Interfacial Thermodynamics of Water and Six Other Liquid Solvents

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Supporting Information

Tables

Table S1: Fitting parameters for fitting the liquid density profile to hyperbolic functions according to eqn. (6)

Liquid	Top surface			Bottom surface		
	a [g/mL]	δ [Å]	z_G [Å]	a [g/mL]	δ [Å]	z_G [Å]
TIP4P/2005	0.49	1.57	74.84	0.49	1.56	37.70
mW	0.44	1.34	87.03	0.44	1.33	50.41
SPC/Ew	0.50	1.59	74.74	0.50	1.64	37.80
TIP3P	0.53	1.68	73.60	0.53	1.69	38.94
acetonitrile	0.35	4.17	73.20	0.35	3.93	36.66
cyclohexane	0.37	3.28	64.52	0.37	3.32	31.53
Dmso	0.55	1.66	66.96	0.55	1.69	33.45
Hexanol	0.41	2.36	64.19	0.41	2.56	32.69
Nma	0.47	1.64	63.78	0.47	1.66	31.77
Toluene	0.42	2.72	65.97	0.42	2.75	32.67

Figures

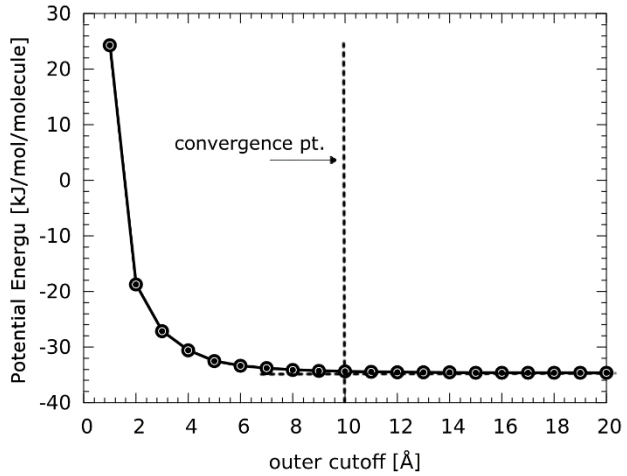

Figure S1: Potential energy [kJ/mol/molecule] of acetonitrile as a function of van der Waals cutoff distance.

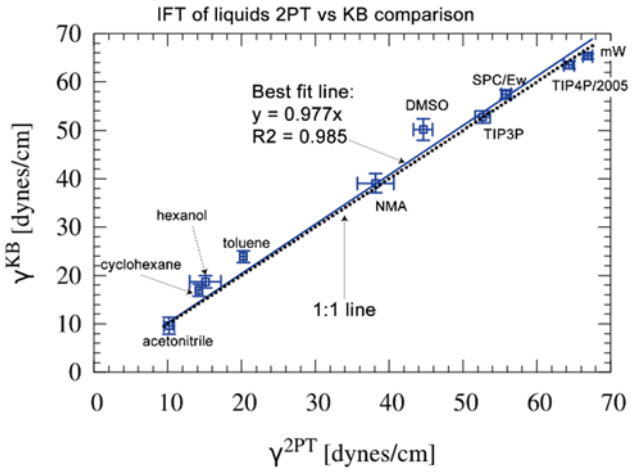

Figure S2: Comparison of the calculated surface tension at 298K calculated using the Kirkwood-Buff (y-axis) and 2PT (x-axis) methods. The average and statistical uncertainty are indicated. The linear best fit line (solid blue line) is indicated, as well as the 1:1 correlation line (dashed black line). Each of the 4 water models and 6 common solvent are indicated.

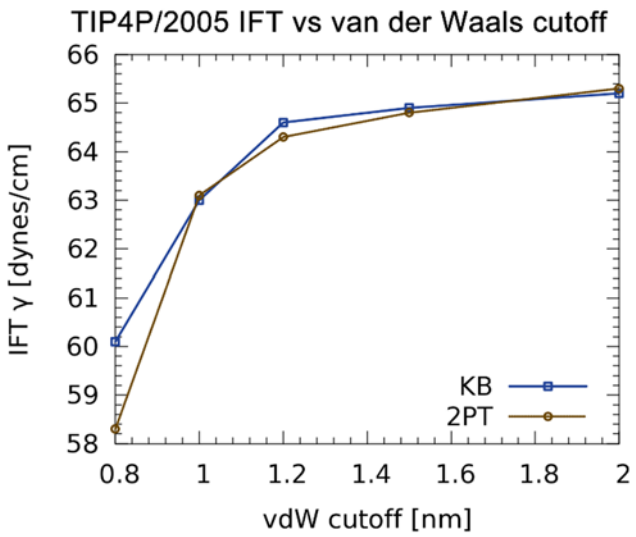

Figure S3: Convergence of the surface tension of TIP4/2005 waters as a function of van der Waals cutoff as calculated using the Kirkwood-Buff (blue open squares) and 2PT (brown open circles) methods. We used a cutoff of xx in our simulations.

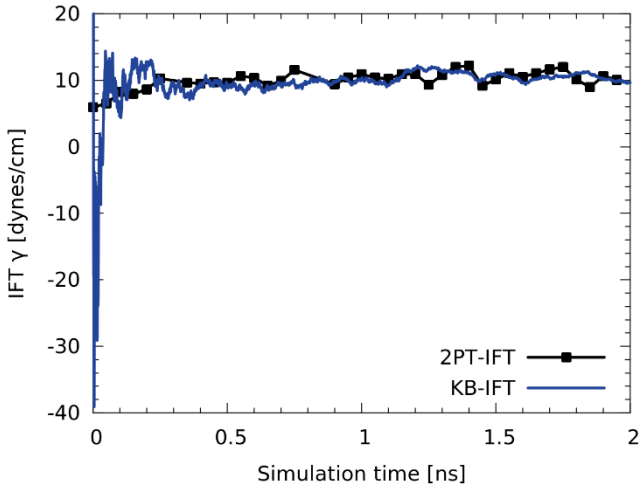

Figure S4: IFT profile of acetonitrile as a function of simulation time from2PT (black squares) and KB (blue line) methods. Note the rapid monotonic convergence for 2PT so that the value at 20 ps is only 12% less than the final value, whereas for KB there are large fluctuations until 400 ps.

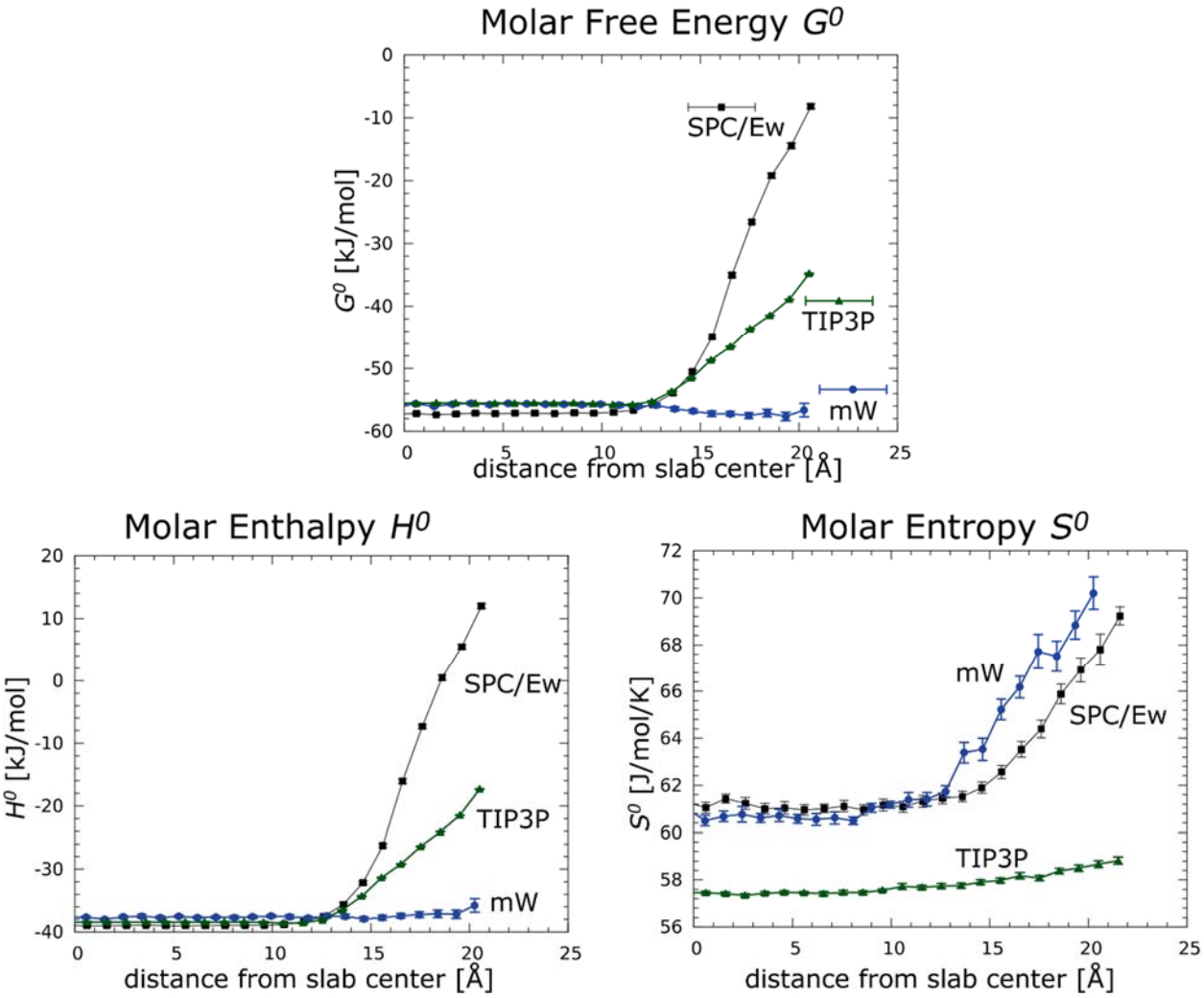

Figure S5: Profile of standard molar free energy G^0, enthalpy H^0 and entropy S^0 of water at 298K as described by the SPC/Ew (black squares), mW (blue circles), and TIP3P (green triangles) water models.