

SUPPLEMENTARY MATERIAL

Influence of Dispersive Long Range Interactions on Properties of Vapour-Liquid Equilibria and Interfaces of Binary Lennard-Jones Mixtures

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Tables

The supplementary material for the publication *Influence of Dispersive Long Range Interactions on Properties of Vapour-Liquid Equilibria and Interfaces of Binary Lennard-Jones Mixtures* contains

- Plots of the density profiles at the planar vapour-liquid interfaces of the investigated LJ mixtures. The results from both MD and DGT are shown for all investigated mixtures, cf. Figs. 1 - 4. The topological behaviour of such density profiles has been discussed in detail elsewhere[41].
- The numeric values of the phase equilibria and interfacial properties of the pure LJ fluid from the coexistence MD simulations and the EOS+DGT (Table 1 & 2)
- The numeric values of the Henry's law constants from MD simulations for the mixture D, E, and F obtained from the LJ and LJTS potential (Table 3 & 4)
- The numeric values of the phase equilibria (Table 5 – 10) and interfacial properties (Table 11 – 16) results of the LJ potential for the mixtures A - F. The results from both the coexistence MD simulations and the EOS+DGT are reported.

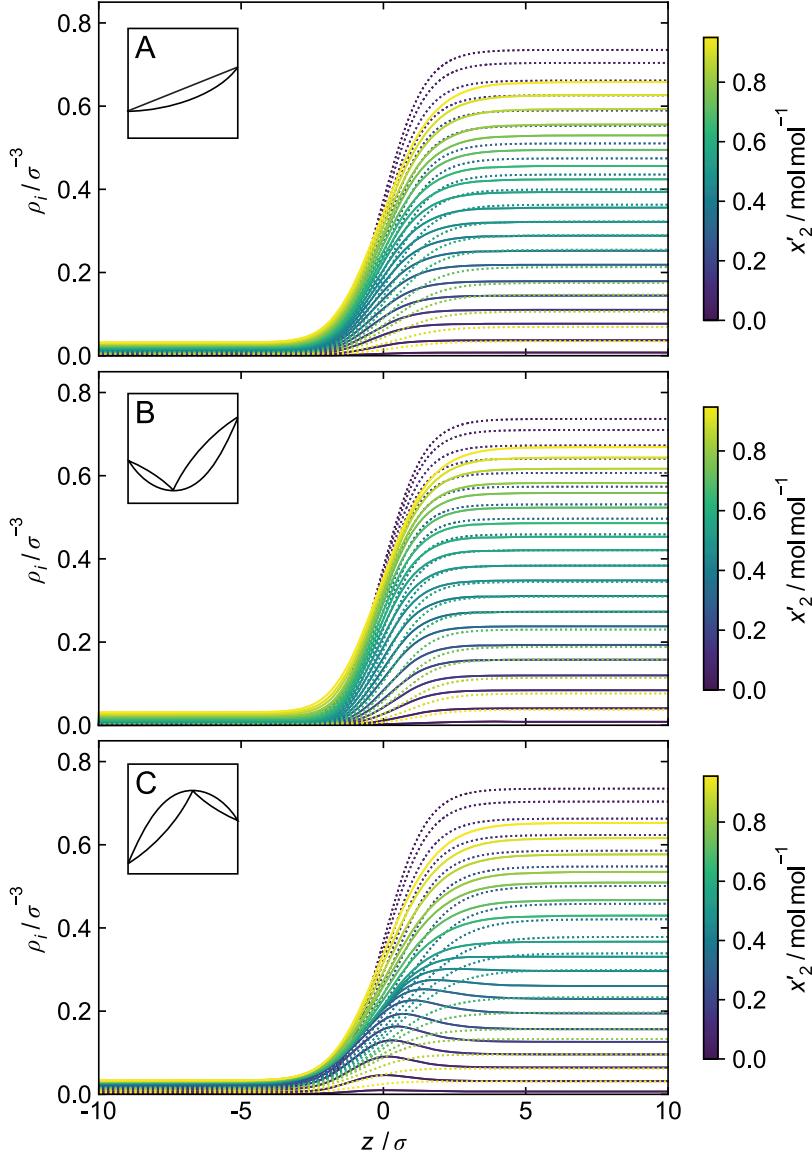


Figure 1. Density profiles of the binary LJ mixtures A, B, and C at $T = 0.92 \varepsilon k_B^{-1}$. Results from DGT. Dashed lines: heavy boiling component 1; solid lines: light boiling component 2. The color indicates the liquid phase composition.

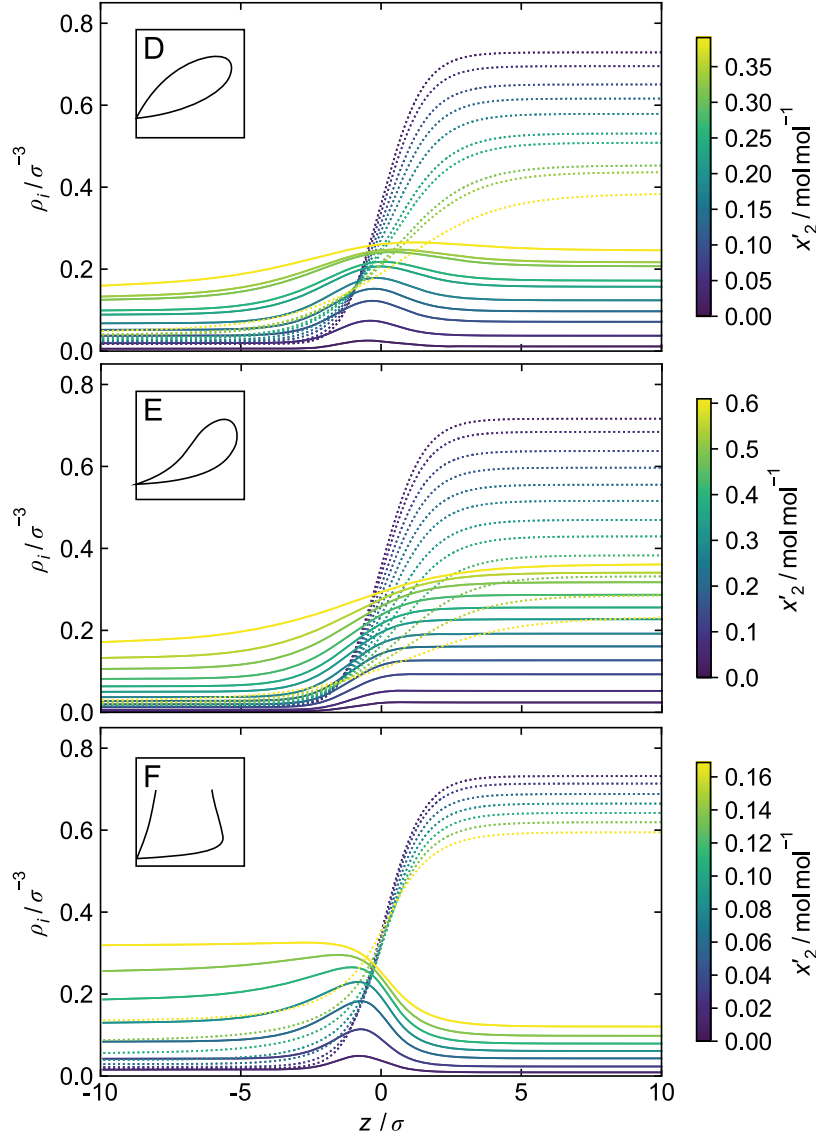


Figure 2. Density profiles of the binary LJ mixtures D, E, and F at $T = 0.92 \varepsilon k_B^{-1}$. Results from DGT. Dashed lines: heavy boiling component 1; solid lines: light boiling component 2. The color indicates the liquid phase composition.

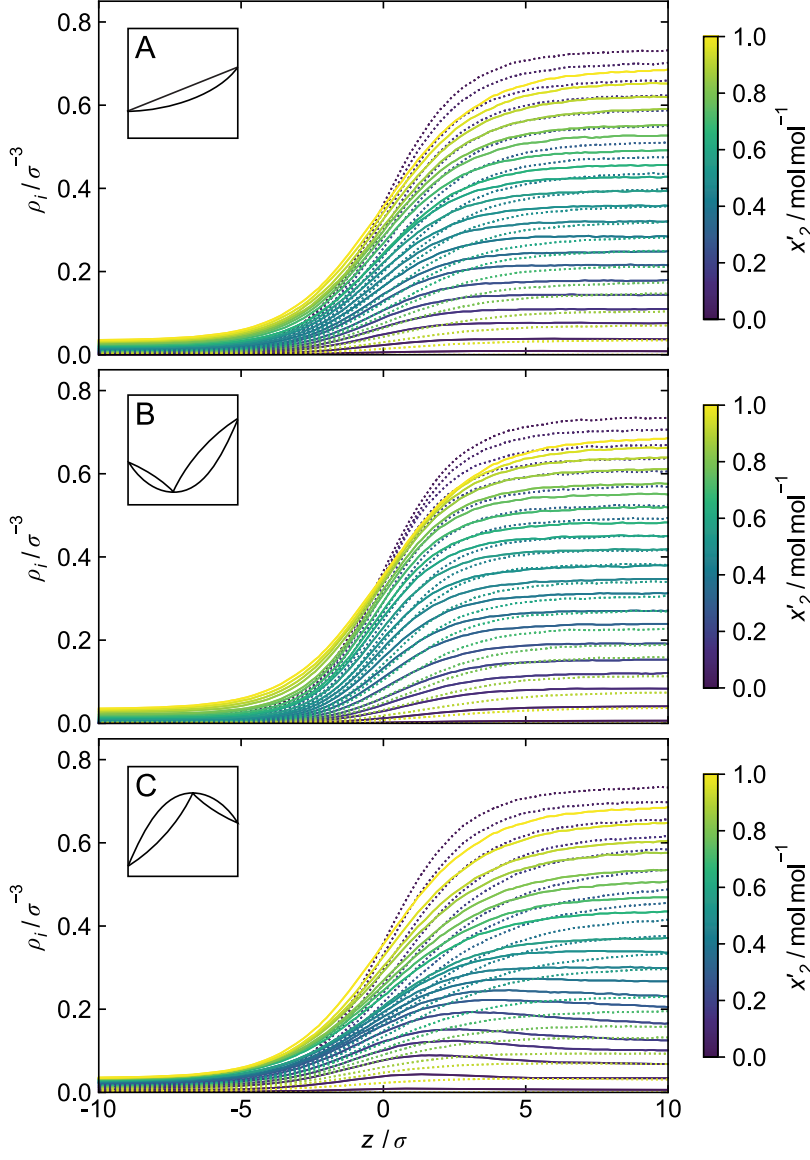


Figure 3. Density profiles of the binary LJ mixtures A, B, and C at $T = 0.92 \epsilon k_B^{-1}$. Results from MD. Dashed lines: heavy boiling component 1; solid lines: light boiling component 2. The color indicates the liquid phase composition.

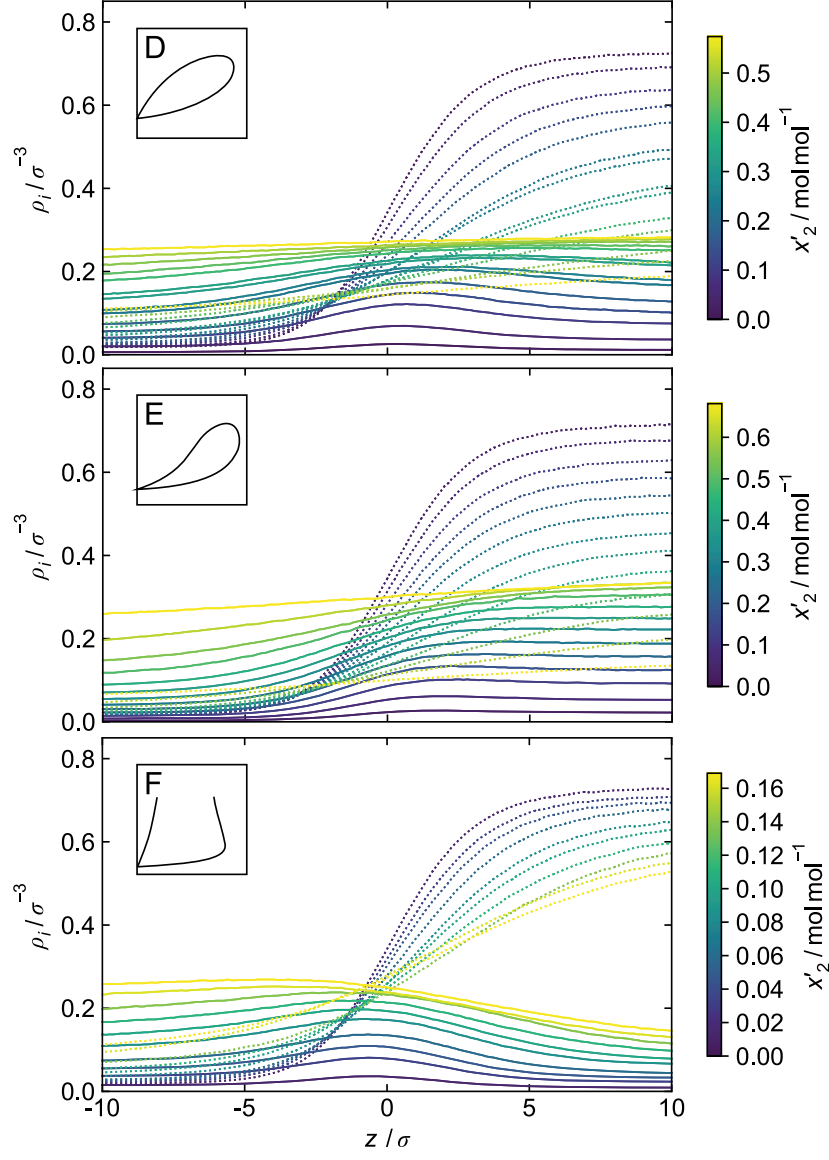


Figure 4. Density profiles of the binary LJ mixtures D, E, and F at $T = 0.92 \epsilon k_B^{-1}$. Results from MD. Dashed lines: heavy boiling component 1; solid lines: light boiling component 2. The color indicates the liquid phase composition.

Table 1. MD and DGT results for the vapour-liquid equilibrium of the pure Lennard-Jones fluid. The columns are from left to right: the temperature, the vapour pressure, saturated liquid and vapour density. The number in the parentheses indicates the statistical uncertainty in the last decimal digit.

T	$p / \varepsilon \sigma^{-3}$		ρ'' / σ^{-3}		ρ' / σ^{-3}	
	MD	EOS	MD	EOS	MD	EOS
0.69	0.00110(10)	0.0012	0.00164(20)	0.0018	0.847(12)	0.8468
0.74	0.00230(10)	0.0023	0.00320(40)	0.0032	0.826(12)	0.8255
0.79	0.00395(10)	0.0042	0.00522(40)	0.0055	0.804(11)	0.8036
0.84	0.0069(2)	0.0069	0.0087(6)	0.0088	0.781(11)	0.7811
0.89	0.0108(1)	0.0109	0.0133(7)	0.0134	0.758(10)	0.7578
0.94	0.0164(1)	0.0162	0.0198(9)	0.0195	0.7327(90)	0.7333
0.99	0.0233(3)	0.0233	0.0276(10)	0.0276	0.7065(80)	0.7073
1.04	0.0323(2)	0.0323	0.0380(10)	0.0380	0.6782(70)	0.6793
1.09	0.0437(1)	0.0434	0.052(1)	0.0515	0.6478(80)	0.6486
1.14	0.0572(4)	0.0570	0.070(2)	0.0691	0.6134(70)	0.6142
1.19	0.0736(7)	0.0733	0.094(2)	0.0925	0.5734(60)	0.5744
1.24	0.0931(5)	0.0925	0.128(3)	0.1249	0.5240(60)	0.5257
1.29	0.1164(3)	0.1150	0.189(4)	0.1753	0.4521(40)	0.4595

Table 2. MD and DGT results for the vapour-liquid interfacial properties of the pure Lennard-Jones fluid. The columns are from left to right: the temperature, surface tension, and interfacial thickness. The number in the parentheses indicates the statistical uncertainty in the last decimal digit.

T	$\gamma / \varepsilon \sigma^{-2}$		L_{10}^{90} / σ	
	MD	DGT	MD	DGT
0.69	1.18(2)	1.207	1.88(2)	2.21
0.74	1.07(3)	1.083	2.06(5)	2.33
0.79	0.95(3)	0.961	2.24(3)	2.47
0.84	0.85(2)	0.844	2.43(3)	2.63
0.89	0.74(2)	0.730	2.72(5)	2.82
0.94	0.62(2)	0.620	3.04(3)	3.05
0.99	0.52(2)	0.515	3.38(5)	3.33
1.04	0.42(3)	0.415	3.84(5)	3.67
1.09	0.32(1)	0.320	4.43(9)	4.13
1.14	0.24(1)	0.232	5.23(8)	4.75
1.19	0.15(1)	0.153	6.5(1)	5.65
1.24	0.08(1)	0.083	8.4(2)	7.21
1.29	0.03(1)	0.028	14.3(9)	10.82

Table 3. MD results for the Henry’s law constants of the LJTS potential for the mixture D, E, and F. The number in the parentheses indicates the statistical uncertainty in the last decimal digit.

T	$H_{2,1} / \varepsilon \sigma^{-3}$		
	D	E	F
0.63	0.2066(57)	0.0224(7)	0.9929(90)
0.68	0.2382(42)	0.0331(6)	0.9937(98)
0.73	0.2595(32)	0.0447(6)	0.9326(92)
0.78	0.2893(23)	0.0583(5)	0.8842(68)
0.83	0.3030(21)	0.0747(5)	0.8350(64)
0.88	0.3137(20)	0.0902(5)	0.7704(59)
0.93	0.3183(20)	0.1060(6)	0.7127(43)
0.98	0.3156(16)	0.1208(5)	0.6300(47)
1.03	0.3045(17)	0.1338(5)	0.5429(44)

Table 4. MD results for the Henry’s law constants of the LJ potential for the mixture D, E, and F. The number in the parentheses indicates the statistical uncertainty in the last decimal digit.

T	$H_{2,1} / \varepsilon \sigma^{-3}$		
	D	E	F
0.74	0.2283(47)	0.0261(6)	1.0999(98)
0.79	0.2538(48)	0.0353(7)	1.0593(90)
0.84	0.2796(27)	0.0468(5)	1.0209(96)
0.89	0.3053(28)	0.0601(5)	0.9902(91)
0.94	0.3302(24)	0.0752(5)	0.9629(73)
0.99	0.3464(21)	0.0903(5)	0.9157(58)
1.04	0.3541(20)	0.1054(5)	0.8538(53)
1.09	0.3664(16)	0.1199(5)	0.8143(48)
1.14	0.3663(17)	0.1357(5)	0.7472(46)
1.19	0.3653(17)	0.1505(5)	0.6912(37)
1.24	0.3539(18)	0.1626(5)	0.6180(39)
1.29	0.3290(26)	0.1703(8)	0.5262(56)

Table 5. MD and LJ-EOS[51] results for the vapour-liquid equilibrium of the binary Lennard-Jones mixture A ($\varepsilon_2/\varepsilon_1 = 0.9$ and $\xi_{12} = 1$). The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$p / \varepsilon \sigma^{-3}$		$x''_2 / \text{mol mol}^{-1}$		ρ' / σ^{-3}		ρ'' / σ^{-3}	
	MD	EOS	MD	EOS	MD	EOS	MD	EOS
0.000	0.0138(1)	0.0139	0.000	0.000	0.743(9)	0.743	0.0167(8)	0.0168
0.010(1)	0.0141(3)	0.0140	0.021(3)	0.018	0.742(4)	0.743	0.0171(8)	0.0170
0.050(1)	0.0145(4)	0.0145	0.089(6)	0.084	0.740(6)	0.741	0.0177(8)	0.0176
0.104(1)	0.0151(2)	0.0151	0.167(12)	0.168	0.738(8)	0.738	0.0184(8)	0.0185
0.150(2)	0.0157(2)	0.0157	0.239(13)	0.234	0.736(9)	0.736	0.0193(8)	0.0192
0.197(2)	0.0163(2)	0.0162	0.299(10)	0.298	0.733(9)	0.734	0.0201(9)	0.0200
0.245(3)	0.0167(3)	0.0168	0.364(14)	0.358	0.731(9)	0.732	0.0206(9)	0.0207
0.300(1)	0.0175(4)	0.0175	0.428(16)	0.424	0.728(11)	0.729	0.0217(12)	0.0216
0.347(1)	0.0178(3)	0.0180	0.473(14)	0.476	0.726(10)	0.727	0.0221(10)	0.0224
0.398(2)	0.0187(4)	0.0186	0.527(14)	0.530	0.723(11)	0.724	0.0233(10)	0.0233
0.446(2)	0.0195(4)	0.0192	0.581(15)	0.577	0.721(11)	0.722	0.0245(11)	0.0240
0.495(2)	0.0197(4)	0.0198	0.626(12)	0.623	0.718(10)	0.719	0.0248(11)	0.0249
0.550(1)	0.0206(2)	0.0205	0.670(7)	0.672	0.715(12)	0.716	0.0261(11)	0.0258
0.594(2)	0.0210(3)	0.0210	0.711(14)	0.710	0.713(11)	0.714	0.0267(11)	0.0266
0.642(2)	0.0214(3)	0.0216	0.747(9)	0.749	0.710(10)	0.711	0.0273(13)	0.0274
0.699(2)	0.0221(4)	0.0223	0.784(8)	0.794	0.706(10)	0.708	0.0282(11)	0.0284
0.752(2)	0.0230(4)	0.0229	0.831(10)	0.833	0.704(10)	0.705	0.0297(12)	0.0294
0.791(1)	0.0234(5)	0.0234	0.859(12)	0.862	0.701(10)	0.702	0.0302(11)	0.0301
0.848(2)	0.0242(3)	0.0241	0.901(9)	0.901	0.698(7)	0.699	0.0315(11)	0.0311
0.900(1)	0.0247(6)	0.0247	0.934(6)	0.936	0.694(7)	0.696	0.0322(11)	0.0321
0.950(1)	0.0253(2)	0.0253	0.968(2)	0.968	0.691(6)	0.693	0.0331(12)	0.0330
1.000	0.0259(3)	0.0259	1.000	1.000	0.688(3)	0.690	0.0342(12)	0.0340

Table 6. MD and LJ-EOS[51] results for the vapour-liquid equilibrium of the binary Lennard-Jones mixture B ($\varepsilon_2/\varepsilon_1 = 0.9$ and $\xi_{12} = 1.2$). The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$p / \varepsilon \sigma^{-3}$		$x''_2 / \text{mol mol}^{-1}$		ρ' / σ^{-3}		ρ'' / σ^{-3}	
	MD	EOS	MD	EOS	MD	EOS	MD	EOS
0.000	0.0138(1)	0.0139	0.000	0.000	0.743(9)	0.743	0.0167(8)	0.0168
0.0111(4)	0.0138(2)	0.0138	0.002(1)	0.002	0.744(4)	0.745	0.0167(8)	0.0166
0.0542(8)	0.0132(2)	0.0132	0.015(3)	0.014	0.749(6)	0.751	0.0159(6)	0.0158
0.1112(9)	0.0124(3)	0.0123	0.039(2)	0.038	0.754(7)	0.757	0.0149(6)	0.0148
0.1575(18)	0.0117(2)	0.0117	0.073(7)	0.067	0.758(8)	0.761	0.0139(7)	0.0139
0.2062(14)	0.0112(2)	0.0110	0.107(8)	0.110	0.761(8)	0.764	0.0133(7)	0.0131
0.2520(17)	0.0105(2)	0.0105	0.167(13)	0.164	0.763(8)	0.767	0.0125(7)	0.0124
0.3094(12)	0.0101(3)	0.0100	0.260(10)	0.252	0.765(9)	0.769	0.0120(7)	0.0118
0.3547(12)	0.0100(2)	0.0098	0.330(20)	0.335	0.765(8)	0.770	0.0118(7)	0.0116
0.4038(15)	0.0099(3)	0.0099	0.445(14)	0.436	0.765(9)	0.770	0.0117(7)	0.0116
0.4528(14)	0.0102(2)	0.0102	0.538(19)	0.540	0.765(9)	0.769	0.0121(7)	0.0120
0.4999(9)	0.0108(3)	0.0107	0.632(7)	0.636	0.763(8)	0.768	0.0128(7)	0.0126
0.5498(12)	0.0115(2)	0.0115	0.724(7)	0.726	0.761(8)	0.765	0.0137(8)	0.0137
0.5943(13)	0.0127(3)	0.0125	0.794(14)	0.793	0.758(8)	0.763	0.0152(7)	0.0149
0.6403(15)	0.0140(4)	0.0137	0.844(13)	0.850	0.754(8)	0.759	0.0169(8)	0.0164
0.6946(8)	0.0154(3)	0.0153	0.899(7)	0.900	0.749(7)	0.753	0.0187(8)	0.0186
0.7479(11)	0.0172(2)	0.0171	0.931(7)	0.935	0.742(8)	0.747	0.0211(8)	0.0210
0.7863(18)	0.0184(3)	0.0185	0.953(4)	0.954	0.737(7)	0.741	0.0228(9)	0.0229
0.8440(13)	0.0207(4)	0.0206	0.972(3)	0.974	0.727(7)	0.731	0.0261(9)	0.0259
0.8938(8)	0.0223(3)	0.0224	0.986(2)	0.986	0.717(6)	0.720	0.0284(9)	0.0286
0.9469(10)	0.0244(5)	0.0243	0.995(1)	0.994	0.704(5)	0.706	0.0317(10)	0.0313
1.0000	0.0259(3)	0.0259	1.000	1.000	0.688(3)	0.690	0.0342(12)	0.0340

Table 7. MD and LJ-EOS[51] results for the vapour-liquid equilibrium of the binary Lennard-Jones mixture C ($\varepsilon_2/\varepsilon_1 = 0.9$ and $\xi_{12} = 0.85$). The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$p / \varepsilon \sigma^{-3}$		$x''_2 / \text{mol mol}^{-1}$		ρ' / σ^{-3}		ρ'' / σ^{-3}	
	MD	EOS	MD	EOS	MD	EOS	MD	EOS
0.000	0.0138(1)	0.0139	0.000	0.000	0.743(9)	0.743	0.0167(8)	0.0168
0.0090(4)	0.0150(2)	0.0150	0.064(8)	0.073	0.741(4)	0.742	0.0183(9)	0.0183
0.0430(10)	0.0182(4)	0.0187	0.230(16)	0.257	0.736(6)	0.735	0.0225(9)	0.0231
0.0886(17)	0.0220(5)	0.0224	0.374(13)	0.388	0.728(9)	0.727	0.0279(12)	0.0284
0.1333(12)	0.0236(3)	0.0251	0.440(8)	0.460	0.721(11)	0.719	0.0302(12)	0.0323
0.1771(18)	0.0255(4)	0.0269	0.480(8)	0.505	0.714(12)	0.712	0.0331(15)	0.0352
0.2222(25)	0.0269(4)	0.0283	0.520(13)	0.537	0.707(13)	0.704	0.0352(13)	0.0375
0.2797(41)	0.0283(4)	0.0295	0.552(11)	0.564	0.699(18)	0.695	0.0375(14)	0.0394
0.3335(46)	0.0288(3)	0.0303	0.566(9)	0.582	0.692(19)	0.687	0.0383(15)	0.0407
0.3821(31)	0.0294(3)	0.0307	0.595(13)	0.595	0.686(15)	0.681	0.0396(17)	0.0415
0.4390(25)	0.0301(3)	0.0311	0.610(10)	0.608	0.680(20)	0.675	0.0411(31)	0.0422
0.4939(51)	0.0305(3)	0.0314	0.617(13)	0.620	0.676(16)	0.670	0.0413(16)	0.0428
0.5510(25)	0.0306(5)	0.0317	0.635(10)	0.634	0.672(20)	0.666	0.0419(27)	0.0432
0.6481(37)	0.0307(5)	0.0319	0.668(8)	0.661	0.668(17)	0.663	0.0417(14)	0.0435
0.7038(9)	0.0308(4)	0.0319	0.695(10)	0.681	0.668(14)	0.664	0.0423(27)	0.0435
0.7647(17)	0.0310(3)	0.0316	0.716(8)	0.710	0.670(12)	0.666	0.0422(16)	0.0431
0.8007(18)	0.0304(5)	0.0314	0.744(10)	0.731	0.670(11)	0.668	0.0412(16)	0.0426
0.8575(23)	0.0298(4)	0.0307	0.792(6)	0.775	0.675(9)	0.673	0.0402(14)	0.0414
0.9085(25)	0.0293(3)	0.0296	0.834(8)	0.830	0.679(10)	0.678	0.0392(14)	0.0396
0.9548(9)	0.0280(5)	0.0280	0.907(7)	0.901	0.683(6)	0.683	0.0373(14)	0.0372
1.0000	0.0259(3)	0.0259	1.000	1.000	0.688(3)	0.690	0.0342(12)	0.0340

Table 8. MD and LJ-EOS[51] results for the vapour-liquid equilibrium of the binary Lennard-Jones mixture D ($\varepsilon_2/\varepsilon_1 = 0.5$ and $\xi_{12} = 1$). The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$p / \varepsilon \sigma^{-3}$		$x''_2 / \text{mol mol}^{-1}$		ρ' / σ^{-3}		ρ'' / σ^{-3}	
	MD	EOS	MD	EOS	MD	EOS	MD	EOS
0.000	0.0138(1)	0.0139	0.000	0.000	0.743(9)	0.743	0.0167(8)	0.0168
0.015(1)	0.0193(4)	0.0190	0.259(13)	0.247	0.739(4)	0.740	0.024(1)	0.0232
0.051(1)	0.0310(3)	0.0305	0.504(10)	0.502	0.731(6)	0.733	0.039(1)	0.0383
0.099(2)	0.0467(6)	0.0452	0.646(9)	0.636	0.719(8)	0.722	0.061(2)	0.0590
0.136(3)	0.0573(6)	0.0559	0.692(7)	0.687	0.708(9)	0.713	0.078(2)	0.0755
0.176(3)	0.0681(5)	0.0669	0.724(7)	0.721	0.697(9)	0.703	0.096(2)	0.0941
0.228(4)	0.0827(8)	0.0803	0.744(6)	0.747	0.681(13)	0.688	0.125(2)	0.1191
0.253(3)	0.0872(6)	0.0863	0.749(7)	0.754	0.672(10)	0.680	0.134(3)	0.1315
0.314(9)	0.0988(3)	0.1002	0.761(5)	0.765	0.644(16)	0.660	0.161(6)	0.1638
0.332(6)	0.1031(9)	0.1040	0.760(7)	0.766	0.642(12)	0.653	0.173(3)	0.1738
0.391(6)	0.1144(9)	0.1157	0.757(10)	0.766	0.616(13)	0.629	0.208(4)	0.2086
0.424(3)	0.1193(7)	0.1217	0.756(7)	0.763	0.599(13)	0.614	0.224(4)	0.2299
0.467(6)	0.1267(7)	0.1288	0.749(11)	0.756	0.576(11)	0.592	0.255(5)	0.2594
0.498(15)	0.1326(17)	0.1334	0.731(43)	0.749	0.558(12)	0.574	0.293(15)	0.2823

Table 9. MD and LJ-EOS[51] results for the vapour-liquid equilibrium of the binary Lennard-Jones mixture E ($\varepsilon_2/\varepsilon_1 = 0.5$ and $\xi_{12} = 1.2$). The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$p / \varepsilon \sigma^{-3}$		$x''_2 / \text{mol mol}^{-1}$		ρ' / σ^{-3}		ρ'' / σ^{-3}	
	MD	EOS	MD	EOS	MD	EOS	MD	EOS
0.000	0.0138(1)	0.0139	0.000	0.000	0.743(9)	0.743	0.0167(8)	0.0168
0.032(1)	0.0161(2)	0.0158	0.146(8)	0.134	0.738(6)	0.740	0.020(1)	0.0192
0.071(2)	0.0197(3)	0.0184	0.312(11)	0.273	0.733(6)	0.737	0.024(1)	0.0227
0.127(1)	0.0248(3)	0.0232	0.462(9)	0.436	0.724(7)	0.730	0.031(1)	0.0289
0.175(1)	0.0301(4)	0.0282	0.557(7)	0.544	0.715(8)	0.724	0.038(1)	0.0357
0.225(2)	0.0357(4)	0.0342	0.633(7)	0.629	0.705(8)	0.716	0.046(1)	0.0441
0.271(1)	0.0430(5)	0.0409	0.691(7)	0.691	0.695(8)	0.708	0.057(2)	0.0536
0.326(2)	0.0518(6)	0.0499	0.740(7)	0.746	0.682(8)	0.697	0.071(2)	0.0671
0.373(2)	0.0612(4)	0.0586	0.777(9)	0.782	0.669(8)	0.685	0.086(2)	0.0811
0.428(3)	0.0714(9)	0.0699	0.803(5)	0.812	0.651(7)	0.670	0.105(2)	0.1005
0.489(1)	0.0847(4)	0.0836	0.825(5)	0.835	0.628(7)	0.649	0.131(3)	0.1270
0.544(3)	0.0971(7)	0.0971	0.834(8)	0.847	0.603(8)	0.626	0.160(4)	0.1568
0.610(3)	0.1116(7)	0.1135	0.835(6)	0.853	0.565(8)	0.592	0.204(5)	0.2010
0.681(6)	0.1290(8)	0.1309	0.826(8)	0.846	0.512(9)	0.541	0.275(7)	0.2650

Table 10. MD and LJ-EOS[51] results for the vapour-liquid equilibrium of the binary Lennard-Jones mixture F ($\varepsilon_2/\varepsilon_1 = 0.5$ and $\xi_{12} = 0.85$). The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$p / \varepsilon \sigma^{-3}$		$x''_2 / \text{mol mol}^{-1}$		ρ' / σ^{-3}		ρ'' / σ^{-3}	
	MD	EOS	MD	EOS	MD	EOS	MD	EOS
0.000	0.0138(1)	0.0139	0.000	0.000	0.743(9)	0.743	0.0167(8)	0.0168
0.012(1)	0.0273(4)	0.0279	0.446(8)	0.454	0.740(4)	0.741	0.033(1)	0.0341
0.032(1)	0.0455(5)	0.0502	0.629(5)	0.655	0.736(6)	0.737	0.058(2)	0.0642
0.048(2)	0.0591(5)	0.0689	0.688(8)	0.719	0.731(7)	0.733	0.078(2)	0.0924
0.059(2)	0.0726(4)	0.0812	0.721(6)	0.743	0.729(8)	0.731	0.099(2)	0.1129
0.084(4)	0.0947(7)	0.1104	0.758(6)	0.769	0.722(8)	0.726	0.138(3)	0.1691
0.101(3)	0.1084(6)	0.1310	0.766(7)	0.771	0.718(9)	0.723	0.165(3)	0.2159
0.110(4)	0.1248(6)	0.1419	0.769(6)	0.769	0.717(11)	0.721	0.202(4)	0.2429
0.137(3)	0.1419(8)	0.1817	0.762(5)	0.745	0.709(10)	0.717	0.246(4)	0.3435

Table 11. Interfacial properties of the binary Lennard-Jones mixture A ($\varepsilon_2/\varepsilon_1 = 0.9$ and $\xi_{12} = 1$). Results from MD and DGT. The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$\gamma / \varepsilon \sigma^{-2}$		$\Gamma_2^{(1)} / \sigma^{-2}$		E_2		L_{10}^{90} / σ	
	MD	DGT	MD	DGT	MD	DGT	MD	DGT
0.000	0.665(21)	0.663	-	-	-	-	2.91(5)	2.95
0.010(1)	0.672(30)	0.661	0.005(13)	0.003	1.2(2)	1.0	2.90(5)	2.96
0.050(1)	0.660(22)	0.650	0.015(15)	0.014	1.07(4)	1.0	2.95(4)	2.98
0.104(1)	0.645(23)	0.636	0.040(23)	0.030	1.05(2)	1.0	2.98(6)	3.02
0.150(2)	0.622(24)	0.624	0.023(4)	0.042	1.03(3)	1.0	3.01(5)	3.06
0.197(2)	0.609(22)	0.612	0.042(4)	0.055	1.03(2)	1.0	3.01(5)	3.08
0.245(3)	0.599(23)	0.600	0.08(6)	0.067	1.03(1)	1.0	3.07(5)	3.12
0.300(1)	0.577(27)	0.586	0.04(5)	0.081	1.01(1)	1.0	3.11(5)	3.16
0.347(1)	0.575(26)	0.575	0.08(6)	0.093	1.02(1)	1.0	3.17(5)	3.2
0.398(2)	0.555(25)	0.562	0.09(9)	0.105	1.02(1)	1.0	3.21(7)	3.24
0.446(2)	0.542(18)	0.551	0.14(10)	0.116	1.02(1)	1.0	3.24(6)	3.28
0.495(2)	0.528(22)	0.539	0.14(6)	0.127	1.02(1)	1.0	3.28(6)	3.32
0.550(1)	0.512(18)	0.527	0.24(9)	0.140	1.02(1)	1.0	3.33(7)	3.34
0.594(2)	0.508(22)	0.516	0.31(10)	0.149	1.02(1)	1.0	3.37(5)	3.4
0.642(2)	0.486(20)	0.505	0.22(7)	0.159	1.01(1)	1.0	3.38(6)	3.42
0.699(2)	0.481(17)	0.492	0.16(18)	0.171	1.01(1)	1.0	3.39(6)	3.48
0.752(2)	0.468(23)	0.481	0.17(16)	0.181	1.01(1)	1.0	3.50(3)	3.52
0.791(1)	0.462(16)	0.472	0.08(17)	0.189	1.01(1)	1.0	3.50(4)	3.54
0.848(2)	0.449(25)	0.459	0.22(26)	0.200	1.01(1)	1.0	3.59(7)	3.6
0.900(1)	0.435(21)	0.448	0.28(28)	0.209	1.01(1)	1.0	3.58(6)	3.64
0.950(1)	0.425(19)	0.437	0.19(42)	0.218	1.01(1)	1.0	3.64(6)	3.68
1.000	0.424(21)	0.427	-	-	-	-	3.67(8)	3.70

Table 12. Interfacial properties of the binary Lennard-Jones mixture B ($\varepsilon_2/\varepsilon_1 = 0.9$ and $\xi_{12} = 1.2$). Results from MD and DGT. The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$\gamma / \varepsilon \sigma^{-2}$		$\Gamma_2^{(1)} / \sigma^{-2}$		E_2		L_{10}^{90} / σ	
	MD	DGT	MD	DGT	MD	DGT	MD	DGT
0.000	0.665(21)	0.663	-	-	-	-	2.91(5)	2.95
0.0111(4)	0.688(28)	0.669	-0.021(8)	-0.006	1.10(8)	1.0	2.90(4)	2.94
0.0542(8)	0.714(28)	0.692	-0.022(24)	-0.026	1.06(4)	1.0	2.84(5)	2.90
0.1112(9)	0.739(24)	0.722	-0.019(19)	-0.042	1.04(1)	1.0	2.77(3)	2.84
0.1575(18)	0.749(27)	0.744	-0.05(5)	-0.048	1.04(2)	1.0	2.77(3)	2.78
0.2062(14)	0.780(26)	0.764	-0.09(5)	-0.048	1.02(1)	1.0	2.73(4)	2.74
0.2520(17)	0.789(28)	0.779	-0.03(4)	-0.042	1.03(1)	1.0	2.67(3)	2.70
0.3094(12)	0.809(29)	0.791	-0.00(6)	-0.027	1.02(1)	1.0	2.65(4)	2.68
0.3547(12)	0.811(28)	0.796	0.02(2)	-0.010	1.02(1)	1.0	2.65(4)	2.68
0.4038(15)	0.808(29)	0.796	0.10(3)	0.014	1.02(1)	1.0	2.64(5)	2.68
0.4528(14)	0.800(25)	0.790	0.09(5)	0.043	1.02(1)	1.0	2.65(5)	2.70
0.4999(9)	0.786(25)	0.778	0.05(6)	0.077	1.02(1)	1.0	2.67(4)	2.72
0.5498(12)	0.768(22)	0.760	0.17(7)	0.118	1.01(1)	1.0	2.73(3)	2.76
0.5943(13)	0.743(33)	0.739	0.21(5)	0.160	1.01(1)	1.0	2.78(3)	2.80
0.6403(15)	0.715(26)	0.713	0.25(10)	0.209	1.01(1)	1.0	2.83(5)	2.86
0.6946(8)	0.684(26)	0.677	0.29(6)	0.275	1.01(1)	1.0	2.92(6)	2.94
0.7479(11)	0.644(23)	0.637	0.27(14)	0.348	1.01(1)	1.0	3.04(3)	3.06
0.7863(18)	0.604(25)	0.606	0.38(12)	0.407	1.01(1)	1.0	3.12(6)	3.14
0.8440(13)	0.558(20)	0.558	0.51(26)	0.506	1.01(1)	1.0	3.28(8)	3.28
0.8938(8)	0.510(18)	0.515	0.68(14)	0.600	1.01(1)	1.0	3.43(7)	3.44
0.9469(10)	0.471(26)	0.470	0.64(27)	0.710	1.01(1)	1.0	3.58(7)	3.58
1.0000	0.426(21)	0.427	-	-	-	-	3.67(8)	3.70

Table 13. Interfacial properties of the binary Lennard-Jones mixture C ($\varepsilon_2/\varepsilon_1 = 0.9$ and $\xi_{12} = 0.85$). Results from MD and DGT. The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$\gamma / \varepsilon \sigma^{-2}$		$\Gamma_2^{(1)} / \sigma^{-2}$		E_2		L_{10}^{90} / σ	
	MD	DGT	MD	DGT	MD	DGT	MD	DGT
0.000	0.665(21)	0.663	-	-	-	-	2.91(5)	2.95
0.0090(4)	0.662(35)	0.649	0.01(1)	0.016	1.31(17)	1.49	2.94(5)	3.00
0.0430(10)	0.604(17)	0.597	0.07(1)	0.078	1.33(10)	1.46	3.09(7)	3.16
0.0886(17)	0.555(23)	0.539	0.18(3)	0.157	1.34(10)	1.41	3.34(6)	3.36
0.1333(12)	0.515(22)	0.493	0.23(5)	0.229	1.25(4)	1.35	3.47(7)	3.54
0.1771(18)	0.479(20)	0.457	0.23(3)	0.290	1.17(5)	1.30	3.60(7)	3.72
0.2222(25)	0.442(23)	0.428	0.36(6)	0.340	1.20(6)	1.24	3.75(7)	3.84
0.2797(41)	0.414(26)	0.401	0.38(12)	0.381	1.11(4)	1.16	3.83(6)	3.98
0.3335(46)	0.406(22)	0.383	0.37(9)	0.393	1.05(2)	1.10	3.87(6)	4.04
0.3821(31)	0.380(22)	0.371	0.28(9)	0.381	1.04(2)	1.06	3.89(8)	4.08
0.4390(25)	0.370(22)	0.361	0.24(11)	0.340	1.03(2)	1.02	3.95(7)	4.10
0.4939(51)	0.351(21)	0.353	0.38(13)	0.279	1.03(1)	1.00	3.99(7)	4.12
0.5510(25)	0.345(18)	0.347	0.15(20)	0.197	1.01(2)	1.00	3.95(4)	4.14
0.6481(37)	0.342(19)	0.343	0.26(22)	0.027	1.02(1)	1.00	3.98(8)	4.16
0.7038(9)	0.342(15)	0.343	-0.13(13)	-0.084	1.01(1)	1.00	4.02(7)	4.14
0.7647(17)	0.338(21)	0.348	-0.14(27)	-0.213	1.01(1)	1.00	4.03(8)	4.12
0.8007(18)	0.354(25)	0.353	-0.09(20)	-0.293	1.01(1)	1.00	3.95(7)	4.12
0.8575(23)	0.366(20)	0.365	-0.04(32)	-0.421	1.01(1)	1.00	3.91(7)	4.06
0.9085(25)	0.373(15)	0.382	-1.25(30)	-0.536	1.01(1)	1.00	3.89(7)	3.96
0.9548(9)	0.393(24)	0.402	-0.72(63)	-0.639	1.01(1)	1.00	3.75(7)	3.86
1.0000	0.423(21)	0.427	-	-	-	-	3.67(8)	3.70

Table 14. Interfacial properties of the binary Lennard-Jones mixture D ($\varepsilon_2/\varepsilon_1 = 0.5$ and $\xi_{12} = 1$). Results from MD and DGT. The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$\gamma / \varepsilon \sigma^{-2}$		$\Gamma_2^{(1)} / \sigma^{-2}$		E_2		L_{10}^{90} / σ	
	MD	DGT	MD	DGT	MD	DGT	MD	DGT
0.000	0.665(21)	0.663	-	-	-	-	2.91(5)	2.95
0.015(1)	0.625(21)	0.620	0.05(1)	0.047	2.2(3)	2.26	3.08(6)	3.06
0.051(1)	0.540(20)	0.529	0.13(2)	0.139	1.8(1)	1.98	3.42(5)	3.38
0.099(2)	0.424(18)	0.427	0.26(3)	0.238	1.68(4)	1.72	3.99(8)	3.80
0.136(3)	0.354(13)	0.360	0.33(4)	0.302	1.52(3)	1.57	4.47(8)	4.18
0.176(3)	0.286(15)	0.296	0.38(4)	0.361	1.40(4)	1.44	5.0(2)	4.64
0.228(4)	0.206(17)	0.226	0.52(6)	0.423	1.30(4)	1.32	5.9(2)	5.34
0.253(3)	0.185(14)	0.196	0.48(3)	0.446	1.24(2)	1.27	6.2(2)	5.72
0.314(9)	0.133(13)	0.135	0.45(11)	0.488	1.14(2)	1.17	7.2(3)	6.82
0.332(6)	0.118(14)	0.119	0.49(9)	0.495	1.12(2)	1.14	7.7(3)	7.22
0.391(6)	0.073(13)	0.076	0.48(5)	0.511	1.06(1)	1.08	9.4(8)	8.76
0.424(3)	0.051(12)	0.056	0.42(7)	0.503	1.04(1)	1.05	10.5(12)	9.86
0.467(6)	0.036(15)	0.034	0.42(10)	0.472	1.03(1)	1.02	13.4(21)	12.00
0.498(15)	0.026(15)	0.023	0.30(17)	0.430	1.02(2)	1.01	14.8(35)	13.90

Table 15. Interfacial properties of the binary Lennard-Jones mixture E ($\varepsilon_2/\varepsilon_1 = 0.5$ and $\xi_{12} = 1.2$). Results from MD and DGT. The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$\gamma / \varepsilon \sigma^{-2}$		$\Gamma_2^{(1)} / \sigma^{-2}$		E_2		L_{10}^{90} / σ	
	MD	DGT	MD	DGT	MD	DGT	MD	DGT
0.000	0.665(21)	0.663	-	-	-	-	2.91(5)	2.95
0.032(1)	0.634(3)	0.637	0.013(14)	0.028	1.1(1)	1.03	3.03(3)	3.02
0.071(2)	0.592(16)	0.603	0.09(2)	0.060	1.2(1)	1.01	3.19(5)	3.14
0.127(1)	0.530(18)	0.551	0.14(3)	0.107	1.09(3)	1.00	3.36(6)	3.30
0.175(1)	0.469(20)	0.504	0.15(3)	0.147	1.05(2)	1.00	3.60(6)	3.48
0.225(2)	0.419(19)	0.453	0.19(4)	0.188	1.03(1)	1.00	3.77(4)	3.70
0.271(1)	0.362(14)	0.403	0.23(5)	0.227	1.03(1)	1.00	4.04(7)	3.94
0.326(2)	0.300(15)	0.343	0.25(4)	0.272	1.02(1)	1.00	4.43(6)	4.28
0.373(2)	0.250(13)	0.291	0.28(5)	0.310	1.01(1)	1.00	4.91(11)	4.64
0.428(3)	0.199(15)	0.231	0.31(8)	0.350	1.01(1)	1.00	5.5(2)	5.20
0.489(1)	0.134(12)	0.168	0.36(5)	0.388	1.01(1)	1.00	6.4(3)	6.02
0.544(3)	0.091(11)	0.116	0.31(6)	0.408	1.01(1)	1.00	7.4(3)	7.10
0.610(3)	0.054(9)	0.063	0.33(6)	0.397	1.01(1)	1.00	9.9(6)	9.10
0.681(6)	0.020(13)	0.023	0.29(8)	0.291	1.01(1)	1.00	16.1(26)	12.68

Table 16. Interfacial properties of the binary Lennard-Jones mixture F ($\varepsilon_2/\varepsilon_1 = 0.5$ and $\xi_{12} = 0.85$). Results from MD and DGT. The number in the parentheses indicates the statistical uncertainty in the last decimal digit. The temperature is $T = 0.92 \varepsilon k_B^{-1}$.

$x'_2 / \text{mol mol}^{-1}$	$\gamma / \varepsilon \sigma^{-2}$		$\Gamma_2^{(1)} / \sigma^{-2}$		E_2		L_{10}^{90} / σ	
	MD	DGT	MD	DGT	MD	DGT	MD	DGT
0.000	0.665(21)	0.663	-	-	-	-	2.91(5)	2.95
0.012(1)	0.600(16)	0.587	0.07(1)	0.082	2.45(7)	3.18	3.15(5)	3.14
0.032(1)	0.519(17)	0.477	0.16(2)	0.199	2.22(3)	2.71	3.59(7)	3.52
0.048(2)	0.455(15)	0.394	0.21(2)	0.284	2.04(5)	2.38	3.92(7)	3.90
0.059(2)	0.400(18)	0.345	0.31(3)	0.333	1.91(4)	2.18	4.38(9)	4.18
0.084(4)	0.311(16)	0.242	0.38(3)	0.418	1.67(3)	1.77	5.1(1)	4.94
0.101(3)	0.268(20)	0.184	0.45(3)	0.443	1.56(2)	1.53	5.8(1)	5.50
0.110(4)	0.207(21)	0.158	0.53(5)	0.432	1.40(2)	1.42	6.6(3)	5.74
0.137(3)	0.166(14)	0.091	0.49(4)	0.322	1.28(1)	1.15	7.3(4)	6.14