Supplementary Information for

Revisiting volumes of lipid components in bilayers

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A. Volume data (in Å^3/molecule) for saturated diCn:0PC lipids

T	DLPC	DMPC	DPPC
ºC	diC12:0	diC14:0	diC16:0
19.999	986.30373	1049.50373	1143.484
20.499	986.01397	1050.1329	1143.95901
21	986.01248	1050.98859	1144.40816
21.499	986.11542	1051.90126	1144.88889
22	986.22217	1052.73482	1145.34374
22.5	986.4603	1053.68202	1145.80093
22.999	986.77809	1054.74294	1146.29082
23.499	987.04704	1056.05788	1146.78413
24	987.39573	1086.33666	1147.24943
24.499	987.69556	1088.30971	1147.71816
25	988.02334	1089.69966	1148.21964
25.5	988.25321	1090.7336	1148.6062
26	988.71189	1091.84666	1149.23085
26.499	989.0727	1092.79896	1149.74059
27	989.3846	1093.61518	1150.22337
27.5	989.77549	1094.37695	1150.73791
28	990.11747	1095.11435	1151.25595
28.5	990.48845	1095.7434	1151.74704
28.999	990.86056	1096.40184	1152.30039
29.501	991.20972	1097.03584	1152.79633
30	991.58696	1097.6443	1153.32518
30.499	991.9663	1098.22721	1153.85648
31	992.34774	1098.84062	1154.39024

31.501	992.70622	1099.4015	1154.92756
32.001	993.11791	1100.07598	1155.52732
32.5	993.4806	1100.58569	1156.19179
33	993.87145	1101.12591	1156.85882
33.501	994.2123	1101.64051	1157.6507
33.999	994.60643	1102.15647	1159.02513
34.499	994.97758	1102.73217	1160.70973
34.999	995.35085	1103.25415	1162.21413
35.499	995.80456	1103.75046	1163.38503
36	996.18212	1104.27736	1164.13014
36.499	996.5357	1104.86302	1164.81666
36.999	996.91753	1105.25412	1165.53649
37.5	997.27536	1105.73211	1166.19768
37.999	997.66051	1106.23964	1166.95243
38.499	998.02263	1106.69435	1167.71102
39	998.41208	1107.20683	1168.50194
39.499	998.80467	1107.63825	1169.35817
40	999.17227	1108.15568	1170.27758
40.499	999.3324	1108.59091	1171.41508
41	999.70422	1109.08507	1173.38612
41.5	1000.05198	1109.58173	1215.8513
42	1000.45436	1109.99608	1217.17186
42.499	1000.8317	1110.46833	1218.21671
43	1001.23845	1110.94417	1219.04971
43.501	1001.59389	1111.39309	1219.82272
44.001	1001.95149	1111.87281	1220.56779
44.5	1002.36286	1112.35393	1221.28368
45	1002.69852	1112.78198	1221.91089
45.5	1003.08797	1113.18303	1222.53975
46.001	1003.47963	1113.7 1223.14052	
46.5	1003.87251	1114.2468	1223.77393
47	1004.24125	1114.6826	1224.37922
47.501	1004.61218	1115.1777	1224.92535
48.001	1004.9853	1115.59009	1225.50535
48.5	1005.35964	1116.00385	1226.11804
49.001	1005.73618	1116.47696	1226.67149
49.501	1006.11493	1116.92415	1227.22779
50	1006.46947	1117.34538	1227.75585
50.501	1006.90353	1117.82385	1228.31538
51.001	1007.23505	1118.24898	1228.78564

51.501	1007.62069	1118.67549	1229.31973
52.001	1007.98207	1119.07599	1229.82551
52.5	1008.2927	1119.5075	1230.33412
53	1008.71049	1119.94041	1230.8755
53.501	1009.10304	1120.40329	1231.51211
54.001	1009.47131	1120.86872	1231.99561
54.501	1009.86833	1121.30811	1232.54439
55.001	1010.21452	1121.69281	1233.03355
55.501	1010.6406	1122.19225	1233.58558
56.001	1010.99024	1122.58085	1234.14176
56.501	1011.3411	1122.99948	1234.637
57.001	1011.74639	1123.47684	1235.19646
57.501	1012.10071	1123.89941	1235.75884
58.001	1012.45726	1124.29583	1236.32413
58.501	1012.84168	1124.72233	1236.98519
59.001	1013.17504	1125.15138	1237.61791
59.501	1013.58863	1125.6382	1238.34531
60.001	1013.92545	1126.04249	1239.01426
60.5	1014.26032	1126.44817	1239.52785
61.001	1014.65157	1126.88404	1239.98019
61.5	1015.01841	1127.32247	1240.27804
62.001	1015.33411	1128.25343	1240.54707
62.501	1015.73112	1128.17708	1240.91197
63.001	1016.12941	1128.56325	1241.27835
63.501	1016.44977	1128.9808	1241.679
64.001	1016.85158	1129.42866	1242.11272
64.501	1017.22792	1129.87797	1242.61113
65.001	1017.57975	1130.30096	1243.04927
65.501	1017.93381	1130.72652	1243.55344
66	1018.31492	1131.15238	1244.02637
66.501	1018.67249	1131.55298	1244.44016
67.001	1019.05714	1132.01182	1244.98085
67.501	1019.41722	1132.44428	1245.46115
68.001	1019.77955	1132.85031	1245.94434
68.501	1020.19591	1133.31468	1246.4596
69	1020.53389	1133.72359	1246.94606
69.502	1020.90102	1134.13507	1247.43543
69.999	1021.24248	1134.51889	1247.92644

B. Expanded lipid simulation system details with some properties.

Lipid	Chains[a]	T °C	N_{LIPIDS}	N_{WATERS}	<A>[b] (Å^2)	<c>[c] (Å)
DLPC	12:0	30	72	2880	63.6 (3)	68.5 (3)
		50			66.2 (2)	67.0 (3)
		70			67.7 (2)	66.8 (2)
DMPC	14:0	30[d]	72	1848	63.0 (4)	59.0 (4)
		50[d]			65.3 (3)	58.0 (2)
		70[d]			67.0 (3)	57.6 (2)
DPPC	16:0	50[d]	72	2189	62.4 (2)	68.7 (2)
		70			66.2 (4)	66.6 (4)
DMOPC	14:1 (9-10)	25	80	3040	68.8 (1)	64.0 (1)
		45			70.4 (1)	63.7 (1)
		65			72.1 (1)	63.4 (1)
DOPC	18:1 (9-10)	25[d]	80	3040	69.0 (2)	70.4 (2)
		45[d]			70.8 (1)	69.5 (3)
		45			70.9 (2)	69.6 (2)
		65[d]			73.3 (1)	68.6 (1)
DEPC	22:1 (13-14)	25	80	3600	65.5 (2)	87.0 (3)
		45			68.4 (2)	84.9 (3)
		65			71.1 (2)	83.4 (3)
MLG	12:0	30	162	2891	33.0 (1)	61.9 (1)
		50			34.6 (1)	60.2 (1)
		70			36.1 (1)	58.9 (1)

[a] Both chains are the same; C=C bond positions are indicated as e.g. (9-10).

[b] Average area/lipid for the last 100 ns; the uncertainty in the last digit is in parentheses.

[c] Average unit cell height for the last 100 ns.

[d] These simulations had $\kappa = 0.32$, the others used $\kappa = 0.34$; DOPC at 45 °C was run twice.

C. Some details regarding component excluded volumes

The following table TS gives the radii for the excluded volumes around atoms. Obtained from the CHARMM potentials.[1]

Atom	σ/2 (Å)
H, alkane CH2	1.194
H, alkane CH3	1.194
polar H for choline CH3	0.624
alkene, vinyl H	1.114
carbonyl C	1.782
C, alkane CH2	1.791
C, alkane CH3	1.817
C, choline CH3	1.835
alkene C	1.862
carbonyl =O	1.515
PO4 =O	1.515
ester -O-	1.470
PO4 -O-	1.470
quaternary N	1.648
PO4 P atom	1.915

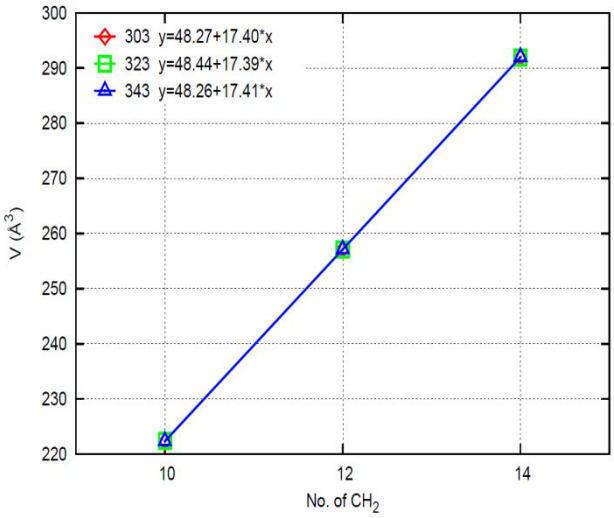

Fig. S1 shows the results of the SIM-0 method applied to alkane excluded volume. The legend shows each temperature (in Kelvin) followed by the linear fit where the intercept is twice the methyl excluded volume and the slope is the methylene excluded volume. Note the negligible temperature difference.

D. SIM-2 results for monolaurin glyceride (MLG)

T(°C)	CH_2	r	esters 2COH	head $C_2O_2H_3$	V_H esters+head	V_L total
30	27.894	1.98125	69.658	79.569	149.227	483.432
50	28.395	2.05487	71.128	80.974	152.102	494.4
70	28.895	2.13899	72.461	82.876	155.337	506.093

E. Results of modified force field cutoffs for alkanes

Figure S1 adds two SIM-1 alkane results to Figs. 6 and 9 in the text. The first result is designated LR, for "Long-Range, (solid squares) in the legends. These calculations utilized a recently developed method for summing the Lennard-Jones interactions to infinity similarly to particle mesh Ewald that is now available in CHARMM.[2] Unfortunately, inclusion of long-range L-D interactions requires reparameterizing the force field and is not presently implemented for lipids. Hence, the effect of long-rang L-J interactions is only shown for the alkanes. The second result is designated LJ10-12 (downward pointing trianges) in the legends; these simulations tapered the Leonard-Jones cutoff from 10 to 12 Å instead of from 8 to 12 Å as was done for all the results in the main text. While tapering the LJ cutoff makes a small difference, a larger difference results from using the LR procedure which agrees much better with experiment.

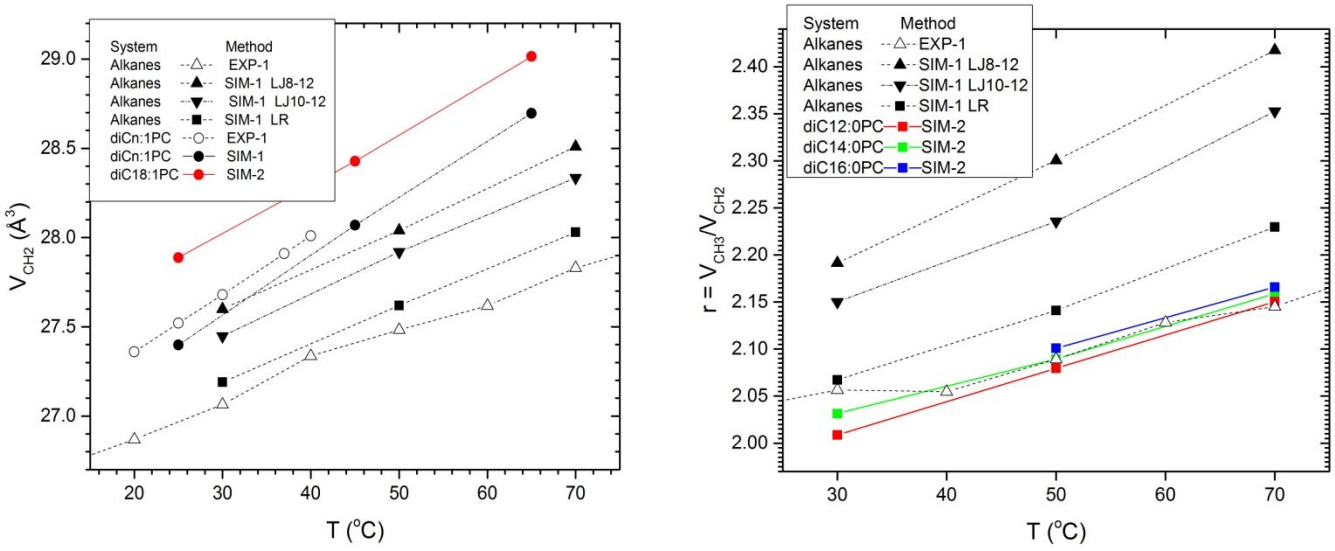

Fig. S2. Effect of cutoffs on alkane methylene volume and on *r*.

Bibliography

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2. Leonard, A. N.; Simmonett, A. C.; Pickard, F. C.; Huang, J.; Venable, R. M.; Klauda, J. B.; Brooks, B. R.; Pastor, R. W., Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. *J Chem Theory Comput* **2018,** *14* (2), 948-958.