethane	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	2.14	1.86	1.99	1.03	7.68	1.99	0.39
498.15	2.47	2.16	3.45	1.32	8.00	2.08	0.42
503.15	2.79	2.45	3.93	1.61	8.32	2.16	0.46
508.15	3.12	2.75	4.40	1.90	8.64	2.25	0.49
513.15	3.45	3.04	4.88	2.19	8.96	2.33	0.53
518.15	3.78	3.34	5.35	2.48	9.28	2.41	0.56
523.15	4.11	3.63	5.83	2.77	9.60	2.50	0.60
528.15	4.43	3.93	6.30	3.06	9.92	2.58	0.63
533.15	4.76	4.22	6.78	3.35	10.24	2.66	0.67

538.15	5.09	4.52	7.25	3.64	10.56	2.75	0.70
543.15	5.42	4.81	7.73	3.93	10.87	2.83	0.74

VDW

T(K)	Dichloromethane	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	0.86	1.24	10.40	12.47	1.27	0.86	0.63
498.15	1.17	1.52	11.39	13.02	1.41	1.10	0.68
503.15	1.47	1.81	12.39	13.57	1.55	1.34	0.73
508.15	1.78	2.09	13.38	14.12	1.69	1.58	0.77
513.15	2.08	2.38	14.38	14.67	1.83	1.82	0.82
518.15	2.39	2.66	15.38	15.22	1.98	2.06	0.87
523.15	2.69	2.95	16.37	15.77	2.12	2.30	0.91
528.15	3.00	3.23	17.37	16.32	2.26	2.54	0.96
533.15	3.30	3.52	18.36	16.87	2.40	2.78	1.01
538.15	3.61	3.80	19.36	17.42	2.54	3.02	1.05
543.15	3.91	4.09	20.36	17.97	2.68	3.26	1.10

Redlich-Kwong

T(K)	Dichloromethane	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	0.30	1.66	1.39	1.64	1.83	1.08	0.22
498.15	0.41	1.77	2.32	2.18	1.98	1.34	0.27
503.15	0.52	1.87	3.24	2.73	2.14	1.60	0.32
508.15	0.63	1.98	4.17	3.27	2.30	1.86	0.38
513.15	0.74	2.08	5.09	3.82	2.45	2.12	0.43
518.15	0.85	2.19	6.02	4.36	2.61	2.38	0.48
523.15	0.96	2.29	6.94	4.91	2.76	2.64	0.53
528.15	1.07	2.40	7.87	5.45	2.92	2.90	0.59
533.15	1.18	2.50	8.79	6.00	3.08	3.16	0.64
538.15	1.29	2.61	9.72	6.54	3.23	3.42	0.69
543.15	1.40	2.71	10.64	7.09	3.39	3.68	0.75

Cylindrical

T(K)	Dichloromethane	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	0.97	0.85	7.63	4.61	1.05	2.29	0.91
498.15	1.10	0.97	8.59	5.14	1.48	2.61	0.94
503.15	1.23	1.09	9.54	5.67	1.91	2.92	0.98
508.15	1.36	1.21	10.50	6.20	2.34	3.24	1.01
513.15	1.49	1.33	11.45	6.73	2.77	3.55	1.04
518.15	1.62	1.45	12.41	7.26	3.20	3.87	1.07
523.15	1.75	1.57	13.36	7.79	3.63	4.18	1.10
528.15	1.88	1.69	14.32	8.32	4.06	4.50	1.14

533.15	2.01	1.81	15.27	8.85	4.49	4.81	1.17
538.15	2.14	1.93	16.23	9.38	4.92	5.13	1.20
543.15	2.27	2.05	17.18	9.91	5.35	5.44	1.23

Hamieh model

T(K)	Dichloromethane	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	6.96	4.59	34.97	7.81	11.31	8.27	2.19
498.15	7.17	4.78	35.78	8.15	11.60	8.41	2.24
503.15	7.39	4.96	36.58	8.48	11.88	8.56	2.29
508.15	7.60	5.15	37.39	8.82	12.16	8.70	2.34
513.15	7.82	5.33	38.20	9.15	12.44	8.84	2.39
518.15	8.03	5.52	39.01	9.49	12.72	8.99	2.44
523.15	8.25	5.70	39.81	9.82	13.00	9.13	2.49
528.15	8.46	5.89	40.62	10.16	13.28	9.27	2.54
533.15	8.68	6.07	41.43	10.49	13.57	9.41	2.59
538.15	8.89	6.26	42.24	10.83	13.85	9.56	2.64
543.15	9.11	6.44	43.04	11.16	14.13	9.70	2.69

Topological index

T(K)	Dichloromethane	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	3.32	3.33	1.61	1.18	1.54	1.65	0.15
498.15	3.45	3.45	2.58	1.98	2.08	1.88	0.18
503.15	3.59	3.58	3.56	2.79	2.61	2.11	0.21
508.15	3.72	3.70	4.53	3.59	3.15	2.34	0.24
513.15	3.86	3.83	5.51	4.40	3.68	2.57	0.27
518.15	3.99	3.95	6.48	5.20	4.22	2.80	0.30
523.15	4.13	4.08	7.46	6.01	4.75	3.03	0.33
528.15	4.26	4.20	8.43	6.81	5.29	3.26	0.36
533.15	4.40	4.33	9.41	7.62	5.82	3.49	0.39
538.15	4.53	4.45	10.38	8.42	6.36	3.72	0.42
543.15	4.67	4.58	11.36	9.23	6.89	3.95	0.45

Deformation polarizability

T(K)	Dichloromethane	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
493.15	10.88055	7.175335	55.64225	42.1912	23.3348	6.354125	2.8137
498.15	10.86555	7.129835	55.21725	41.8312	23.0948	6.241625	2.40518
503.15	10.85055	7.084335	54.79225	41.4712	22.8548	6.129125	2.39118
508.15	10.83555	7.038835	54.36725	41.1112	22.6148	6.016625	2.37718
513.15	10.82055	6.993335	53.94225	40.7512	22.3748	5.904125	2.36318
518.15	10.80555	6.947835	53.51725	40.3912	22.1348	5.791625	2.34918
523.15	10.79055	6.902335	53.09225	40.0312	21.8948	5.679125	2.33518

528.15	10.77555	6.856835	52.66725	39.6712	21.6548	5.566625	2.32118
533.15	10.76055	6.811335	52.24225	39.3112	21.4148	5.454125	2.30718
538.15	10.74555	6.765835	51.81725	38.9512	21.1748	5.341625	2.29318
543.15	10.73055	6.720335	51.39225	38.5912	20.9348	5.229125	2.27918

Vapor pressure							
T(K)	**Dichloromethane**	**Chloroform**	**THF**	**Ether**	**Acetonitrile**	**Toluene**	**Benzene**
493.15	6.60275	5.08905	63.7285	55.10965	43.42375	11.637	1.50685
498.15	6.52775	5.02405	63.2785	54.66465	43.04875	11.537	1.50185
503.15	6.45275	4.95905	62.8285	54.21965	42.67375	11.437	1.49685
508.15	6.37775	4.89405	62.3785	53.77465	42.29875	11.337	1.49185
513.15	6.30275	4.82905	61.9285	53.32965	41.92375	11.237	1.48685
518.15	6.22775	4.76405	61.4785	52.88465	41.54875	11.137	1.48185
523.15	6.15275	4.69905	61.0285	52.43965	41.17375	11.037	1.47685
528.15	6.07775	4.63405	60.5785	51.99465	40.79875	10.937	1.47185
533.15	6.00275	4.56905	60.1285	51.54965	40.42375	10.837	1.46685
538.15	5.92775	4.50405	59.6785	51.10465	40.04875	10.737	1.46185
543.15	5.85275	4.43905	59.2285	50.65965	39.67375	10.637	1.45685

Table S8. Values (in kJ/mol) of the specific free energy ($-\Delta G_a^{sp}(T)$) of the various polar solvents adsorbed on UiO-66(NH_2) material surface for different temperatures by using the various IGC models and methods.

Kiselev				
T (K)	**Dichloromethane**	**Chloroform**	**Toluene**	**Benzene**
493.15	0.010	3.831	1.889	–0.268
498.15	–0.107	3.662	1.642	–0.284
503.15	–0.223	3.494	1.394	–0.300
508.15	–0.340	3.325	1.147	–0.316
513.15	–0.456	3.157	0.899	–0.332
518.15	–0.573	2.988	0.652	–0.348
523.15	–0.689	2.820	0.404	–0.364
528.15	–0.806	2.651	0.157	–0.380
533.15	–0.922	2.483	–0.091	–0.396
538.15	–1.039	2.314	–0.338	–0.412
543.15	–1.155	2.146	–0.586	–0.428
Spherical				
T (K)	**Dichloromethane**	**Chloroform**	**Toluene**	**Benzene**
493.15	5.137	10.533	–4.630	0.221
498.15	5.037	11.329	–4.960	0.206
503.15	4.937	11.593	–5.290	0.191
508.15	4.837	11.513	–5.620	0.176
513.15	4.737	11.262	–5.950	0.161
518.15	4.637	9.947	–6.280	0.146
523.15	4.537	6.512	–6.610	0.131
528.15	4.437	7.512	–6.940	0.116
533.15	4.337	8.512	–7.270	0.101
538.15	4.237	9.512	–7.600	0.086

543.15	4.137	10.512	–7.930	0.071
		Geometric		
T (K)	**Dichloromethane**	**Chloroform**	**Toluene**	**Benzene**
493.15	–3.412	10.750	22.663	0.634
498.15	–3.622	10.715	25.070	0.609
503.15	–3.832	10.680	27.045	0.584
508.15	–4.042	10.645	28.848	0.559
513.15	–4.252	10.610	30.583	0.534
518.15	–4.462	10.575	31.660	0.509
523.15	–4.672	10.540	32.282	0.484
528.15	–4.882	10.505	33.282	0.459
533.15	–5.092	10.470	34.282	0.434
538.15	–5.302	10.435	35.282	0.409
543.15	–5.512	10.400	36.282	0.384
		VDW		
T (K)	**Dichloromethane**	**Chloroform**	**Toluene**	**Benzene**
493.15	15.554	10.937	16.137	1.821
498.15	15.541	11.957	16.001	1.818
503.15	15.528	12.457	15.864	1.814
508.15	15.515	12.632	15.728	1.811
513.15	15.502	12.668	15.591	1.807
518.15	15.489	11.704	15.455	1.804
523.15	15.476	8.828	15.318	1.800
528.15	15.463	9.828	15.182	1.797
533.15	15.450	10.828	15.045	1.793
538.15	15.437	11.828	14.909	1.790
543.15	15.424	12.828	14.772	1.786
		Redlich-Kwong		
T (K)	**Dichloromethane**	**Chloroform**	**Toluene**	**Benzene**
493.15	4.245	8.109	12.480	2.157
498.15	4.120	7.994	12.290	2.152
503.15	3.995	7.878	12.100	2.147
508.15	3.870	7.763	11.910	2.142
513.15	3.745	7.647	11.720	2.137
518.15	3.620	7.532	11.530	2.132
523.15	3.495	7.416	11.340	2.127
528.15	3.370	7.301	11.150	2.122
533.15	3.245	7.185	10.960	2.117
538.15	3.120	7.070	10.770	2.112
543.15	2.995	6.954	10.580	2.107
		Cylindrical		
T (K)	**Dichloromethane**	**Chloroform**	**Toluene**	**Benzene**
493.15	9.975	9.654	5.986	0.314
498.15	9.876	9.544	5.826	0.312
503.15	9.778	9.434	5.666	0.309
508.15	9.679	9.324	5.506	0.307
513.15	9.581	9.214	5.346	0.304
518.15	9.482	9.104	5.186	0.302
523.15	9.384	8.994	5.026	0.299
528.15	9.285	8.884	4.866	0.297
533.15	9.187	8.774	4.706	0.294

538.15	9.088	8.664	4.546	0.292
543.15	8.990	8.554	4.386	0.289
		Hamieh model		
T (K)	**Dichloromethane**	**Chloroform**	**Toluene**	**Benzene**
493.15	3.541	7.722	10.278	0.760
498.15	3.511	7.691	10.185	0.753
503.15	3.481	7.660	10.091	0.746
508.15	3.451	7.629	9.998	0.739
513.15	3.421	7.598	9.904	0.732
518.15	3.391	7.567	9.811	0.725
523.15	3.361	7.536	9.717	0.718
528.15	3.331	7.505	9.624	0.711
533.15	3.301	7.474	9.530	0.704
538.15	3.271	7.443	9.437	0.697
543.15	3.241	7.412	9.343	0.690
		Topological index		
T (K)	**Dichloromethane**	**Chloroform**	**Toluene**	**Benzene**
493.15	18.234	15.884	3.606	3.751
498.15	18.110	15.783	3.441	3.780
503.15	17.986	15.683	3.276	3.810
508.15	17.862	15.582	3.111	3.839
513.15	17.738	15.482	2.946	3.869
518.15	17.614	15.381	2.781	3.898
523.15	17.490	15.281	2.616	3.928
528.15	17.366	15.180	2.451	3.957
533.15	17.242	15.080	2.286	3.987
538.15	17.118	14.979	2.121	4.016
543.15	16.994	14.879	1.956	4.046
		Deformation polarizability		
T (K)	**Dichloromethane**	**Chloroform**	**Toluene**	**Benzene**
493.15	4.923	10.264	7.179	0.508
498.15	4.940	10.230	7.085	0.502
503.15	4.956	10.197	6.990	0.496
508.15	4.973	10.163	6.896	0.490
513.15	4.989	10.130	6.801	0.484
518.15	5.006	10.096	6.707	0.478
523.15	5.022	10.063	6.612	0.472
528.15	5.039	10.029	6.518	0.466
533.15	5.055	9.996	6.423	0.460
538.15	5.072	9.962	6.329	0.454
543.15	5.088	9.929	6.234	0.448
		Vapor pressure		
T (K)	**Dichloromethane**	**Chloroform**	**Toluene**	**Benzene**
493.15	10.312	6.465	5.629	0.057
498.15	10.287	6.456	5.557	0.052
503.15	10.264	6.447	5.484	0.047
508.15	10.255	6.442	5.412	0.042
513.15	10.254	6.439	5.339	0.037
518.15	10.270	6.455	5.267	0.032
523.15	10.271	6.462	5.194	0.027
528.15	10.325	6.490	5.122	0.022

533.15	10.351	6.577	5.049	0.017
538.15	10.389	6.537	4.977	0.012
543.15	10.484	6.607	4.904	0.007

Table S9. Values of the specific enthalpy ($-\Delta H_a^{sp}$ in kJ mol^{-1}) of the various polar solvents adsorbed on UiO-66-00 by using the various molecular models, Hamieh model, topological index, deformation polarizability and vapor pressure methods compared to global average.

Probes	DCM	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
Kiselev	12.35	11.66	52.33	47.80	39.15	8.54	1.80
Spherical	26.15	13.08	53.70	53.09	45.34	4.00	1.00
Geometric	30.21	27.23	43.87	27.57	23.78	6.24	0.30
VDW	24.35	16.17	92.23	33.84	21.61	27.65	3.30
Redlich-Kwong	24.44	16.25	67.90	55.00	21.63	15.20	2.40
Cylindrical	10.23	9.82	44.23	43.21	39.15	6.88	0.75
Hamieh model	14.25	13.65	44.67	25.23	16.45	5.80	2.74
Topological index	10.00	8.08	35.65	7.39	40.52	8.67	1.26
Deformation polarizability	5.23	3.37	38.50	10.00	42.60	8.61	1.92
Vapor pressure	4.80	3.10	30.97	31.64	29.48	7.02	1.06
Average values	18.23	16.22	44.96	32.10	31.97	9.86	1.65

Table S10. Values of the specific entropy ($-\Delta S_a^{sp}$in J $K^{-1}mol^{-1}$) of the various polar solvents adsorbed on UiO-66-00 by using the various molecular models, Hamieh model, topological index, deformation polarizability and vapor pressure methods compared to global average.

Probes	DCM	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
Kiselev	27.8	26.5	162.0	98.0	95.0	31.0	8.0
Spherical	115.7	74.2	155.0	120.0	100.0	14.0	4.0
Geometric	65.6	59.0	95.0	58.0	63.8	16.7	1.8
VDW	87.3	84.6	200.0	120.0	48.2	66.5	7.1
Redlich-Kwong	60.0	45.0	210.0	115.0	72.0	37.0	13.0
Cylindrical	23.6	22.7	138.7	92.0	88.0	27.0	7.3
Hamieh model	43.0	37.0	161.5	67.0	56.3	28.5	10.7
Topological index	1.5	3.3	40.0	7.0	40.5	15.0	2.0
Deformation polarizability	3.5	2.8	31.0	15.0	42.5	15.0	0.0
Vapor pressure	4.0	2.0	22.0	22.1	18.3	4.9	0.2
Average values	27.8	26.5	162.0	98.0	95.0	31.0	8.0

Table S11. Values of the specific enthalpy ($-\Delta H_a^{sp}$ in kJ mol^{-1}) of the various polar solvents adsorbed on UiO-66-AA by using the various molecular models, Hamieh model, topological index, deformation polarizability and vapor pressure methods compared to global average.

Probes	DCM	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
Kiselev	18.395	17.889	57.460	27.537	14.866	9.905	3.500
Spherical	11.698	9.831	35.462	35.462	47.097	5.003	4.512
Geometric	13.331	2.736	39.241	29.071	36.339	1.311	1.980
VDW	10.158	30.327	34.814	22.105	30.363	3.383	2.346
Redlich-Kwong	10.084	30.240	44.450	22.101	30.395	3.379	2.346
Cylindrical	14.708	21.070	54.630	18.580	37.971	7.919	3.120
Hamieh model	15.724	12.062	48.334	47.263	39.197	7.600	1.120
Topological index	16.072	13.155	21.753	33.863	40.644	6.600	2.395
Deformation polarizability	5.539	7.727	24.018	45.741	49.862	6.200	2.395

Vapor pressure	7.317	5.893	21.262	28.191	22.724	3.609	3.174
Average values	12.303	15.093	38.142	30.991	34.946	5.491	2.689

Table S12. Values of the specific entropy ($-\Delta S_a^{sp}$ in $J\,K^{-1}mol^{-1}$) of the various polar solvents adsorbed on UiO-66-AA by using the various molecular models, Hamieh model, topological index, deformation polarizability and vapor pressure methods compared to global average.

Probes	DCM	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
Kiselev	23	22.6	64.33	32.8	30.3	20	2.1
Spherical	10.6	9	49.8	49.8	93.2	11.5	11.2
Geometric	12.1	18.5	63	35.2	68.1	3.4	3.2
VDW	7.2	63.6	47.5	37.4	56.5	6.8	6.3
Redlich-Kwong	6.9	63	89.3	37.3	56.6	6.8	6.3
Cylindrical	14.2	33.1	75.3	29.7	72.3	13.9	3.5
Hamieh model	21.8	20.3	44.8	47.1	6.5	12.1	0.5
Topological index	11.9	7	37.6	39.9	68.4	2.1	1.2
Deformation polarizability	2.1	1.1	40.9	60.8	84.9	5.6	4.2
Vapor pressure	8.1	9.4	36.5	32.3	42.4	5	0.3
Average values	11.79	24.76	54.9	40.23	57.92	8.72	3.88

Table S13. Values of the specific enthalpy ($-\Delta H_a^{sp}$ in $kJ\ mol^{-1}$) of the various polar solvents adsorbed on UiO-66-FA by using the various molecular models, Hamieh model, topological index, deformation polarizability and vapor pressure methods compared to global average.

Probes	DCM	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
Kiselev	12.35	11.66	52.33	47.80	39.15	8.54	1.80
Spherical	26.15	13.08	53.70	53.09	45.34	4.00	1.00
Geometric	30.21	27.23	43.87	27.57	23.78	6.24	0.30
VDW	24.35	16.17	92.23	33.84	21.61	27.65	3.30
Redlich-Kwong	24.44	16.25	67.90	55.00	21.63	15.20	2.40
Cylindrical	10.23	9.82	44.23	43.21	39.15	6.88	0.75
Hamieh model	14.25	13.65	44.67	25.23	16.45	5.80	2.74
Topological index	10.00	8.08	35.65	7.39	40.52	8.67	1.26
Deformation polarizability	5.23	3.37	38.50	10.00	42.60	8.61	1.92
Vapor pressure	4.80	3.10	30.97	31.64	29.48	7.02	1.06
Average values	18.23	16.22	44.96	32.10	31.97	9.86	1.65

Table S14. Values of the specific entropy ($-\Delta S_a^{sp}$ in $J\,K^{-1}mol^{-1}$) of the various polar solvents adsorbed on UiO-66-FA by using the various molecular models, Hamieh model, topological index, deformation polarizability and vapor pressure methods compared to global average.

Probes	DCM	Chloroform	THF	Ether	Acetonitrile	Toluene	Benzene
Kiselev	35.0	31.0	180.0	143.0	88.0	44.0	6.0
Spherical	41.0	38.0	201.0	148.0	97.0	46.0	6.7
Geometric	27.0	22.0	162.0	127.0	95.0	31.0	7.0
VDW	61.0	57.0	199.0	110.0	28.0	48.0	9.4
Redlich-Kwong	22.0	21.0	185.0	109.0	31.0	52.0	10.6
Cylindrical	26.0	24.0	191.0	136.0	86.0	53.0	6.4
Hamieh model	27.0	25.0	195.0	161.0	107.0	46.0	6.0
Topological index	23.4	20.0	66.0	33.0	46.7	22.5	1.5
Deformation polarizability	3.0	9.1	85.0	72.0	48.0	22.5	2.8

Vapor pressure	15.0	13.0	90.0	89.0	75.0	20.0	1.0
Average values	28.0	26.0	155.4	112.8	70.2	38.5	5.7

Table S15. Values of the specific enthalpy ($-\Delta H_a^{sp}$ in kJ mol^{-1}) of the various polar solvents adsorbed on UiO-66(NH_2) by using the various molecular models, Hamieh model, topological index, deformation polarizability and vapor pressure methods compared to global average.

Model or method	DCM	Chloroform	Toluene	Benzene
Kiselev	20.45	11.50	1.31	26.30
Spherical	29.14	15.00	1.70	27.91
Geometric	14.20	17.30	3.10	32.43
Van der Waals	19.71	16.84	2.17	29.60
Redlich-Kwong	19.50	16.57	2.65	31.22
Cylindrical	20.50	19.69	0.56	21.77
Hamieh model	10.78	6.50	1.45	19.50
Topological index	15.38	17.61	0.84	19.88
Deformation polarizability	10.10	5.01	1.10	16.50
Vapor pressure	6.49	10.32	0.55	12.78
Average values	16.63	13.63	1.54	23.79

Table S16. Values of the specific entropy ($-\Delta S_a^{sp}$in J $K^{-1}mol^{-1}$) of the various polar solvents adsorbed on UiO-66(NH_2) by using the various molecular models, Hamieh model, topological index, deformation polarizability and vapor pressure methods compared to global average.

Model or method	DCM	Chloroform	Toluene	Benzene
Kiselev	34	23	3	50
Spherical	52	20	3	66
Geometric	7	42	5	78
Van der Waals	24	3	1	27
Redlich-Kwong	23	25	1	38
Cylindrical	22	20	1	32
Hamieh model	6	6	1	19
Topological index	0	0	0	0
Deformation polarizability	7	3	1	19
Vapor pressure	0	0	0	0
Average value	17	14	2	33

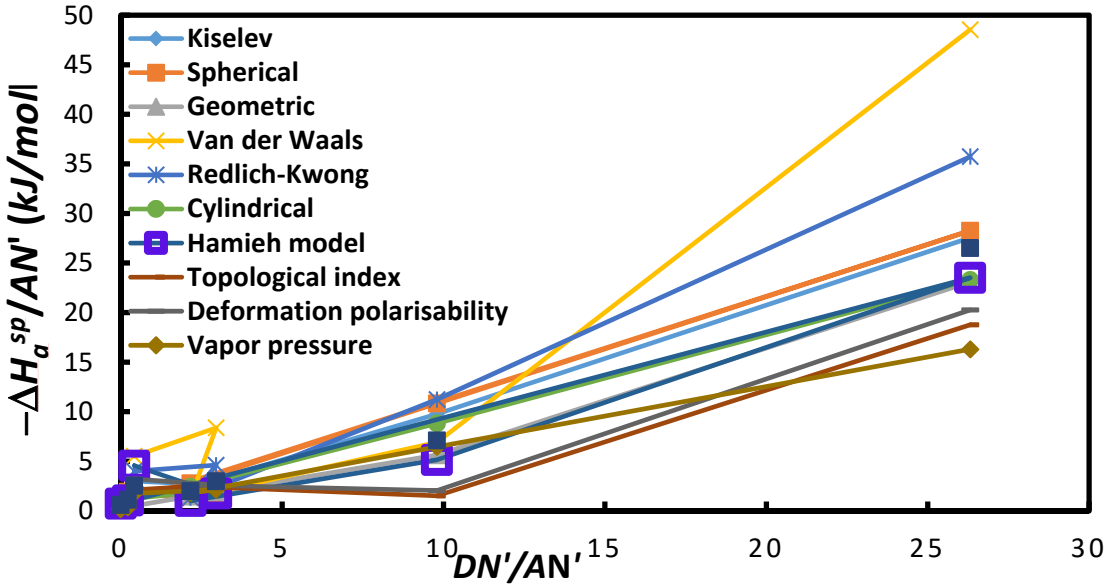

Figure S2. Variations of $\left(\frac{-\Delta H_a^{sp}}{AN'}\right)$ as a function of $\left(\frac{DN'}{AN'}\right)$ of UiO-66-00 for different models and IGC methods.

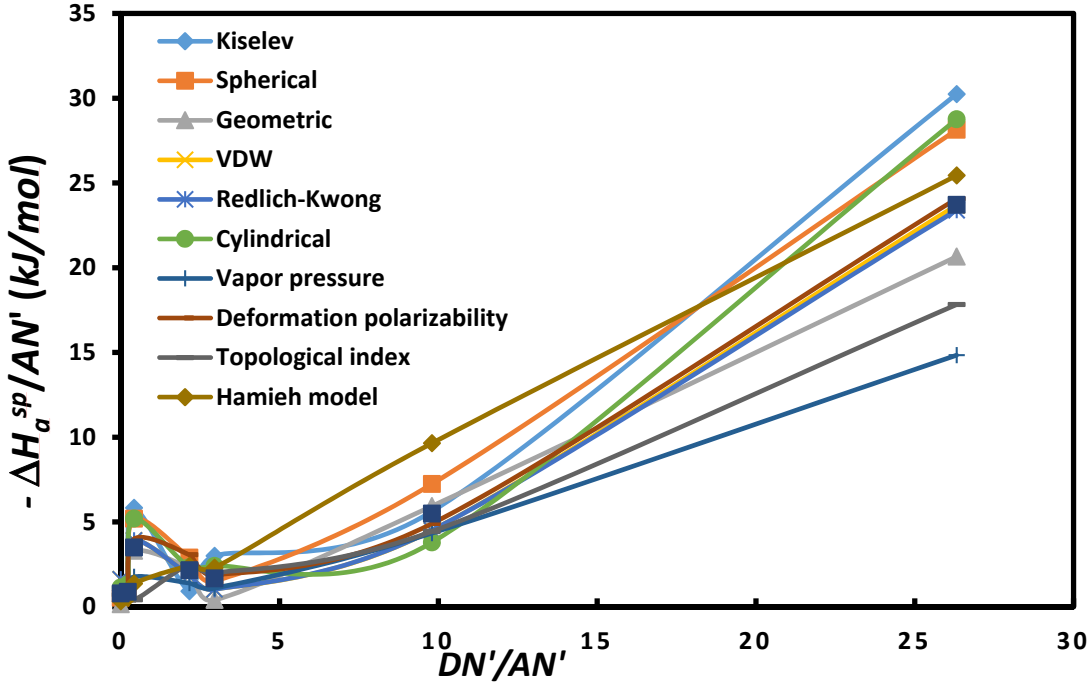

Figure S3. Variations of $\left(\frac{-\Delta H_a^{sp}}{AN'}\right)$ as a function of $\left(\frac{DN'}{AN'}\right)$ of UiO-66-AA for different models and IGC methods.

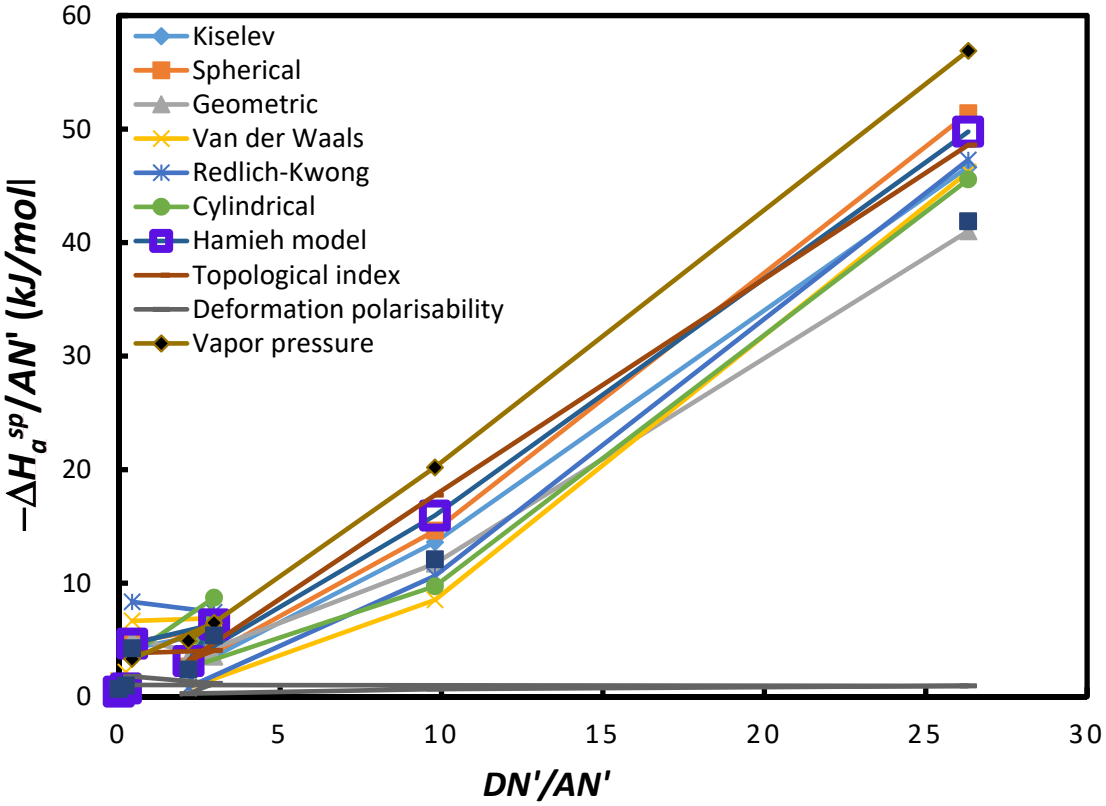

Figure S4. Variations of $\left(\frac{-\Delta H_a^{sp}}{AN'}\right)$ as a function of $\left(\frac{DN'}{AN'}\right)$ of UiO-66-FA for different models and IGC methods.

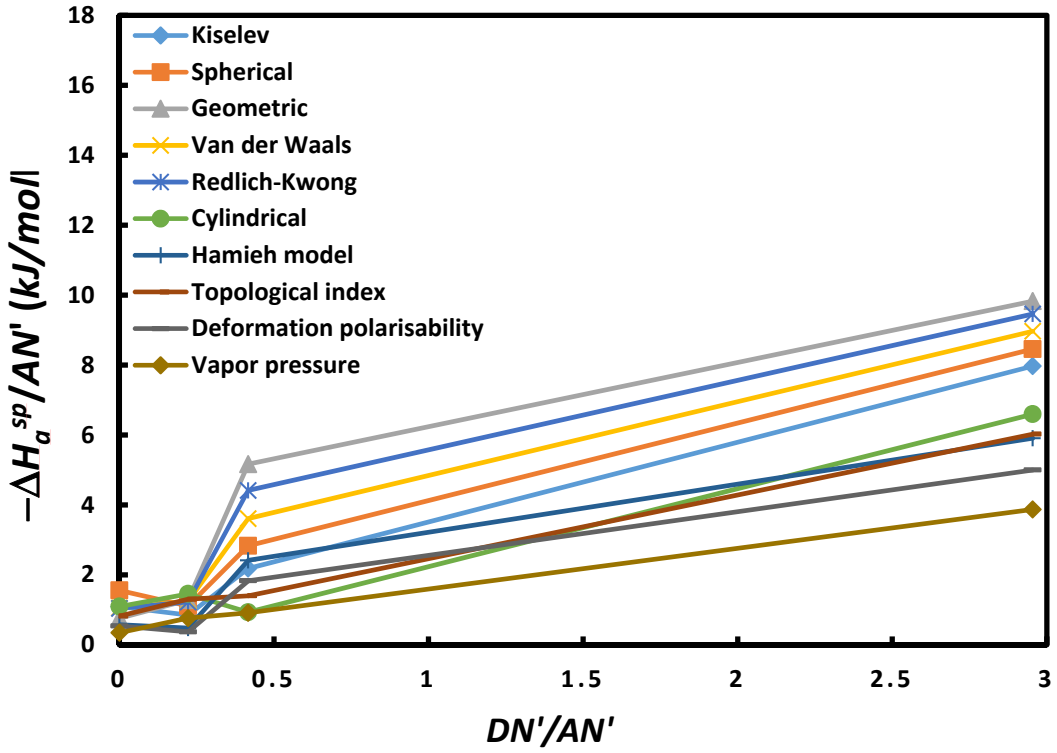

Figure S5. Variations of $\left(\frac{-\Delta H_a^{sp}}{AN'}\right)$ as a function of $\left(\frac{DN'}{AN'}\right)$ of UiO-66(NH_2) for different models and IGC methods.

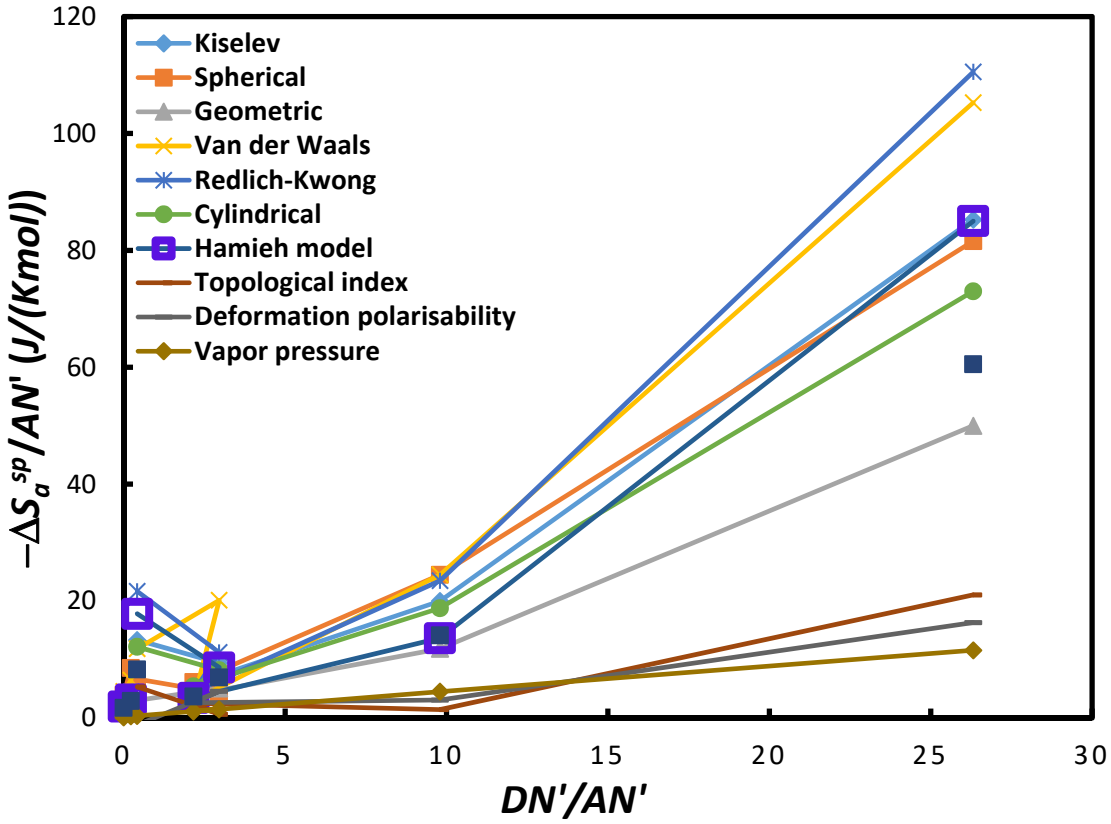

Figure S6. Variations of $\left(\frac{-\Delta S_a^{sp}}{AN'}\right)$ as a function of $\left(\frac{DN'}{AN'}\right)$ of UiO-66-00 for different models and IGC methods.

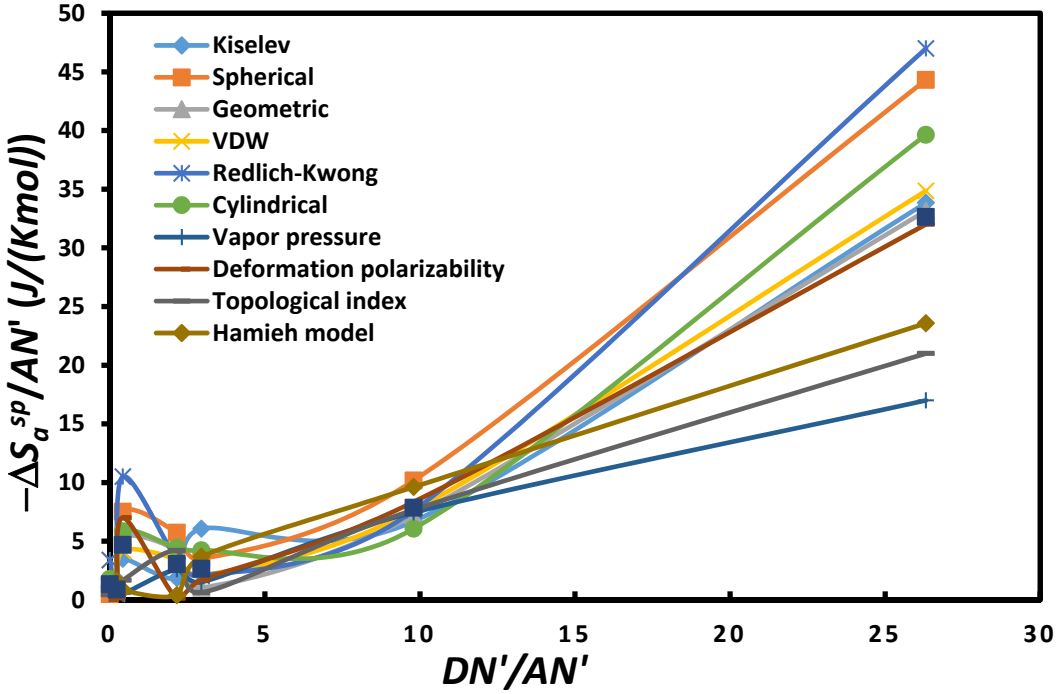

Figure S7. Variations of $\left(\frac{-\Delta S_a^{sp}}{AN'}\right)$ as a function of $\left(\frac{DN'}{AN'}\right)$ of UiO-66-AA for different models and IGC methods.

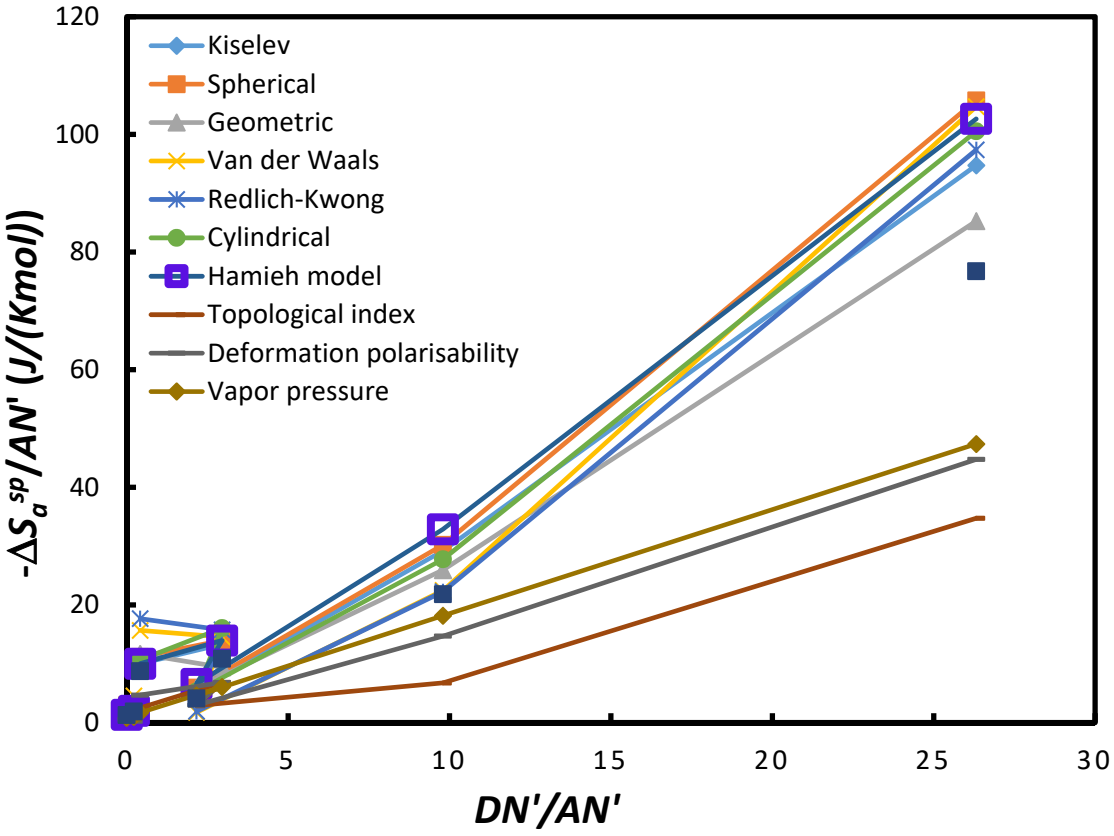

Figure S8. Variations of $\left(\frac{-\Delta S_a^{sp}}{AN'}\right)$ as a function of $\left(\frac{DN'}{AN'}\right)$ of UiO-66-FA for different models and IGC methods.

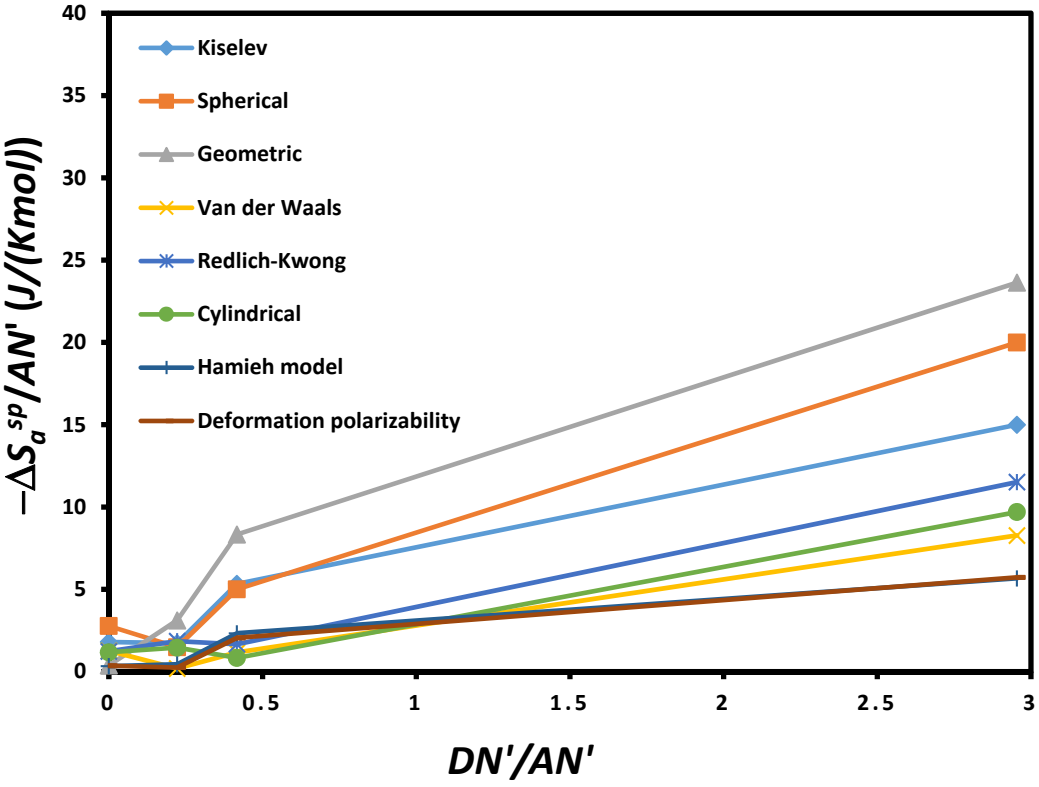

Figure S9. Variations of $\left(\frac{-\Delta S_a^{sp}}{AN'}\right)$ as a function of $\left(\frac{DN'}{AN'}\right)$ of UiO-66(NH_2) for different models and IGC methods.