Supporting Information: Molecular modeling of interfacial properties of the hydrogen+water+decane mixture in three-phase equilibrium

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Table S1: PC-SAFT parameters for H_2, H_2O, and n-$C_{10}H_{22}$.

Comp.	m	σ(Å)	ϵ/k (K)	$\epsilon_{PC-SAFT}/k$ (K)	$\kappa_{PC-SAFT}$	Ref.
H_2	0.6800	3.5400	31.57	-	-	S1
H_2O	2.1945	2.2290	141.66	1804.17	0.2039	S2
$C_{10}H_{22}$	4.6627	3.8384	243.87	-	-	S3

Table S2: PC-SAFT binary interaction parameter (k_{ij}) for pairs (T is temperature in K). The references for experimental data used for parameter fitting are marked as 'Expt.'

Pair	k_{ij}	Ref.
H_2-H_2O	-1.0158e-05·T^2 + 9.1742e-03 ·T - 2.1375	Expt. (S4)
H_2-$C_{10}H_{22}$	2.5037e-04 ·T - 1.9778e-02	Expt. (S5)
H_2O-$C_{10}H_{22}$	-3.5305e-6·T^2 + 2.9134e-3 ·T - 3.7739e-1	S6

Table S3: DGT (PC-SAFT) influence parameters (c_{ii}) for H_2, H_2O, and n-$C_{10}H_{22}$.

Comp.	c_{ii} (10^{-20} J m^5 mol^{-2})	Ref.
H_2	0.0350	S7
H_2O	1.4412	S8
$C_{10}H_{22}$	90.8954	S6

Table S4: DGT (PC-SAFT) binary interaction coefficient (β_{ij}) for pairs.

Pair	β_{ij}	Ref.
H_2-H_2O	0.99	Expt. (S9,S10)
H_2-$C_{10}H_{22}$	0.20	-
H_2O-$C_{10}H_{22}$	7.5941e-06·T^2 - 6.4833e-03·T + 1.7825	Expt. (S11)

Table S5: IFTs from MD in two-component two-phase systems for Figs. S2-S4. The 'wv','wo', and 'ov' stand for the 'water+vapor (H_2) system','water+oil (n-decane) system', and 'oil+vapor(H_2) system',respectively.

Type	T (K)	P (MPa)	IFT (mN/m)	Error
wv	298	4.9	70.03	0.38
wv	298	20.0	68.73	0.38
wv	298	40.0	67.98	0.46
wv	298	70.0	67.17	0.13
wv	298	99.9	66.75	0.14
wv	333	5.0	64.25	0.24
wv	333	19.8	63.77	0.09
wv	333	39.9	63.33	0.20
wv	333	70.0	63.09	0.65
wv	333	99.8	63.12	0.15
wv	373	5.0	58.03	0.12
wv	373	19.9	56.73	0.32
wv	373	40.0	57.00	0.21
wv	373	70.1	57.11	0.28
wv	373	100.1	56.78	0.43
wo	298	4.9	50.08	0.94
wo	298	19.2	51.35	0.32
wo	298	39.9	53.19	0.08
wo	298	67.0	56.05	1.00
wo	298	99.4	57.82	0.43
wo	333	4.8	47.61	0.59
wo	333	19.9	48.46	0.75
wo	333	39.9	50.16	0.76
wo	333	69.9	52.30	0.66

wo	333	100.1	54.30	0.62
wo	373	5.0	41.97	0.42
wo	373	19.6	43.83	0.22
wo	373	39.9	45.60	0.61
wo	373	69.6	48.30	0.46
wo	373	100.0	50.89	0.34
ov	298	5.0	23.99	0.32
ov	298	19.9	22.25	0.43
ov	298	40.0	18.85	0.16
ov	298	70.0	16.99	0.28
ov	298	100.1	15.37	0.34
ov	333	5.0	20.27	0.14
ov	333	20.0	18.27	0.56
ov	333	40.0	16.49	0.28
ov	333	70.1	14.69	0.30
ov	333	99.9	12.10	0.23
ov	373	5.0	16.66	0.24
ov	373	20.0	15.25	0.28
ov	373	40.1	13.43	0.19
ov	373	70.2	11.39	0.47
ov	373	100.2	9.64	0.26

Table S6: Solubilities from MD in two-component two-phase systems for Figs. S5-S7. The 'wv','wo', and 'ov' stand for the 'water+vapor (H_2) system','water+oil (n-decane) system', and 'oil+vapor(H_2) system',respectively.

Type	T(K)	P(MPa)	H_2(-)	Error	H_2O(-)	Error	Oil(-)	Error
wv	298	4.9	2.13E-04	4.15E-05	1.28E-01	2.83E-03	-	-
wv	298	20.0	7.18E-04	2.80E-04	3.98E-02	1.63E-03	-	-
wv	298	40.0	1.46E-03	2.92E-05	2.33E-02	3.09E-04	-	-
wv	298	70.0	2.18E-03	1.89E-04	1.73E-02	8.04E-04	-	-
wv	298	99.9	2.85E-03	4.15E-04	1.46E-02	2.43E-04	-	-
wv	333	5.0	2.48E-04	1.27E-04	2.53E-01	1.95E-03	-	-
wv	333	19.8	1.19E-03	2.90E-04	7.17E-02	1.46E-03	-	-
wv	333	39.9	2.14E-03	8.58E-05	4.39E-02	1.76E-03	-	-
wv	333	70.0	2.99E-03	1.92E-04	3.12E-02	8.44E-04	-	-
wv	333	99.8	4.56E-03	3.66E-04	2.48E-02	5.47E-04	-	-
wv	373	5.0	2.55E-04	6.38E-05	4.78E-01	2.42E-03	-	-
wv	373	19.9	1.60E-03	2.19E-04	1.40E-01	3.61E-03	-	-
wv	373	40.0	3.13E-03	1.05E-04	7.99E-02	1.00E-03	-	-
wv	373	70.1	4.68E-03	7.05E-04	5.60E-02	3.71E-04	-	-
wv	373	100.1	6.48E-03	2.58E-04	4.47E-02	1.87E-03	-	-
wo	298	4.9	-	-	9.51E-02	6.98E-03	0.00E+00	0.00E+00
wo	298	19.2	-	-	8.36E-02	9.38E-03	0.00E+00	0.00E+00
wo	298	39.9	-	-	7.17E-02	7.21E-03	0.00E+00	0.00E+00
wo	298	67.0	-	-	7.73E-02	7.82E-03	0.00E+00	0.00E+00
wo	298	99.4	-	-	6.97E-02	6.09E-03	0.00E+00	0.00E+00
wo	333	4.8	-	-	1.37E-01	3.67E-03	0.00E+00	0.00E+00
wo	333	19.9	-	-	1.29E-01	9.67E-03	0.00E+00	0.00E+00
wo	333	39.9	-	-	1.13E-01	9.52E-03	0.00E+00	0.00E+00
wo	333	69.9	-	-	1.16E-01	3.21E-03	0.00E+00	0.00E+00

wo	333	100.1	-	-	9.82E-02	1.65E-03	0.00E+00	0.00E+00
wo	373	5.0	-	-	2.13E-01	6.53E-03	0.00E+00	0.00E+00
wo	373	19.6	-	-	1.87E-01	7.69E-03	0.00E+00	0.00E+00
wo	373	39.9	-	-	1.91E-01	2.82E-03	0.00E+00	0.00E+00
wo	373	69.6	-	-	1.70E-01	8.64E-03	0.00E+00	0.00E+00
wo	373	100.0	-	-	1.58E-01	5.07E-03	0.00E+00	0.00E+00
ov	298	5.0	2.78E-02	5.03E-04	-	-	8.05E-05	1.13E-04
ov	298	19.9	1.18E-01	4.69E-03	-	-	1.05E-04	1.38E-04
ov	298	40.0	2.03E-01	5.40E-03	-	-	8.16E-05	7.56E-05
ov	298	70.0	2.87E-01	1.17E-02	-	-	1.55E-04	1.58E-04
ov	298	100.1	3.53E-01	5.56E-03	-	-	1.83E-04	9.11E-05
ov	333	5.0	3.72E-02	1.02E-03	-	-	3.71E-04	1.20E-04
ov	333	20.0	1.35E-01	6.46E-03	-	-	3.77E-04	3.04E-04
ov	333	40.0	2.28E-01	2.55E-03	-	-	2.79E-04	1.36E-04
ov	333	70.1	3.35E-01	3.83E-03	-	-	4.83E-04	3.36E-05
ov	333	99.9	4.14E-01	6.91E-03	-	-	5.73E-04	2.27E-04
ov	373	5.0	4.53E-02	1.53E-03	-	-	3.12E-03	3.67E-04
ov	373	20.0	1.60E-01	4.07E-04	-	-	1.12E-03	1.09E-04
ov	373	40.1	2.77E-01	5.22E-03	-	-	1.37E-03	1.56E-04
ov	373	70.2	3.87E-01	1.02E-02	-	-	1.35E-03	2.98E-04
ov	373	100.2	4.81E-01	5.00E-03	-	-	1.73E-03	1.47E-04

Table S7: Enrichments from MD in two-component two-phase systems for Figs. S11-S13. The 'wv','wo', and 'ov' stand for the 'water+vapor (H_2) system','water+oil (n-decane) system', and 'oil+vapor(H_2) system',respectively.

Type	T(K)	P (MPa)	Enrichment	Error
wv	298	4.9	1.244	0.027
wv	298	20.0	1.144	0.001
wv	298	40.0	1.102	0.009
wv	298	70.0	1.068	0.007
wv	298	99.9	1.041	0.005
wv	333	5.0	1.169	0.011
wv	333	19.8	1.089	0.016
wv	333	39.9	1.081	0.009
wv	333	70.0	1.053	0.011
wv	333	99.8	1.035	0.001
wv	373	5.0	1.141	0.004
wv	373	19.9	1.065	0.005
wv	373	40.0	1.045	0.009
wv	373	70.1	1.034	0.004
wv	373	100.1	1.030	0.007
wo	298	4.9	1.030	0.010
wo	298	19.2	1.024	0.000
wo	298	39.9	1.025	0.003
wo	298	67.0	1.028	0.005
wo	298	99.4	1.027	0.006
wo	333	4.8	1.021	0.005
wo	333	19.9	1.022	0.000
wo	333	39.9	1.025	0.003
wo	333	69.9	1.020	0.004

wo	333	100.1	1.020	0.005
wo	373	5.0	1.019	0.001
wo	373	19.6	1.022	0.001
wo	373	39.9	1.022	0.005
wo	373	69.6	1.018	0.001
wo	373	100.0	1.022	0.004
ov	298	5.0	1.167	0.016
ov	298	19.9	1.105	0.005
ov	298	40.0	1.058	0.008
ov	298	70.0	1.032	0.003
ov	298	100.1	1.026	0.002
ov	333	5.0	1.097	0.021
ov	333	20.0	1.065	0.011
ov	333	40.0	1.038	0.009
ov	333	70.1	1.022	0.002
ov	333	99.9	1.022	0.004
ov	373	5.0	1.073	0.005
ov	373	20.0	1.045	0.005
ov	373	40.1	1.037	0.007
ov	373	70.2	1.024	0.000
ov	373	100.2	1.021	0.002

Table S8: Surface excesses from MD in two-component two-phase systems for Figs. S14-S16. The 'wv','wo', and 'ov' stand for the 'water+vapor (H_2) system','water+oil (n-decane) system', and 'oil+vapor(H_2) system',respectively.

Type	T(K)	P (MPa)	Surface Excess (mol/m^2)	Error
wv	298	4.9	2.39E-07	3.93E-08
wv	298	20.0	4.20E-07	1.88E-07
wv	298	40.0	3.65E-07	1.11E-07
wv	298	70.0	1.48E-07	8.26E-08
wv	298	99.9	-1.04E-07	1.58E-07
wv	333	5.0	1.39E-07	3.58E-08
wv	333	19.8	4.04E-07	9.25E-08
wv	333	39.9	2.39E-07	7.33E-08
wv	333	70.0	8.06E-08	2.32E-07
wv	333	99.8	-2.17E-07	3.28E-07
wv	373	5.0	5.64E-08	1.29E-07
wv	373	19.9	1.95E-07	1.85E-07
wv	373	40.0	-1.87E-08	7.62E-08
wv	373	70.1	-1.85E-07	8.51E-08
wv	373	100.1	-3.88E-07	1.67E-07
wo	298	4.9	-4.75E-07	3.31E-08
wo	298	19.2	-4.29E-07	2.03E-08
wo	298	39.9	-4.07E-07	2.05E-08
wo	298	67.0	-3.63E-07	1.55E-08
wo	298	99.4	-3.53E-07	3.03E-08
wo	333	4.8	-5.22E-07	4.94E-09
wo	333	19.9	-4.86E-07	2.42E-08
wo	333	39.9	-4.48E-07	8.33E-09
wo	333	69.9	-4.06E-07	2.36E-08

wo	333	100.1	-3.71E-07	1.66E-08
wo	373	5.0	-5.54E-07	1.99E-08
wo	373	19.6	-5.45E-07	1.74E-08
wo	373	39.9	-4.82E-07	2.13E-08
wo	373	69.6	-4.24E-07	1.46E-09
wo	373	100.0	-3.96E-07	2.13E-09
ov	298	5.0	4.33E-07	2.63E-08
ov	298	19.9	1.03E-06	1.13E-07
ov	298	40.0	1.20E-06	1.71E-07
ov	298	70.0	1.22E-06	5.16E-08
ov	298	100.1	1.20E-06	1.82E-07
ov	333	5.0	2.85E-07	1.79E-08
ov	333	20.0	8.85E-07	1.62E-07
ov	333	40.0	1.04E-06	1.13E-07
ov	333	70.1	1.09E-06	1.07E-07
ov	333	99.9	1.06E-06	3.57E-07
ov	373	5.0	1.61E-07	4.31E-08
ov	373	20.0	8.04E-07	2.35E-07
ov	373	40.1	7.23E-07	1.63E-07
ov	373	70.2	8.72E-07	1.24E-07
ov	373	100.2	7.32E-07	1.87E-07

Table S9: IFTs from MD in the three-component three-phase system for Figs. 2, 6, and 10. The 'wv','wo', and 'ov' stand for the 'water+vapor interface','water+oil interface', and 'oil+vapor interface',respectively.

Type	T(K)	P (MPa)	IFT (mN/m)	Error
wv	298	6	69.63	1.13
wv	298	21	68.74	0.33
wv	298	42	67.97	0.46
wv	298	72	66.82	0.29
wv	298	102	66.61	0.19
wv	333	6	63.81	0.29
wv	333	21	63.38	1.00
wv	333	42	62.40	0.15
wv	333	72	62.15	0.48
wv	333	103	61.39	0.91
wv	373	6	55.60	0.41
wv	373	21	55.33	0.61
wv	373	41	55.08	1.13
wv	373	71	55.03	0.37
wv	373	102	56.28	0.34
wo	298	6	49.88	0.18
wo	298	21	51.27	1.63
wo	298	42	52.74	0.56
wo	298	72	53.37	1.18
wo	298	102	55.02	0.34
wo	333	6	47.06	0.52
wo	333	21	47.92	0.16
wo	333	42	48.91	0.37
wo	333	72	49.98	0.91

wo	333	103	51.54	0.42
wo	373	6	41.91	0.87
wo	373	21	42.68	0.21
wo	373	41	44.19	0.44
wo	373	71	45.26	0.39
wo	373	102	46.96	0.53
ov	298	6	23.10	0.29
ov	298	21	20.95	0.70
ov	298	42	18.55	0.34
ov	298	72	15.64	0.31
ov	298	102	14.10	0.72
ov	333	6	19.45	0.36
ov	333	21	17.38	0.06
ov	333	42	15.43	0.29
ov	333	72	13.57	0.22
ov	333	103	11.23	0.27
ov	373	6	14.90	0.32
ov	373	21	13.72	0.54
ov	373	41	11.31	0.49
ov	373	71	9.89	0.76
ov	373	102	8.34	0.56

Table S10: Solubilities from MD in the three-component three-phase system for Fig. S18. The 'v','w', and 'o' stand for the 'vapor phase','water-rich phase', and 'oil-rich phase',respectively.

Type	T(K)	P (MPa)	H_2 (-)	Error	H_2O (-)	Error	Oil (-)	Error
v	298	6	-	-	1.21E-01	2.77E-03	1.24E-04	8.74E-05
v	298	21	-	-	3.76E-02	1.01E-03	1.09E-04	3.02E-05
v	298	42	-	-	2.34E-02	5.75E-04	6.83E-05	5.41E-05
v	298	72	-	-	1.66E-02	3.77E-04	7.25E-05	1.06E-05
v	298	102	-	-	1.46E-02	1.81E-04	1.24E-04	3.40E-05
v	333	6	-	-	2.30E-01	2.99E-03	4.08E-04	4.88E-05
v	333	21	-	-	7.01E-02	1.94E-03	3.92E-04	1.16E-04
v	333	42	-	-	4.35E-02	1.39E-03	4.13E-04	3.28E-04
v	333	72	-	-	3.00E-02	8.70E-04	5.04E-04	1.53E-04
v	333	103	-	-	2.49E-02	4.39E-04	4.83E-04	6.01E-05
v	373	6	-	-	4.39E-01	1.78E-03	5.62E-03	1.17E-03
v	373	21	-	-	1.38E-01	1.18E-03	2.05E-03	6.91E-05
v	373	41	-	-	7.79E-02	2.15E-03	1.46E-03	7.39E-05
v	373	71	-	-	5.51E-02	1.67E-03	2.11E-03	4.08E-04
v	373	102	-	-	4.46E-02	3.41E-04	2.10E-03	5.24E-04
w	298	6	1.96E-04	5.10E-05	-	-	0.00E+00	0.00E+00
w	298	21	8.93E-04	6.47E-05	-	-	0.00E+00	0.00E+00
w	298	42	1.59E-03	1.22E-04	-	-	0.00E+00	0.00E+00
w	298	72	2.44E-03	3.01E-04	-	-	0.00E+00	0.00E+00
w	298	102	3.24E-03	2.07E-04	-	-	0.00E+00	0.00E+00
w	333	6	2.75E-04	2.36E-05	-	-	0.00E+00	0.00E+00
w	333	21	1.15E-03	1.11E-04	-	-	0.00E+00	0.00E+00
w	333	42	2.17E-03	1.38E-04	-	-	0.00E+00	0.00E+00
w	333	72	3.43E-03	2.87E-04	-	-	0.00E+00	0.00E+00

w	333	103	4.42E-03	1.38E-04	-	-	0.00E+00	0.00E+00
w	373	6	3.04E-04	2.38E-05	-	-	0.00E+00	0.00E+00
w	373	21	1.49E-03	1.31E-04	-	-	0.00E+00	0.00E+00
w	373	41	2.87E-03	2.02E-04	-	-	0.00E+00	0.00E+00
w	373	71	5.05E-03	1.86E-04	-	-	0.00E+00	0.00E+00
w	373	102	6.41E-03	2.70E-04	-	-	0.00E+00	0.00E+00
o	298	6	2.82E-02	1.40E-03	8.55E-02	4.10E-03	-	-
o	298	21	1.23E-01	1.29E-02	9.28E-02	5.58E-03	-	-
o	298	42	1.98E-01	1.70E-02	9.16E-02	1.01E-02	-	-
o	298	72	2.94E-01	5.74E-03	9.14E-02	6.04E-03	-	-
o	298	102	3.63E-01	9.32E-03	8.35E-02	7.38E-03	-	-
o	333	6	3.56E-02	9.60E-04	1.39E-01	2.38E-03	-	-
o	333	21	1.41E-01	1.14E-02	1.41E-01	5.69E-03	-	-
o	333	42	2.39E-01	1.30E-02	1.36E-01	6.55E-03	-	-
o	333	72	3.50E-01	1.38E-02	1.37E-01	6.59E-03	-	-
o	333	103	4.07E-01	7.21E-03	1.36E-01	1.88E-02	-	-
o	373	6	3.26E-02	1.32E-03	2.19E-01	4.70E-03	-	-
o	373	21	1.49E-01	5.25E-03	2.11E-01	4.35E-03	-	-
o	373	41	2.83E-01	7.83E-03	2.18E-01	4.02E-03	-	-
o	373	71	4.10E-01	3.05E-03	2.07E-01	1.68E-03	-	-
o	373	102	5.12E-01	1.80E-03	2.14E-01	4.46E-03	-	-

Table S11: Enrichments from MD in the three-component three-phase system for Figs. 4, 8, and 12. The 'wv','wo', and 'ov' stand for the 'water+vapor interface','water+oil interface', and 'oil+vapor interface',respectively.

Type	T(K)	P (MPa)	H_2 (-)	Error	H_2O (-)	Error	Oil (-)	Error
wv	298	6	1.206	0.001	-	-	2883.286	1977.716
wv	298	21	1.101	0.004	-	-	1760.557	2185.726
wv	298	42	1.080	0.012	-	-	781.795	519.620
wv	298	72	1.044	0.008	-	-	157.444	23.976
wv	298	102	1.019	0.004	-	-	236.546	115.390
wv	333	6	1.144	0.006	-	-	399.033	169.777
wv	333	21	1.080	0.010	-	-	308.000	127.012
wv	333	42	1.045	0.014	-	-	113.998	41.116
wv	333	72	1.027	0.004	-	-	69.219	30.782
wv	333	103	1.015	0.001	-	-	89.345	33.877
wv	373	6	1.058	0.012	-	-	182.379	58.924
wv	373	21	1.046	0.009	-	-	98.918	23.073
wv	373	41	1.026	0.007	-	-	95.699	18.944
wv	373	71	1.017	0.000	-	-	31.340	2.139
wv	373	102	1.019	0.005	-	-	20.586	5.609
wo	298	6	1.461	0.251	-	-	1.017	0.006
wo	298	21	1.445	0.018	-	-	1.012	0.003
wo	298	42	1.427	0.069	-	-	1.017	0.002
wo	298	72	1.436	0.139	-	-	1.019	0.001
wo	298	102	1.393	0.071	-	-	1.015	0.002
wo	333	6	1.374	0.110	-	-	1.014	0.003
wo	333	21	1.303	0.069	-	-	1.012	0.003
wo	333	42	1.293	0.054	-	-	1.013	0.003
wo	333	72	1.238	0.038	-	-	1.014	0.002

wo	333	103	1.199	0.063	-	-	1.018	0.004
wo	373	6	1.294	0.148	-	-	1.013	0.003
wo	373	21	1.172	0.127	-	-	1.012	0.005
wo	373	41	1.169	0.042	-	-	1.021	0.005
wo	373	71	1.198	0.022	-	-	1.012	0.002
wo	373	102	1.130	0.019	-	-	1.015	0.002
ov	298	6	1.148	0.011	1.637	0.074	-	-
ov	298	21	1.079	0.011	1.554	0.207	-	-
ov	298	42	1.047	0.008	1.427	0.112	-	-
ov	298	72	1.021	0.003	1.354	0.077	-	-
ov	298	102	1.016	0.001	1.351	0.194	-	-
ov	333	6	1.084	0.009	1.375	0.013	-	-
ov	333	21	1.038	0.012	1.372	0.101	-	-
ov	333	42	1.027	0.003	1.354	0.071	-	-
ov	333	72	1.016	0.001	1.357	0.020	-	-
ov	333	103	1.014	0.000	1.345	0.105	-	-
ov	373	6	1.066	0.006	1.261	0.017	-	-
ov	373	21	1.027	0.002	1.307	0.052	-	-
ov	373	41	1.021	0.002	1.227	0.055	-	-
ov	373	71	1.013	0.001	1.257	0.034	-	-
ov	373	102	1.015	0.002	1.195	0.044	-	-

Table S12: Surface excesses in unit of mol/m^2 from MD in the three-component three-phase system for Figs. 5, 9, and 13. The 'wv','wo', and 'ov' stand for the 'water+vapor interface','water+oil interface', and 'oil+vapor interface',respectively.

Type	T(K)	P (MPa)	H_2	Error	H_2O	Error	Oil	Error
wv	298	6	1.90E-07	5.84E-08	-	-	1.26E-07	3.25E-08
wv	298	21	1.11E-07	2.10E-07	-	-	2.71E-07	3.16E-08
wv	298	42	2.32E-07	4.70E-07	-	-	1.50E-07	1.31E-07
wv	298	72	-9.89E-08	3.34E-07	-	-	8.34E-08	5.69E-08
wv	298	102	-7.33E-07	4.36E-07	-	-	2.70E-07	7.02E-08
wv	333	6	1.05E-07	3.24E-08	-	-	1.93E-07	2.33E-08
wv	333	21	2.80E-07	3.59E-07	-	-	2.65E-07	1.63E-07
wv	333	42	-1.95E-07	3.21E-07	-	-	2.73E-07	7.72E-08
wv	333	72	-7.65E-07	3.62E-07	-	-	3.32E-07	6.16E-08
wv	333	103	-9.86E-07	5.78E-08	-	-	1.93E-07	3.16E-08
wv	373	6	-2.04E-07	2.54E-08	-	-	8.99E-07	2.37E-07
wv	373	21	-7.20E-07	3.03E-07	-	-	1.07E-06	3.54E-07
wv	373	41	-1.29E-06	6.09E-07	-	-	1.04E-06	3.65E-07
wv	373	71	-2.08E-06	2.23E-07	-	-	6.88E-07	1.31E-07
wv	373	102	-2.72E-06	1.32E-06	-	-	7.37E-07	3.81E-07
wo	298	6	5.96E-08	5.53E-08	-	-	-4.60E-07	2.44E-08
wo	298	21	3.19E-07	1.97E-08	-	-	-4.92E-07	7.19E-09
wo	298	42	4.29E-07	2.62E-07	-	-	-4.36E-07	3.66E-08
wo	298	72	1.06E-06	5.72E-07	-	-	-5.18E-07	1.04E-07
wo	298	102	1.37E-06	1.91E-07	-	-	-4.85E-07	3.69E-08
wo	333	6	8.60E-08	2.75E-08	-	-	-5.03E-07	1.27E-08
wo	333	21	2.98E-07	7.57E-08	-	-	-5.38E-07	3.17E-08
wo	333	42	5.80E-07	1.12E-07	-	-	-5.25E-07	2.19E-08
wo	333	72	8.63E-07	1.95E-07	-	-	-4.91E-07	4.91E-08

wo	333	103	1.35E-06	2.09E-07	-	-	-5.74E-07	2.98E-08
wo	373	6	7.49E-08	6.83E-08	-	-	-5.62E-07	2.11E-08
wo	373	21	2.64E-07	8.47E-08	-	-	-5.51E-07	2.77E-08
wo	373	41	5.49E-07	4.46E-08	-	-	-5.58E-07	1.44E-08
wo	373	71	9.40E-07	1.60E-07	-	-	-5.45E-07	4.49E-08
wo	373	102	1.25E-06	3.12E-07	-	-	-5.81E-07	7.42E-08
ov	298	6	3.52E-07	1.46E-08	3.49E-07	7.53E-08	-	-
ov	298	21	1.05E-06	1.74E-07	3.94E-07	2.00E-07	-	-
ov	298	42	1.22E-06	1.50E-07	2.27E-07	9.63E-08	-	-
ov	298	72	1.24E-06	2.37E-07	1.73E-07	1.02E-07	-	-
ov	298	102	1.14E-06	1.86E-07	2.54E-07	1.60E-07	-	-
ov	333	6	1.93E-07	4.35E-08	4.76E-07	4.65E-08	-	-
ov	333	21	7.32E-07	3.72E-07	4.95E-07	1.25E-07	-	-
ov	333	42	9.43E-07	2.24E-07	4.56E-07	8.19E-08	-	-
ov	333	72	9.37E-07	2.64E-07	3.83E-07	9.39E-08	-	-
ov	333	103	9.11E-07	2.99E-07	5.57E-07	3.39E-07	-	-
ov	373	6	9.62E-08	3.70E-08	6.32E-07	1.19E-07	-	-
ov	373	21	5.08E-07	1.27E-07	7.38E-07	2.63E-08	-	-
ov	373	41	7.07E-07	3.64E-07	6.50E-07	3.41E-07	-	-
ov	373	71	7.41E-07	1.27E-07	5.15E-07	8.80E-08	-	-
ov	373	102	5.83E-07	3.18E-07	5.85E-07	4.81E-07	-	-

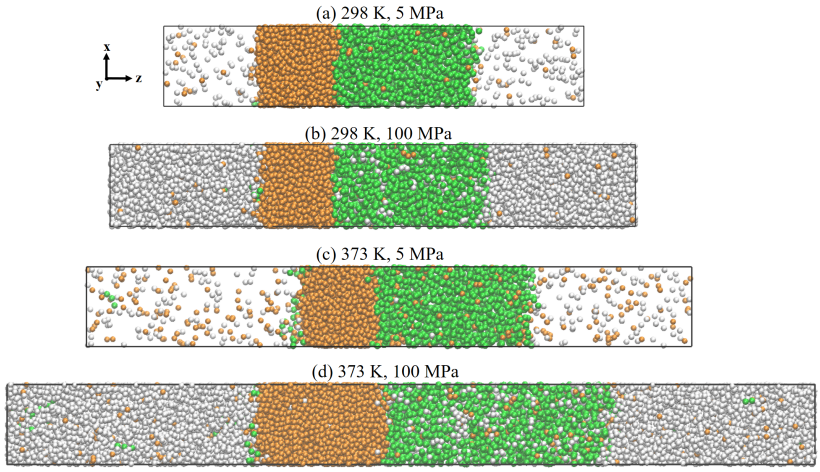

Figure S1: Equilibrium snapshots of the H_2+H_2O+n-decane three-phase system at different temperature and pressure conditions. Color code: H_2, white; H_2O, orange; n-decane segment, green.

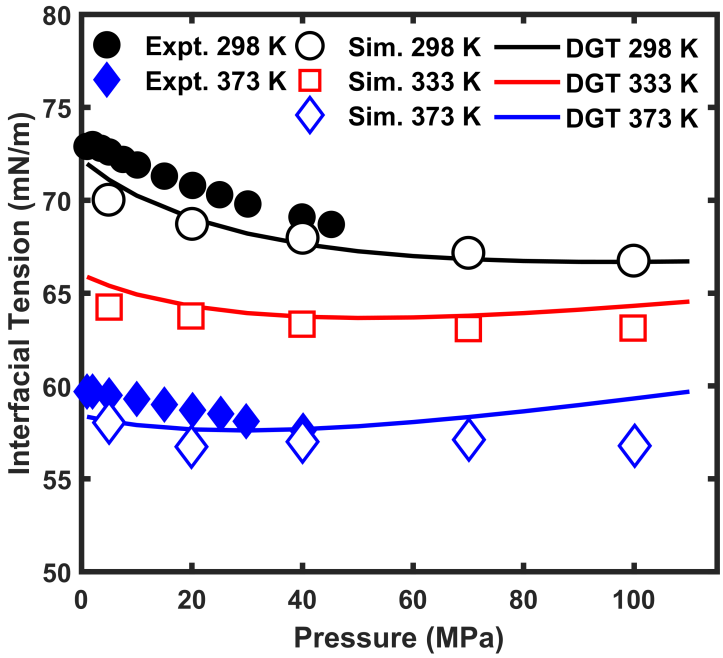

Figure S2: Pressure dependence of IFT in the H_2+H_2O 2-phase system at various temperatures from MD simulation (open symbols) and DGT with the PC-SAFT EoS (lines). The experimental data from ref. S9 and S10 are shown as solid symbols.

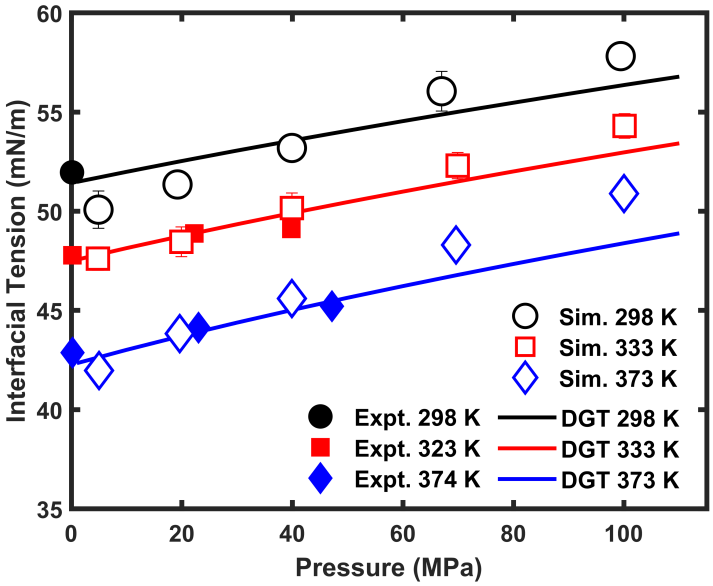

Figure S3: Pressure dependence of IFT in the H_2O+decane 2-phase system at various temperatures from MD simulation (open symbols) and DGT with the PC-SAFT EoS (lines). The experimental data from ref. S11 are shown as solid symbols.

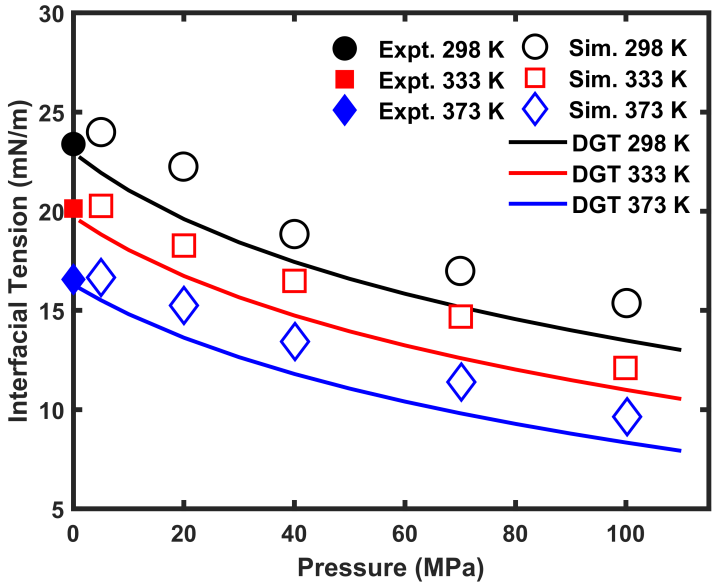

Figure S4: Pressure dependence of IFT in the H_2+decane 2-phase system at various temperatures from MD simulation (open symbols) and DGT with the PC-SAFT EoS (lines). The experimental data for pure decane system from ref. S12 are shown as solid symbols.

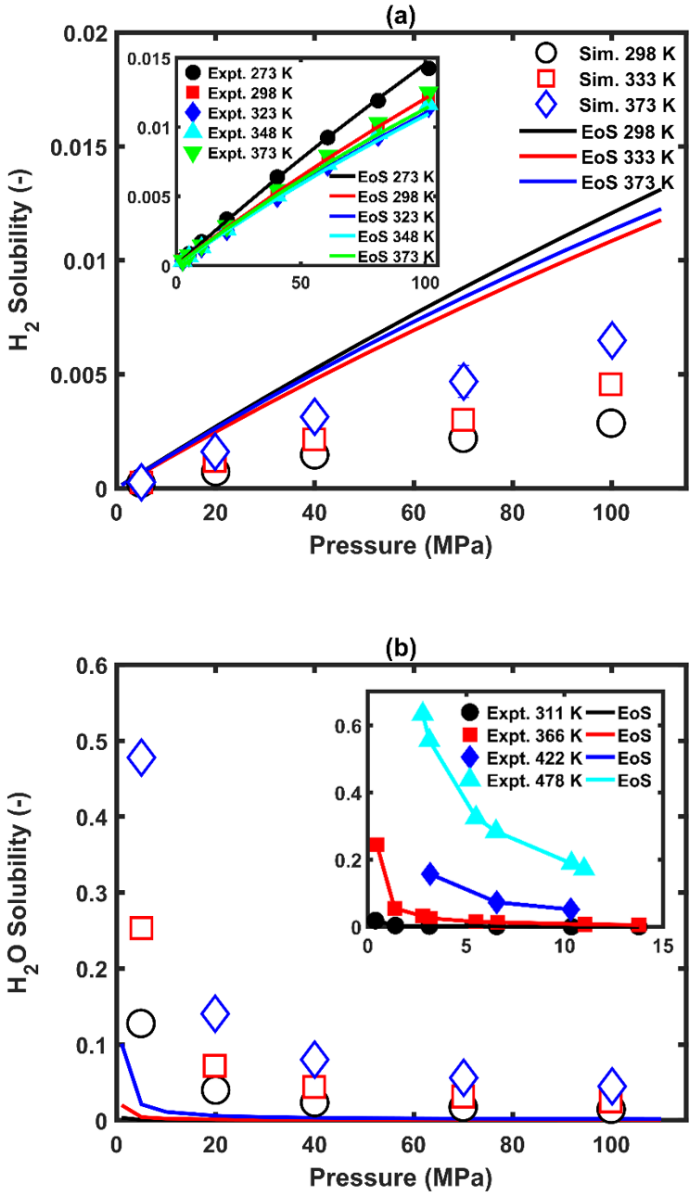

Figure S5: Component solubilities (dimensionless mole fractions) in the H_2+H_2O 2-phase system at different temperatures and pressures. The results from MD simulation and the PC-SAFT EoS are shown as open symbols and lines, respectively. The experimental data shown in inset figures are from ref. S4 and S13.

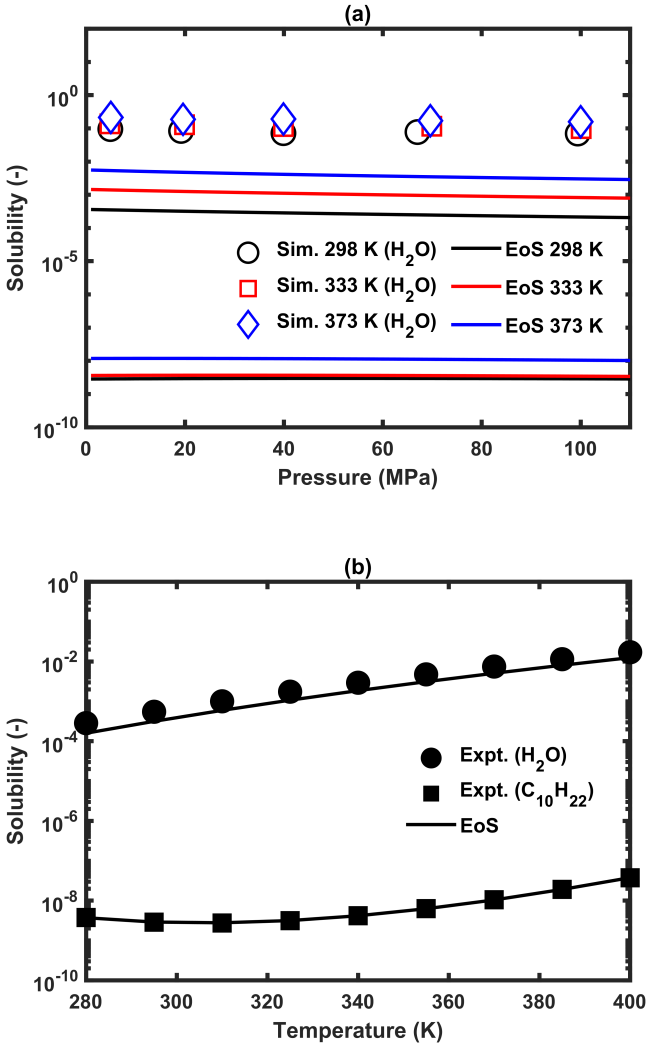

Figure S6: Component solubilities (dimensionless mole fractions) in the H_2O+decane 2-phase system at different temperatures and pressures. The results from MD simulation, experiment (ref. S14) and the PC-SAFT EoS are shown as open symbols, solid symbols and lines, respectively. The decane solublities in the water-rich phase are zeros and not shown in logarithmic scale.

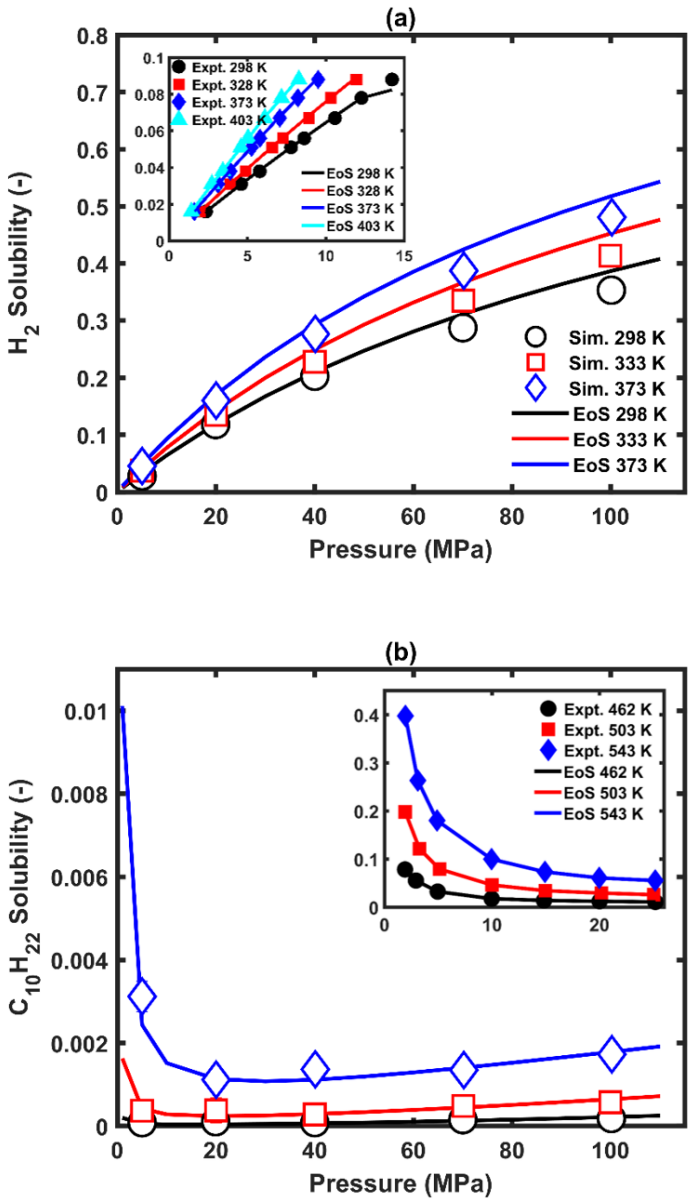

Figure S7: Component solubilities (dimensionless mole fractions) in the H_2+decane 2-phase system at different temperatures and pressures. The results from MD simulation and the PC-SAFT EoS are shown as open symbols and lines, respectively. The experimental data shown in inset figures are from ref. S5 and S15.

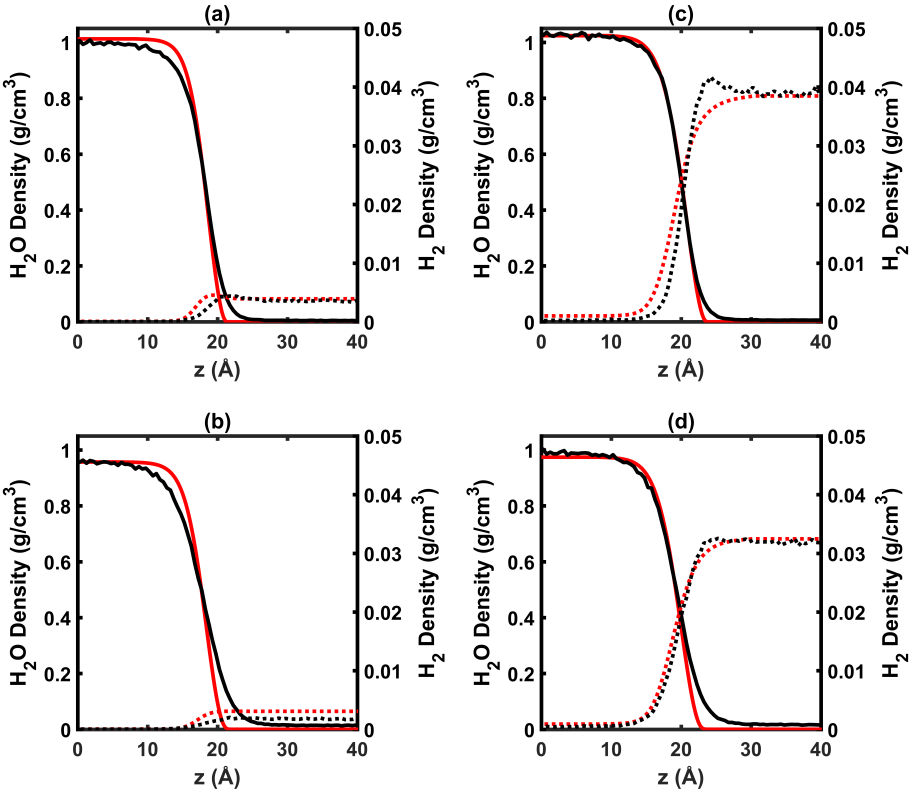

Figure S8: Equilibrium distributions of different species in the H_2+H_2O 2-phase system at (a) 298 K and 5 MPa, (b) 373 K and 5 MPa, (c) 298 K and 70 MPa, and (d) 373 K and 70 MPa. The black and red colors represent MD simulation and DGT with the PC-SAFT EoS, respectively. The solid and dotted lines denote H_2O and H_2, respectively.

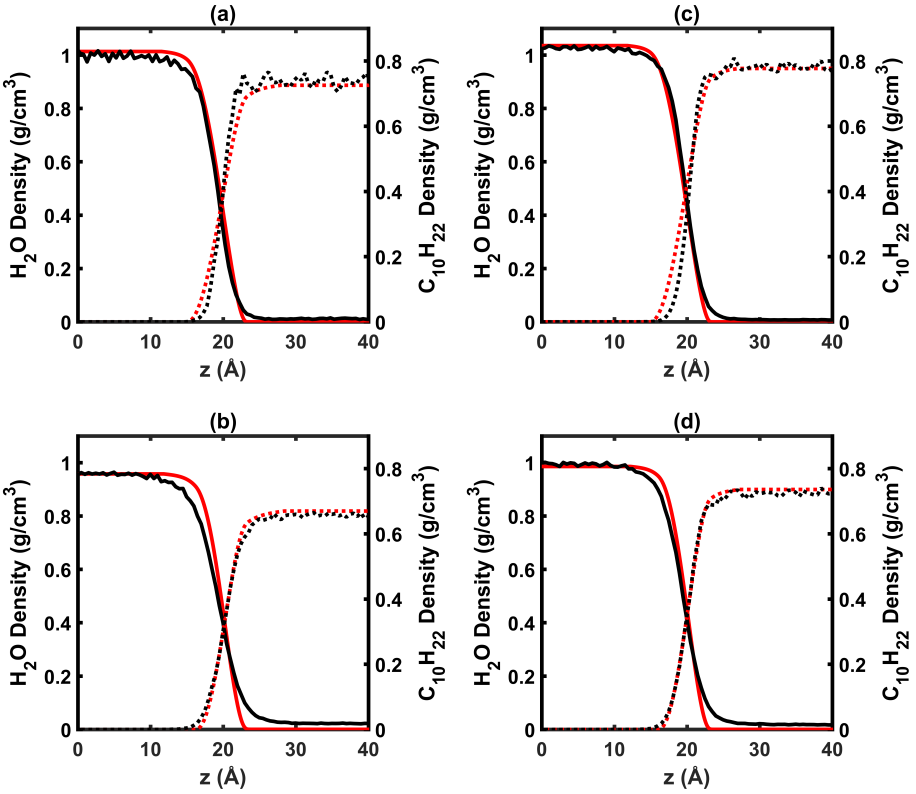

Figure S9: Equilibrium distributions of different species in the H_2O+decane 2-phase system at (a) 298 K and 5 MPa, (b) 373 K and 5 MPa, (c) 298 K and 70 MPa, and (d) 373 K and 70 MPa. The black and red colors represent MD simulation and DGT with the PC-SAFT EoS, respectively. The solid and dotted lines denote H_2O and decane, respectively.

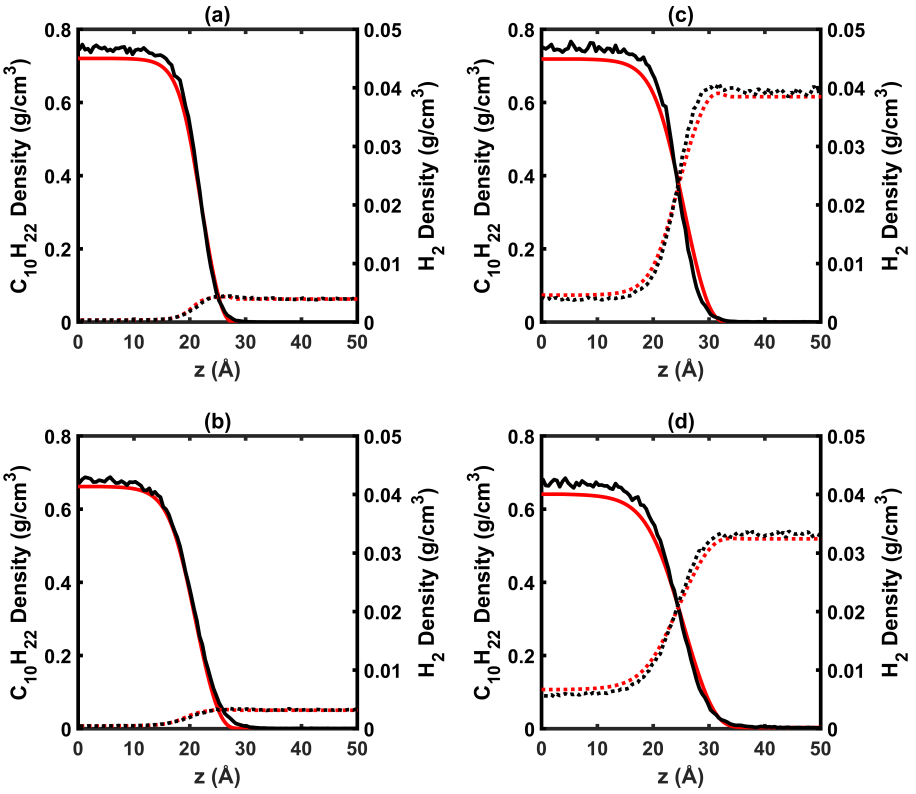

Figure S10: Equilibrium distributions of different species in the H_2+decane 2-phase system at (a) 298 K and 5 MPa, (b) 373 K and 5 MPa, (c) 298 K and 70 MPa, and (d) 373 K and 70 MPa. The black and red colors represent MD simulation and DGT with the PC-SAFT EoS, respectively. The solid and dotted lines denote H_2 and decane, respectively.

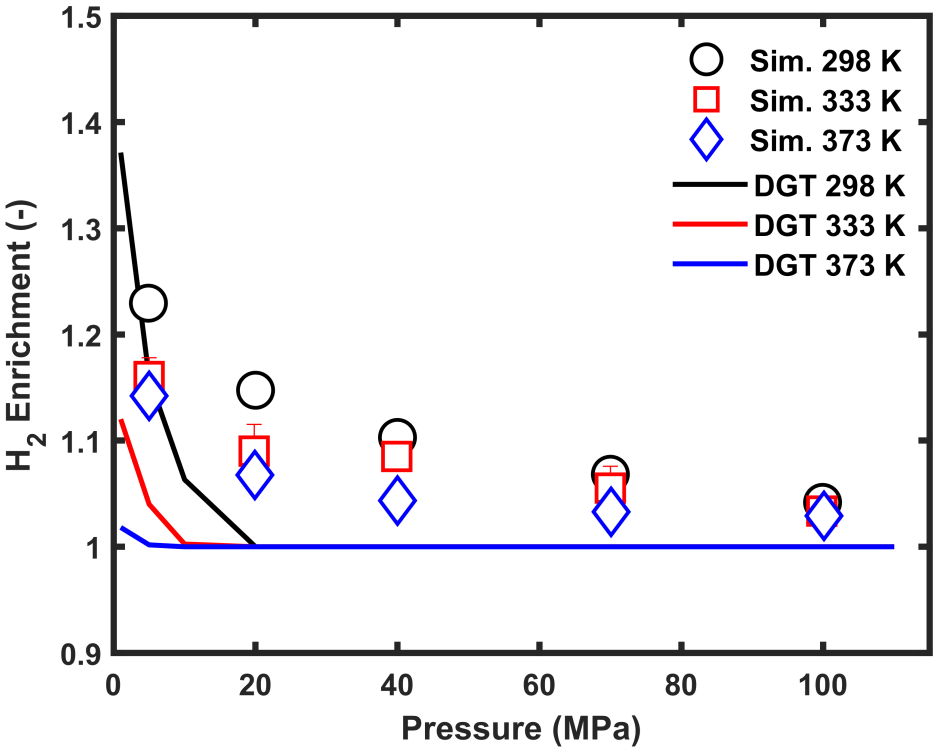

Figure S11: Enrichments in the H_2+H_2O 2-phase system at different temperatures and pressures. The results from MD simulation and the PC-SAFT EoS are shown as open symbols and lines, respectively.

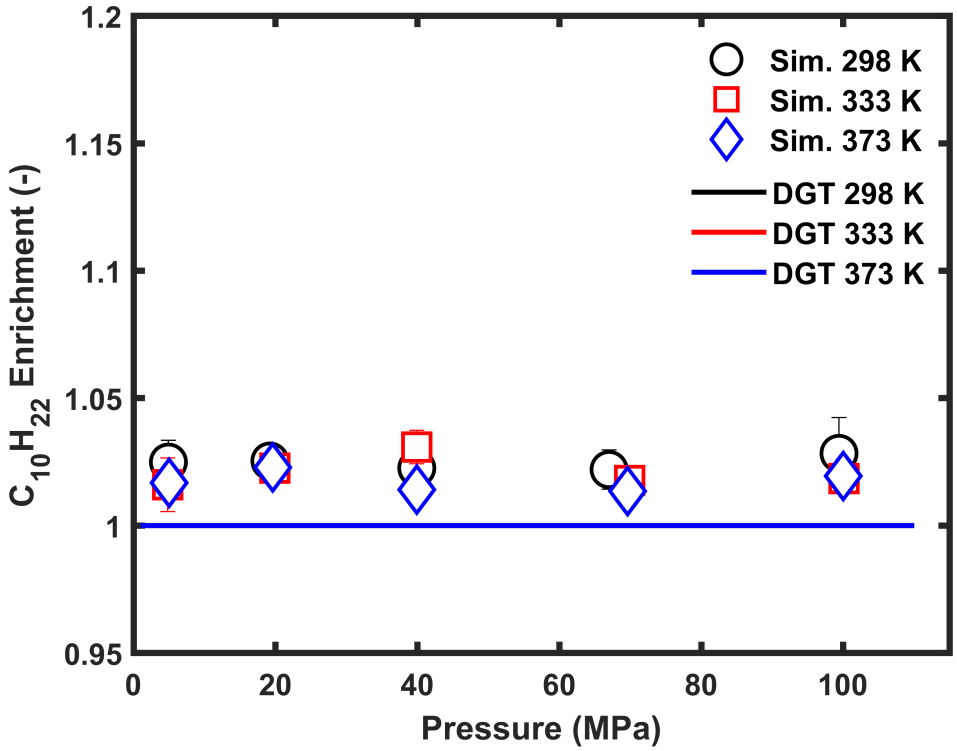

Figure S12: Enrichments in the H_2O+decane 2-phase system at different temperatures and pressures. The results from MD simulation and the PC-SAFT EoS are shown as open symbols and lines, respectively.

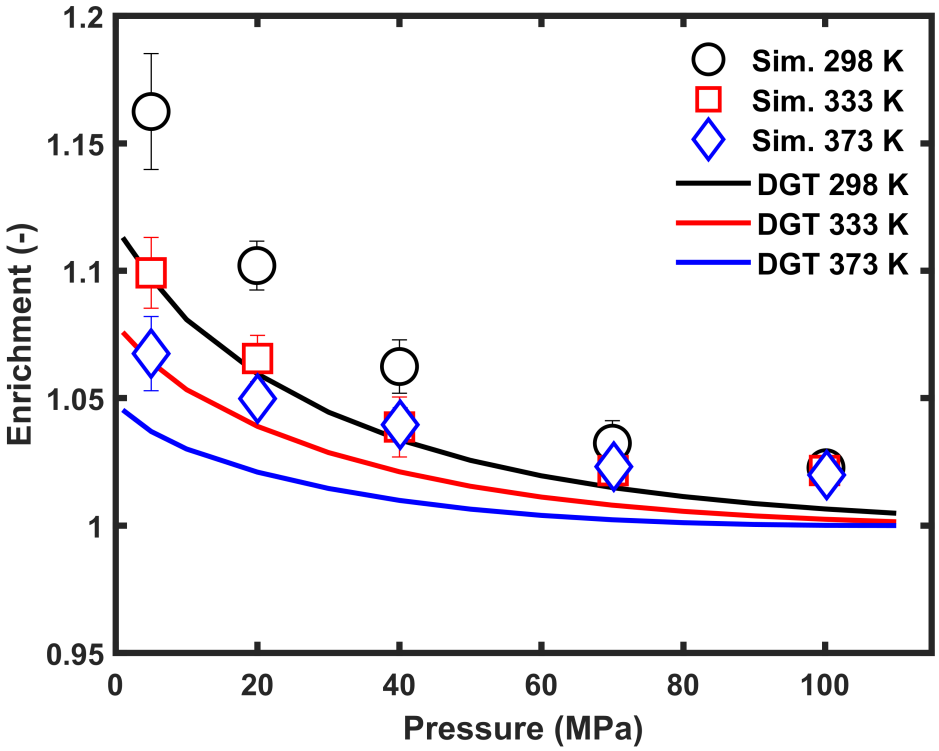

Figure S13: Enrichments in the H_2+decane 2-phase system at different temperatures and pressures. The results from MD simulation and the PC-SAFT EoS are shown as open symbols and lines, respectively.

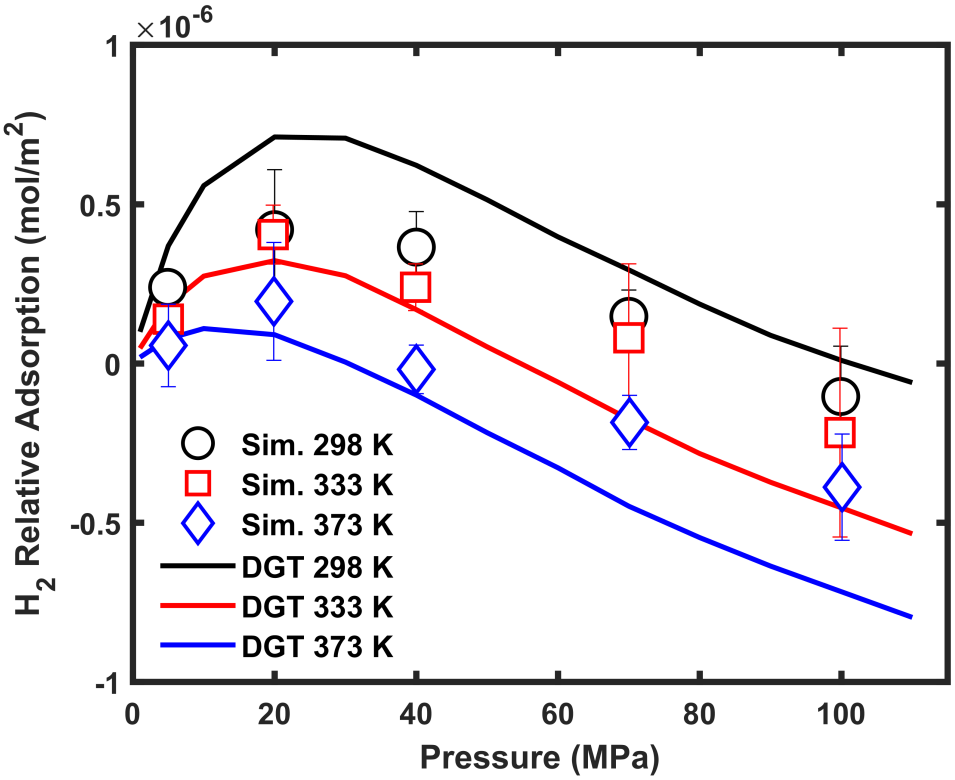

Figure S14: Surface excesses in the H_2+H_2O 2-phase system at different temperatures and pressures. The results from MD simulation and the PC-SAFT EoS are shown as open symbols and lines, respectively.

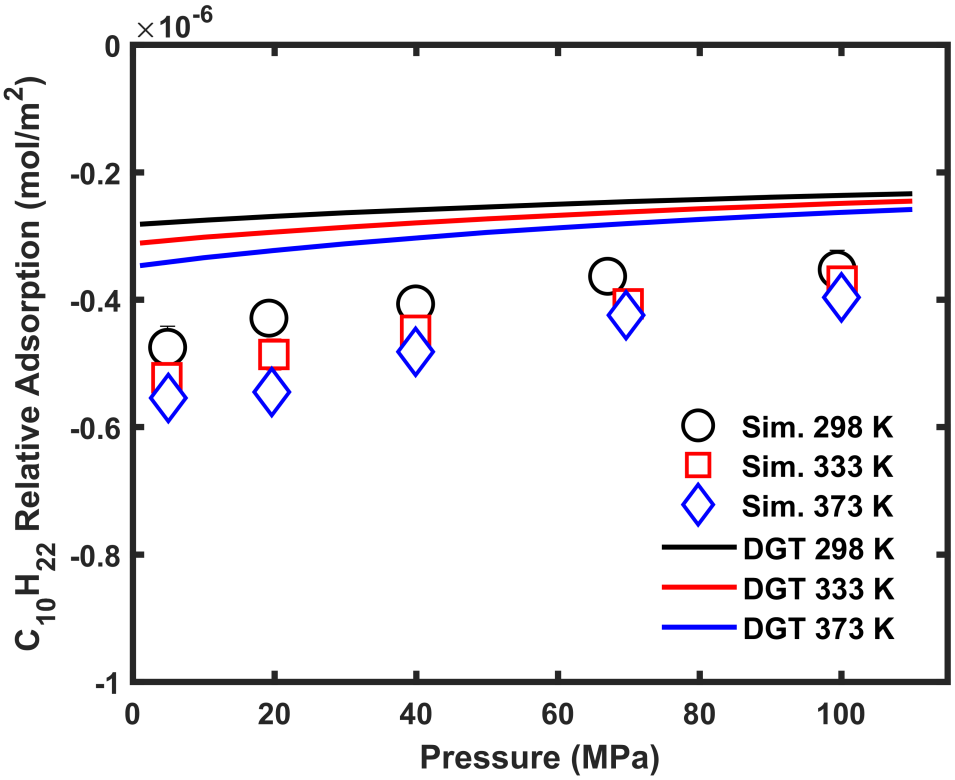

Figure S15: Surface excesses in the H_2O+decane 2-phase system at different temperatures and pressures. The results from MD simulation and the PC-SAFT EoS are shown as open symbols and lines, respectively.

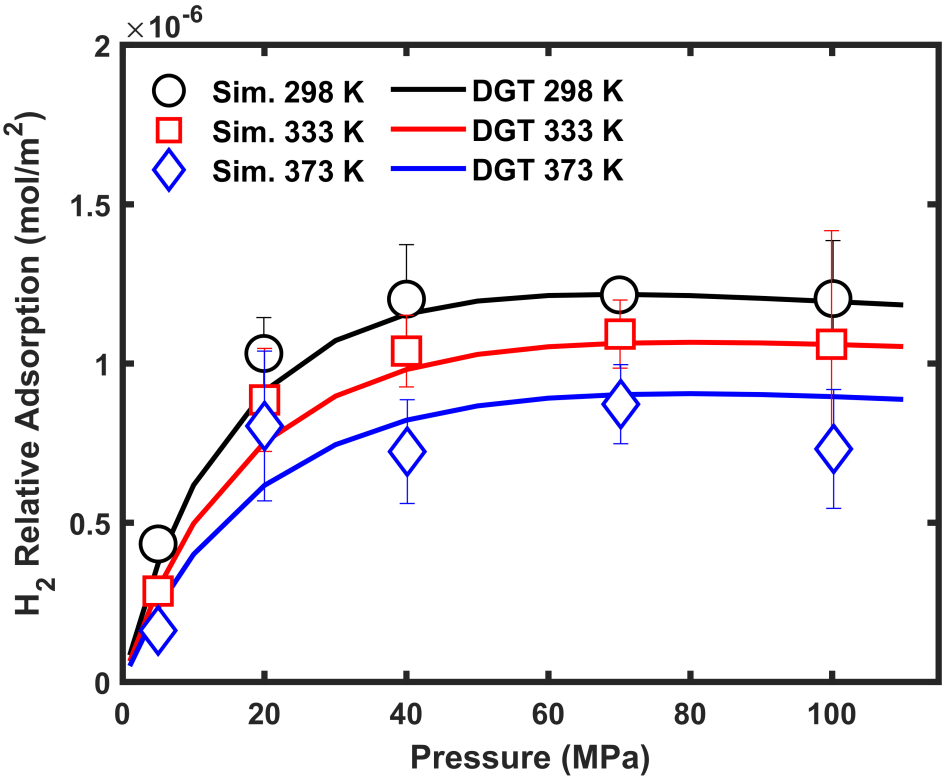

Figure S16: Surface excesses in the H_2+decane 2-phase system at different temperatures and pressures. The results from MD simulation and the PC-SAFT EoS are shown as open symbols and lines, respectively.

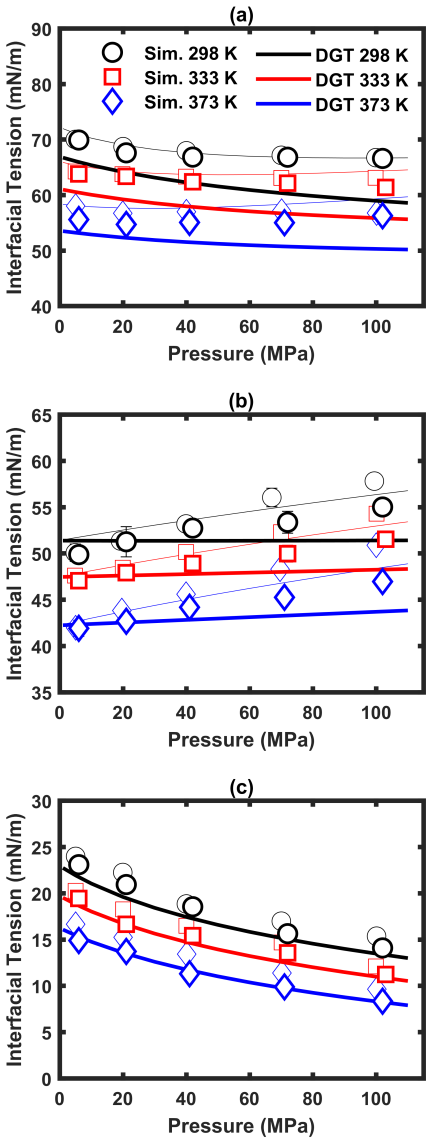

Figure S17: IFTs in (a), (b), and (c) are same as those in Fig. 2, 4, and 6, respectively, but in comparison with corresponding 2-phase IFTs from Fig. S1-3. The 2-phase IFTs from simulations and DGT are displayed as open symbols and lines with thin line width.

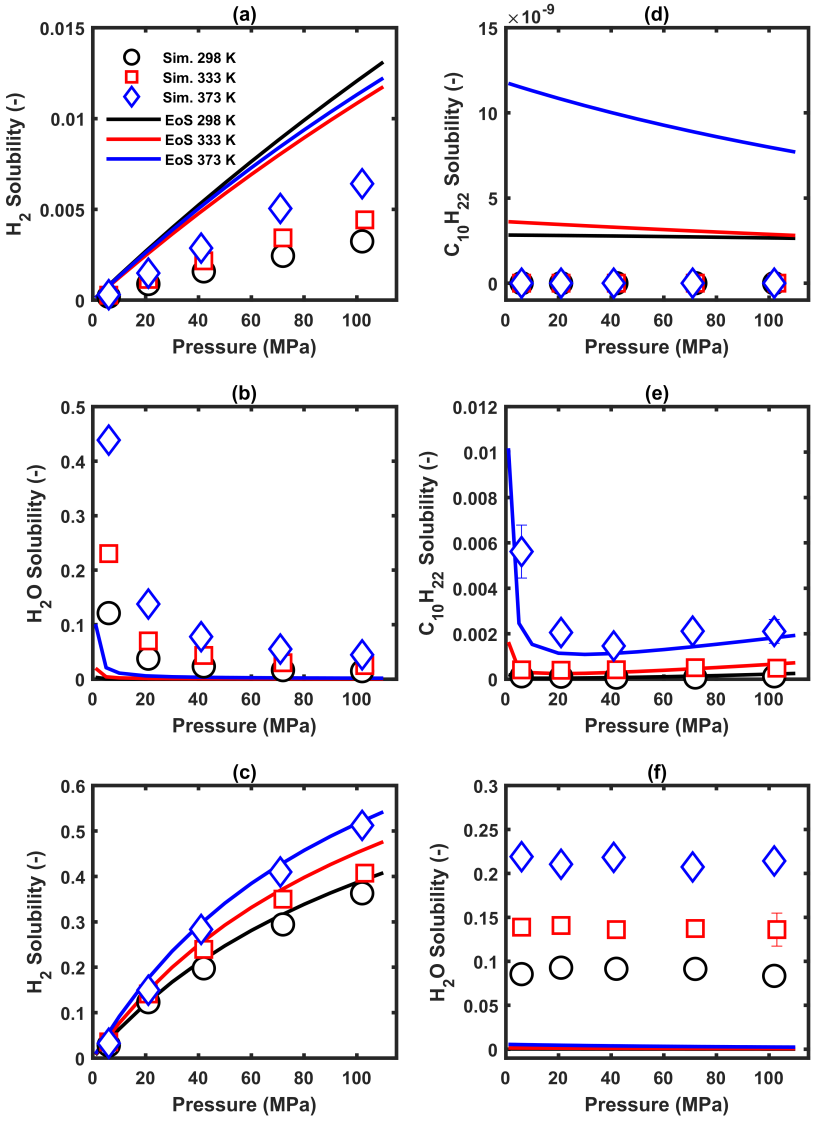

Figure S18: Solubilities (dimensionless mole fractions) in the H_2+H_2O+$C_{10}H_{22}$ 3-phase system. Top, middle, and bottom panels show solubilities in H_2O-rich, H_2-rich, and $C_{10}H_{22}$-rich phases, respectively. The results from MD simulation and the PC-SAFT EoS are shown as open symbols and lines, respectively.

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