Supporting information

New physicochemical methodology for the determination of the surface thermodynamic properties of solid particles

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Table S1. Values (in kJ/mol) of the specific free energy ($-\Delta G_a^{sp}(T)$) of the various polar solvents adsorbed on alumina particles surface for different temperatures by using the various molecular models and IGC methods.

ΔG_a^{sp} (T) (in kJ/mol)	Kiselev model					
T(K)	CCl4	CHCl3	CH2Cl2	Diethyl ether	THF	Toluene
T(K)	5.14	34.92	15.80	42.47	32.33	10.89
323.15	4.81	33.27	15.41	40.36	30.57	9.48
343.15	4.48	31.83	15.83	38.35	28.89	8.29
363.15	4.22	30.37	13.54	36.79	27.54	7.56
383.15	3.83	29.45	11.08	34.90	25.85	6.55
403.15	3.32	25.97	7.36	31.58	24.01	5.67
423.15	3.18	23.80	5.70	30.20	23.36	4.28
443.15	3.24	21.56	3.00	27.92	22.22	3.14

ΔG_a^{sp} (T) (in kJ/mol)	Spherical model					
T(K)	CCl4	CHCl3	CH2Cl2	Diethyl ether	THF	Toluene
323.15	5.76	37.36	19.27	41.89	35.52	15.12
343.15	5.25	35.40	18.53	39.92	33.30	13.18
363.15	4.76	33.66	18.60	38.05	31.20	11.53
383.15	4.37	31.94	16.48	36.65	29.47	10.41
403.15	3.85	30.70	13.21	34.94	27.34	8.95
423.15	3.24	27.12	9.39	33.44	25.02	7.60
443.15	2.99	25.02	7.60	31.53	24.07	6.12
463.15	2.77	21.63	4.00	28.44	22.21	4.96

ΔG_a^{sp} (T) (in kJ/mol)	Geometric model					
T(K)	CCl4	CHCl3	CH2Cl2	Diethyl ether	THF	Toluene

323.15	10.65	38.43	20.49	39.68	33.31	13.30
343.15	9.92	36.10	18.40	37.92	31.48	11.84
363.15	9.23	33.97	16.73	36.23	29.75	10.60
383.15	8.69	31.76	14.84	34.97	28.36	9.83
403.15	7.85	29.79	11.85	33.45	26.62	8.66
423.15	6.75	26.76	8.56	32.03	24.70	7.49
443.15	6.27	24.35	6.91	30.35	23.85	6.17
463.15	5.40	21.61	3.62	27.72	21.93	4.43

ΔG_a^{sp} (T) (in kJ/mol)	Van de Waals (VDW) model					
T(K)	CCl4	CHCl3	CH2Cl2	Diethyl ether	THF	Toluene
323.15	5.10	35.58	18.23	40.52	35.03	14.37
343.15	5.29	34.39	17.83	39.29	33.50	13.15
363.15	4.89	32.76	17.47	37.48	31.44	11.62
383.15	4.57	31.11	15.21	36.13	29.75	10.61
403.15	4.11	29.95	11.89	34.48	27.65	9.21
423.15	3.52	26.89	8.44	32.99	25.34	7.86
443.15	3.29	24.05	6.91	31.07	24.37	6.41
463.15	3.10	21.37	3.71	28.17	22.53	5.24

ΔG_a^{sp} (T) (in kJ/mol)	Redlich-Kwong (R-K) model					
T(K)	CCl4	CHCl3	CH2Cl2	Diethyl ether	THF	Toluene
323.15	5.73	36.29	18.92	41.21	35.69	14.93
343.15	5.32	34.43	17.85	39.31	33.52	13.15
363.15	4.91	32.79	17.49	37.50	31.46	11.61
383.15	4.59	31.14	15.42	36.15	29.77	10.60
403.15	4.13	29.96	12.67	34.49	27.67	9.20
423.15	3.53	26.60	8.88	33.00	25.36	7.86
443.15	3.23	24.19	7.05	30.77	24.25	6.44
463.15	2.97	21.26	3.54	27.85	22.28	5.27

ΔG_a^{sp} (T) (in kJ/mol)	Cylindrical model					
T(K)	CCl4	CHCl3	CH2Cl2	Diethyl ether	THF	Toluene
323.15	5.78	39.62	21.30	39.67	31.00	9.14
343.15	5.42	37.16	19.35	37.95	29.40	7.91
363.15	5.07	34.91	17.92	36.33	27.88	6.89
383.15	4.80	32.61	16.82	35.15	26.66	6.29
403.15	4.37	30.58	13.44	33.71	25.15	5.43
423.15	3.79	27.11	9.27	32.48	23.50	4.73
443.15	3.18	23.21	5.96	29.02	22.41	4.21
463.15	3.08	20.89	3.02	26.87	21.10	3.09

ΔG_a^{sp} (T) (in kJ/mol)	Hamieh model

T(K)	CCl4	CH2Cl2	CHCl3	Diethyl ether	THF	Toluene
323.15	6.25	27.30	19.07	41.10	35.83	7.21
343.15	6.16	27.20	17.16	38.72	34.56	6.50
363.15	6.04	27.00	15.20	36.22	33.11	5.56
383.15	5.92	26.90	13.10	34.40	32.03	5.08
403.15	5.80	26.80	11.35	32.18	30.76	4.38
423.15	5.68	26.60	9.33	29.96	29.50	3.67
443.15	5.56	26.51	7.25	27.74	28.13	2.96
463.15	5.44	26.37	5.22	25.52	26.76	2.25

ΔG_a^{sp} (T) (in kJ/mol)	Topological index method					
T(K)	CCl4	CH2Cl2	CHCl3	Diethyl ether	THF	Toluene
323.15	13.21	42.10	22.94	40.41	37.51	16.80
343.15	12.72	39.74	20.34	38.50	35.53	15.59
363.15	12.31	37.59	17.91	36.66	33.68	14.62
383.15	12.17	35.42	16.07	35.20	32.28	14.25
403.15	11.74	33.32	13.66	33.37	30.46	13.37
423.15	11.07	30.70	10.86	31.20	28.46	12.39
443.15	11.05	28.88	9.75	29.83	27.56	11.64
463.15	10.56	26.42	6.98	27.99	25.48	10.80

ΔG_a^{sp} (T) (in kJ/mol)	Deformation polarizability method					
T(K)	CCl4	CH2Cl2	CHCl3	Diethyl ether	THF	Toluene
323.15	14.67	30.37	17.97	41.98	40.62	16.74
343.15	14.10	28.70	15.66	39.98	38.45	15.52
363.15	13.61	27.16	13.49	38.05	36.44	14.56
383.15	13.43	25.37	11.81	36.55	34.94	14.19
403.15	12.91	23.90	9.67	34.63	32.95	13.32
423.15	12.15	22.08	7.21	32.35	30.74	12.34
443.15	12.09	20.48	6.20	30.96	29.78	11.60
463.15	11.51	18.78	3.75	29.01	27.50	10.76

ΔG_a^{sp} (T) (in kJ/mol)	Vapor pressure method					
T(K)	CCl4	CH2Cl2	CHCl3	Diethyl ether	THF	Toluene
323.15	4.97	33.95	14.53	39.89	33.87	13.00
343.15	4.98	32.19	12.43	38.10	32.01	11.96
363.15	5.00	30.58	10.45	36.37	30.26	11.16
383.15	5.01	28.79	8.88	35.01	28.90	10.89
403.15	5.02	27.22	6.94	33.28	27.20	10.20
423.15	5.04	25.23	4.71	31.19	25.40	9.47
443.15	5.05	23.66	3.78	29.90	24.51	8.79
463.15	5.06	21.78	1.55	28.12	22.64	8.20

ΔG_a^{sp} (T) (in kJ/mol)	Boiling point method					
T(K)	CCl4	CH2Cl2	CHCl3	Diethyl ether	THF	Toluene
323.15	4.76	34.05	13.51	39.96	33.81	12.72
343.15	4.78	32.17	11.47	38.09	32.05	11.74
363.15	4.81	30.45	9.54	36.28	30.40	10.99
383.15	4.95	28.55	8.00	34.84	29.12	10.74
403.15	4.97	26.89	6.11	33.04	27.50	10.09
423.15	4.88	24.82	3.95	30.90	25.76	9.38
443.15	5.03	23.16	3.03	29.55	24.93	8.72
463.15	5.08	21.22	0.87	27.74	23.10	8.14

ΔG_a^{sp} (T) (in kJ/mol)	Method of enthalpy of vaporization (ΔHvap(298K))					
T(K)	CCl4	CH2Cl2	CHCl3	Diethyl ether	THF	Toluene
323.15	5.231835	31.53	14.10	39.21	33.22	13.43
343.15	5.249835	29.79	12.02	37.37	31.49	12.41
363.15	5.267835	28.20	10.06	35.60	29.87	11.62
383.15	5.285835	26.37	8.49	34.18	28.60	11.36
403.15	5.303835	24.84	6.57	32.41	27.01	10.66
423.15	5.321835	22.94	4.36	30.32	25.31	9.91
443.15	5.36	21.32	3.43	28.98	24.49	9.23
463.15	5.38	19.54	1.23	27.21	22.69	8.61

ΔG_a^{sp} (T) (in kJ/mol)	Method of thermic enthalpy of vaporization ΔHvap(T)					
T(K)	CCl4	CH2Cl2	CHCl3	Diethyl ether	THF	Toluene
323.15	4.33	31.53	13.25	38.41	32.46	13.43
343.15	4.03	29.41	10.26	35.61	29.92	12.20
363.15	3.46	27.49	7.52	33.02	27.61	11.22
383.15	3.01	25.35	5.20	30.84	25.67	10.72
403.15	2.77	23.65	2.92	28.62	23.78	10.08
423.15	2.43	21.61	0.43	26.23	21.82	9.25
443.15	2.13	19.80	-0.90	24.44	20.65	8.50
463.15	1.82	18.10	-2.94	22.77	19.03	8.06