Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Molecular dynamics simulations of discotic ionic liquid crystals: comparison of a full-charge and a scaled-charge force field

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Electronic Supporting Information

Reference pdb structure of the cation of **2[BF_4]** salt with atom names as in Table S1

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ATOM     3 C02 LC  X  1    62.110  6.590 10.950 0.00 0.00
ATOM     4 C03 LC  X  1    61.310  5.530 10.570 0.00 0.00
ATOM     5 C04 LC  X  1    59.910  5.700 10.580 0.00 0.00
ATOM     6 C05 LC  X  1    59.350  6.950 10.870 0.00 0.00
ATOM     7 O06 LC  X  1    62.380  8.890 11.520 0.00 0.00
ATOM     8 C07 LC  X  1    61.520  9.950 11.720 0.00 0.00
ATOM     9 C08 LC  X  1    62.320 11.170 12.070 0.00 0.00
ATOM    10 C09 LC  X  1    61.390 12.330 12.300 0.00 0.00
ATOM    11 C0A LC  X  1    62.190 13.550 12.630 0.00 0.00
ATOM    12 C0B LC  X  1    61.270 14.700 12.860 0.00 0.00
ATOM    13 C0C LC  X  1    62.060 15.930 13.210 0.00 0.00
ATOM    14 C0D LC  X  1    61.130 17.090 13.420 0.00 0.00
ATOM    15 C0E LC  X  1    61.860 18.240 13.690 0.00 0.00
ATOM    16 C0F LC  X  1    60.990 19.460 13.990 0.00 0.00
ATOM    17 C0G LC  X  1    61.790 20.690 14.340 0.00 0.00
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ATOM    26 C0Q LC  X  1    69.530 10.170 12.260 0.00 0.00
ATOM    27 C0R LC  X  1    70.080 11.520 12.620 0.00 0.00
ATOM    28 C0S LC  X  1    71.580 11.460 12.700 0.00 0.00
ATOM    29 C0T LC  X  1    72.120 12.820 13.050 0.00 0.00
ATOM    30 C0U LC  X  1    73.610 12.750 13.120 0.00 0.00
ATOM    31 C0V LC  X  1    74.150 14.100 13.480 0.00 0.00
ATOM    32 C0W LC  X  1    75.650 14.040 13.560 0.00 0.00
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ATOM    34 N0Y LC  X  1    58.200  4.980  8.990 0.00 0.00
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ATOM    52 C1G LC  X  1    57.260  3.860  8.620 0.00 0.00
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ATOM    61 H1Q LC  X  1    57.940  8.520 12.060 0.00 0.00
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ATOM    63 H1S LC  X  1    65.850  7.300 10.450 0.00 0.00
ATOM    64 H1T LC  X  1    65.710  9.660 11.010 0.00 0.00
ATOM    65 H1U LC  X  1    65.600  9.240 12.710 0.00 0.00
ATOM    66 H1V LC  X  1    67.780  8.180 12.590 0.00 0.00
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ATOM   69 H1Y LC X  1    67.640 10.540 13.140 0.00 0.00
ATOM   70 H1Z LC X  1    69.820  9.470 13.010 0.00 0.00
ATOM   71 H20 LC X  1    69.920  9.860 11.320 0.00 0.00
ATOM   72 H21 LC X  1    69.790 12.240 11.870 0.00 0.00
ATOM   73 H22 LC X  1    69.680 11.830 13.570 0.00 0.00
ATOM   74 H23 LC X  1    71.860 10.750 13.440 0.00 0.00
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ATOM   80 H29 LC X  1    62.890 11.000 12.960 0.00 0.00
ATOM   81 H2A LC X  1    62.990 11.410 11.260 0.00 0.00
ATOM   82 H2B LC X  1    60.830 12.520 11.410 0.00 0.00
ATOM   83 H2C LC X  1    60.730 12.090 13.110 0.00 0.00
ATOM   84 H2D LC X  1    62.760 13.380 13.530 0.00 0.00
ATOM   85 H2E LC X  1    62.850 13.780 11.820 0.00 0.00
ATOM   86 H2F LC X  1    60.690 14.880 11.970 0.00 0.00
ATOM   87 H2G LC X  1    60.600 14.480 13.670 0.00 0.00
ATOM   88 H2H LC X  1    62.620 15.750 14.100 0.00 0.00
ATOM   89 H2I LC X  1    62.730 16.160 12.390 0.00 0.00
ATOM   90 H2J LC X  1    60.560 17.260 12.530 0.00 0.00
ATOM   91 H2K LC X  1    60.470 16.850 14.240 0.00 0.00
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ATOM   93 H2N LC X  1    62.580 18.540 12.940 0.00 0.00
ATOM   94 H2O LC X  1    60.420 19.650 13.100 0.00 0.00
ATOM   95 H2P LC X  1    60.330 19.230 14.800 0.00 0.00
ATOM   96 H2Q LC X  1    62.350 20.510 15.210 0.00 0.00
ATOM   97 H2R LC X  1    62.460 20.920 13.520 0.00 0.00
ATOM   98 H2S LC X  1    58.030 10.890 12.610 0.00 0.00
ATOM   99 H2T LC X  1    58.140 11.280 10.920 0.00 0.00
ATOM  100 H2U LC X  1    55.980 10.250 10.540 0.00 0.00
ATOM  101 H2V LC X  1    55.880  9.830 12.240 0.00 0.00
ATOM  102 H2W LC X  1    55.980 12.190 12.810 0.00 0.00
ATOM  103 H2X LC X  1    56.080 12.600 11.120 0.00 0.00
ATOM  104 H2Y LC X  1    53.930 11.550 10.730 0.00 0.00
ATOM  105 H2Z LC X  1    53.810 11.160 12.430 0.00 0.00
ATOM  106 H30 LC X  1    53.920 13.510 12.990 0.00 0.00
ATOM  107 H31 LC X  1    54.030 13.920 11.290 0.00 0.00
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ATOM  109 H33 LC X  1    51.760 12.470 12.610 0.00 0.00
ATOM  110 H34 LC X  1    51.860 14.820 13.180 0.00 0.00
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ATOM  112 H36 LC X  1    49.810 14.190 11.090 0.00 0.00
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ATOM  117 H3B LC X  1    58.290  4.410 11.020 0.00 0.00
ATOM  118 H3C LC X  1    56.710  4.140  7.740 0.00 0.00
ATOM  119 H3D LC X  1    57.820  2.970  8.420 0.00 0.00
ATOM  120 H3E LC X  1    56.730  6.040 10.060 0.00 0.00
ATOM  121 H3F LC X  1    58.090  7.020  9.530 0.00 0.00
ATOM  122 H3G LC X  1    58.600  5.490  6.990 0.00 0.00
ATOM  123 H3H LC X  1    59.820  6.020  8.110 0.00 0.00
ATOM  124 H3I LC X  1    60.310 22.030 13.660 0.00 0.00
ATOM  125 H3J LC X  1    60.200 21.630 15.350 0.00 0.00
ATOM  126 H3K LC X  1    61.000 23.900 15.050 0.00 0.00
ATOM  127 H3M LC X  1    62.230 22.890 15.790 0.00 0.00
ATOM  128 H3N LC X  1    62.330 23.300 14.080 0.00 0.00
ATOM  129 H3O LC X  1    73.860 14.810 12.730 0.00 0.00
ATOM  130 H3P LC X  1    73.750 14.410 14.430 0.00 0.00
ATOM  131 H3Q LC X  1    76.030 15.010 13.820 0.00 0.00
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ATOM  138 H3X LC X  1    47.860 17.870 11.840 0.00 0.00
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END

Table S1. FF parameters obtained from the LigParGen web site[1]

name	Mass / a.u.	ε / kJmol^{-1}	σ / nm	q / e
C00	12.0110	3.55000E-01	2.92880E-01	0.3271
C01	12.0110	3.55000E-01	2.92880E-01	0.0099
C02	12.0110	3.55000E-01	2.92880E-01	0.3271
C03	12.0110	3.55000E-01	2.92880E-01	-0.3970
C04	12.0110	3.55000E-01	2.92880E-01	0.1075
C05	12.0110	3.55000E-01	2.92880E-01	-0.3970
O06	15.9990	2.90000E-01	5.85760E-01	-0.3624
C07	12.0110	3.50000E-01	2.76144E-01	0.2313
C08	12.0110	3.50000E-01	2.76144E-01	-0.1006
C09	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0A	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0B	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0C	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0D	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0E	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0F	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0G	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0H	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0I	12.0110	3.50000E-01	2.76144E-01	-0.2220
O0J	15.9990	2.90000E-01	5.85760E-01	-0.2994
C0K	12.0110	3.50000E-01	2.76144E-01	0.3207
C0M	12.0110	3.50000E-01	2.76144E-01	-0.2190
C0N	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0O	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0P	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0Q	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0R	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0S	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0T	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0U	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0V	12.0110	3.50000E-01	2.76144E-01	-0.1480
C0W	12.0110	3.50000E-01	2.76144E-01	-0.2220
C0X	12.0110	3.50000E-01	2.76144E-01	-0.0079
N0Y	14.0070	3.25000E-01	7.11280E-01	0.2035
C0Z	12.0110	3.50000E-01	2.76144E-01	-0.2118
H10	1.0080	2.50000E-01	1.25520E-01	0.1261
O11	15.9990	2.90000E-01	5.85760E-01	-0.2994
C12	12.0110	3.50000E-01	2.76144E-01	0.3207
C13	12.0110	3.50000E-01	2.76144E-01	-0.2190
C14	12.0110	3.50000E-01	2.76144E-01	-0.1480
C15	12.0110	3.50000E-01	2.76144E-01	-0.1480
C16	12.0110	3.50000E-01	2.76144E-01	-0.1480
C17	12.0110	3.50000E-01	2.76144E-01	-0.1480
C18	12.0110	3.50000E-01	2.76144E-01	-0.1480
C19	12.0110	3.50000E-01	2.76144E-01	-0.1480
C1A	12.0110	3.50000E-01	2.76144E-01	-0.1480
C1B	12.0110	3.50000E-01	2.76144E-01	-0.1480
C1C	12.0110	3.50000E-01	2.76144E-01	-0.1480
C1D	12.0110	3.50000E-01	2.76144E-01	-0.2220
C1E	12.0110	3.50000E-01	2.76144E-01	-0.2118
H1F	1.0080	2.50000E-01	1.25520E-01	0.1261
C1G	12.0110	3.50000E-01	2.76144E-01	-0.2118
H1H	1.0080	2.50000E-01	1.25520E-01	0.1261
H1I	1.0080	2.42000E-01	1.25520E-01	0.1443
H1J	1.0080	2.42000E-01	1.25520E-01	0.1443
H1K	1.0080	2.50000E-01	1.25520E-01	-0.0101
H1M	1.0080	2.50000E-01	1.25520E-01	-0.0101
H1N	1.0080	2.50000E-01	1.25520E-01	-0.0012
H1O	1.0080	2.50000E-01	1.25520E-01	-0.0012
H1P	1.0080	2.50000E-01	1.25520E-01	-0.0101

H1Q	1.0080	2.50000E-01	1.25520E-01	-0.0101
H1R	1.0080	2.50000E-01	1.25520E-01	0.1095
H1S	1.0080	2.50000E-01	1.25520E-01	0.1095
H1T	1.0080	2.50000E-01	1.10000E-01	0.0740
H1U	1.0080	2.50000E-01	1.10000E-01	0.0740
H1V	1.0080	2.50000E-01	1.10000E-01	0.0740
H1W	1.0080	2.50000E-01	1.10000E-01	0.0740
H1X	1.0080	2.50000E-01	1.10000E-01	0.0740
H1Y	1.0080	2.50000E-01	1.10000E-01	0.0740
H1Z	1.0080	2.50000E-01	1.10000E-01	0.0740
H20	1.0080	2.50000E-01	1.10000E-01	0.0740
H21	1.0080	2.50000E-01	1.10000E-01	0.0740
H22	1.0080	2.50000E-01	1.10000E-01	0.0740
H23	1.0080	2.50000E-01	1.10000E-01	0.0740
H24	1.0080	2.50000E-01	1.10000E-01	0.0740
H25	1.0080	2.50000E-01	1.10000E-01	0.0740
H26	1.0080	2.50000E-01	1.10000E-01	0.0740
H27	1.0080	2.50000E-01	1.10000E-01	0.0740
H28	1.0080	2.50000E-01	1.10000E-01	0.0740
H29	1.0080	2.50000E-01	1.25520E-01	0.0503
H2A	1.0080	2.50000E-01	1.25520E-01	0.0503
H2B	1.0080	2.50000E-01	1.10000E-01	0.0740
H2C	1.0080	2.50000E-01	1.10000E-01	0.0740
H2D	1.0080	2.50000E-01	1.10000E-01	0.0740
H2E	1.0080	2.50000E-01	1.10000E-01	0.0740
H2F	1.0080	2.50000E-01	1.10000E-01	0.0740
H2G	1.0080	2.50000E-01	1.10000E-01	0.0740
H2H	1.0080	2.50000E-01	1.10000E-01	0.0740
H2I	1.0080	2.50000E-01	1.10000E-01	0.0740
H2J	1.0080	2.50000E-01	1.10000E-01	0.0740
H2K	1.0080	2.50000E-01	1.10000E-01	0.0740
H2M	1.0080	2.50000E-01	1.10000E-01	0.0740
H2N	1.0080	2.50000E-01	1.10000E-01	0.0740
H2O	1.0080	2.50000E-01	1.10000E-01	0.0740
H2P	1.0080	2.50000E-01	1.10000E-01	0.0740
H2Q	1.0080	2.50000E-01	1.10000E-01	0.0740
H2R	1.0080	2.50000E-01	1.10000E-01	0.0740
H2S	1.0080	2.50000E-01	1.25520E-01	0.1095
H2T	1.0080	2.50000E-01	1.25520E-01	0.1095
H2U	1.0080	2.50000E-01	1.10000E-01	0.0740
H2V	1.0080	2.50000E-01	1.10000E-01	0.0740
H2W	1.0080	2.50000E-01	1.10000E-01	0.0740
H2X	1.0080	2.50000E-01	1.10000E-01	0.0740
H2Y	1.0080	2.50000E-01	1.10000E-01	0.0740
H2Z	1.0080	2.50000E-01	1.10000E-01	0.0740
H30	1.0080	2.50000E-01	1.10000E-01	0.0740
H31	1.0080	2.50000E-01	1.10000E-01	0.0740
H32	1.0080	2.50000E-01	1.10000E-01	0.0740
H33	1.0080	2.50000E-01	1.10000E-01	0.0740
H34	1.0080	2.50000E-01	1.10000E-01	0.0740
H35	1.0080	2.50000E-01	1.10000E-01	0.0740
H36	1.0080	2.50000E-01	1.10000E-01	0.0740
H37	1.0080	2.50000E-01	1.10000E-01	0.0740
H38	1.0080	2.50000E-01	1.10000E-01	0.0740
H39	1.0080	2.50000E-01	1.10000E-01	0.0740
H3A	1.0080	2.50000E-01	1.25520E-01	0.0850
H3B	1.0080	2.50000E-01	1.25520E-01	0.0850
H3C	1.0080	2.50000E-01	1.25520E-01	0.1261
H3D	1.0080	2.50000E-01	1.25520E-01	0.1261
H3E	1.0080	2.50000E-01	1.25520E-01	0.1261
H3F	1.0080	2.50000E-01	1.25520E-01	0.1261
H3G	1.0080	2.50000E-01	1.25520E-01	0.1261
H3H	1.0080	2.50000E-01	1.25520E-01	0.1261
H3I	1.0080	2.50000E-01	1.10000E-01	0.0740
H3J	1.0080	2.50000E-01	1.10000E-01	0.0740
H3K	1.0080	2.50000E-01	1.10000E-01	0.0740
H3M	1.0080	2.50000E-01	1.10000E-01	0.0740
H3N	1.0080	2.50000E-01	1.10000E-01	0.0740

H3O	1.0080	2.50000E-01	1.10000E-01	0.0740
H3P	1.0080	2.50000E-01	1.10000E-01	0.0740
H3Q	1.0080	2.50000E-01	1.10000E-01	0.0740
H3R	1.0080	2.50000E-01	1.10000E-01	0.0740
H3S	1.0080	2.50000E-01	1.10000E-01	0.0740
H3T	1.0080	2.50000E-01	1.10000E-01	0.0740
H3U	1.0080	2.50000E-01	1.10000E-01	0.0740
H3V	1.0080	2.50000E-01	1.25520E-01	0.0740
H3W	1.0080	2.50000E-01	1.10000E-01	0.0740
H3X	1.0080	2.50000E-01	1.10000E-01	0.0740
B	10.810	0.355000	0.29288	1.177448
F	18.9984	0.31181	0.25522	-0.544362

[1] a) Potential energy functions for atomic-level simulations of water and organic and biomolecular systems. Jorgensen, W. L.; Tirado-Rives, J. Proc. Nat. Acad. Sci. USA 2005, 102, 6665-6670

b) 1.14*CM1A-LBCC: Localized Bond-Charge Corrected CM1A Charges for Condensed-Phase Simulations. Dodda, L. S.; Vilseck, J. Z.; Tirado-Rives, J.; Jorgensen, W. L. J. Phys. Chem. B, 2017, 121 (15), pp 3864-3870

c) LigParGen web server: An automatic OPLS-AA parameter generator for organic ligands. Dodda, L. S.;Cabeza de Vaca, I.; Tirado-Rives, J.; Jorgensen, W. L. Nucleic Acids Research, Volume 45, Issue W1, 3 July 2017, Pages W331-W336

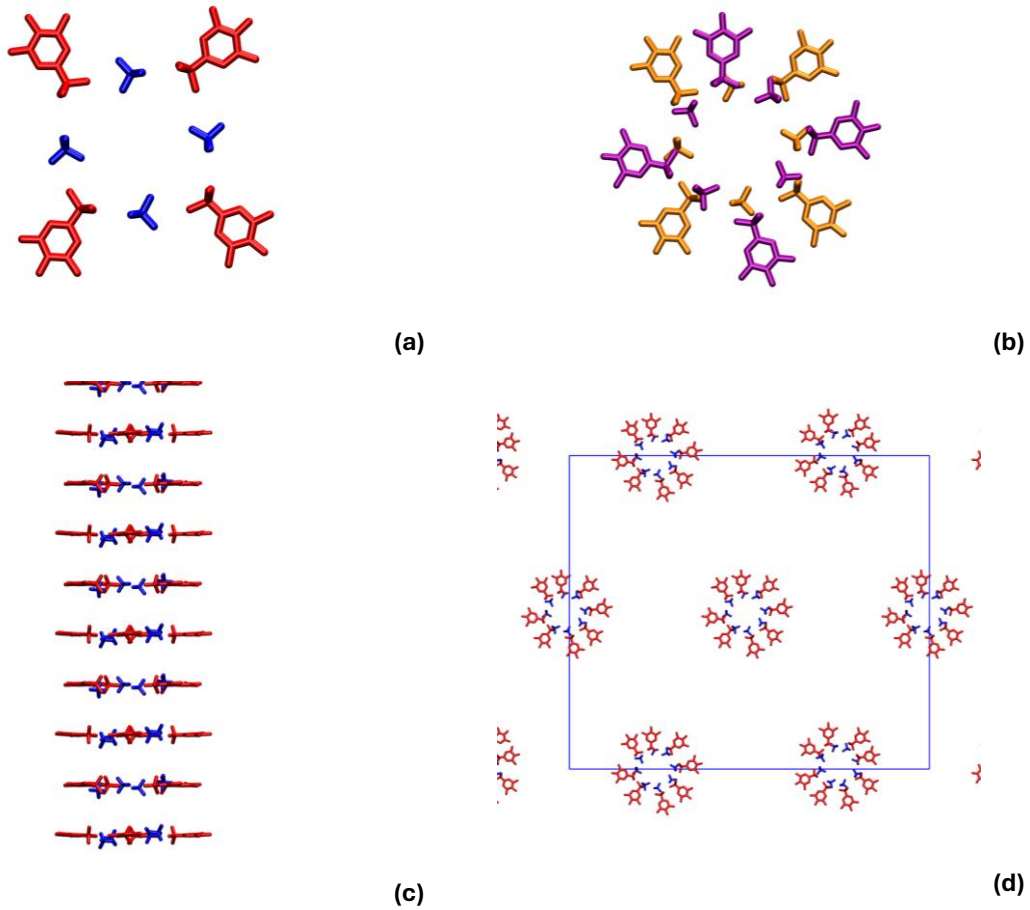


Figure S1. Discotic unit composed of 4 gallic acid derivatives (this example for compound **1** in Figure 1 of the main text) and 4 tetrafluoroborate anions, (a), respectively represented as red and blue sticks. Two discotic units stacked one on top of the other, (b), with the orange unit being below the purple one. Multiple stacked disks forming the column, (c), with the same color code of (a). Hexagonal arrangement of the columns seen from above with the simulation box indicated as blue line and with the closest periodic images represented, (d). In all these images the alkyl chains are not shown for the sake of clarity.

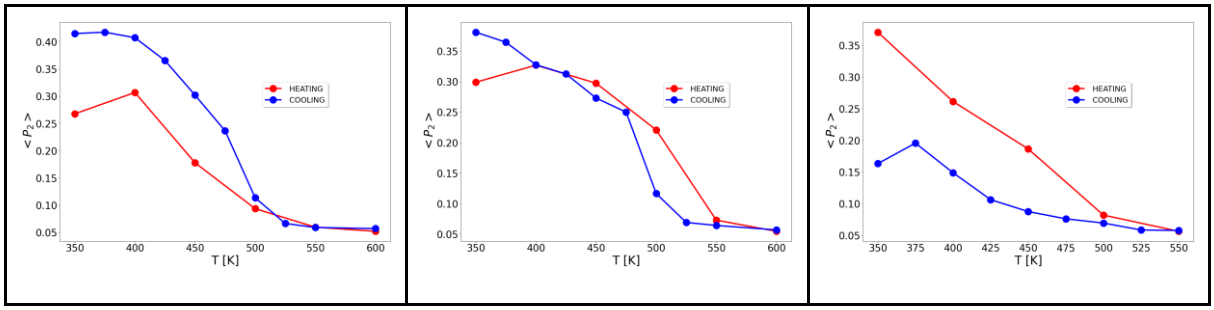


Figure S2. Orientational order parameters, <P_2>, in heating (red circles) and cooling (blue circles) run. The lines are a guide to the eye. From left to right: **1[BF_4]**, **2[BF_4]** and **3[BF_4]**. Small boxes made of 320 ion pars.

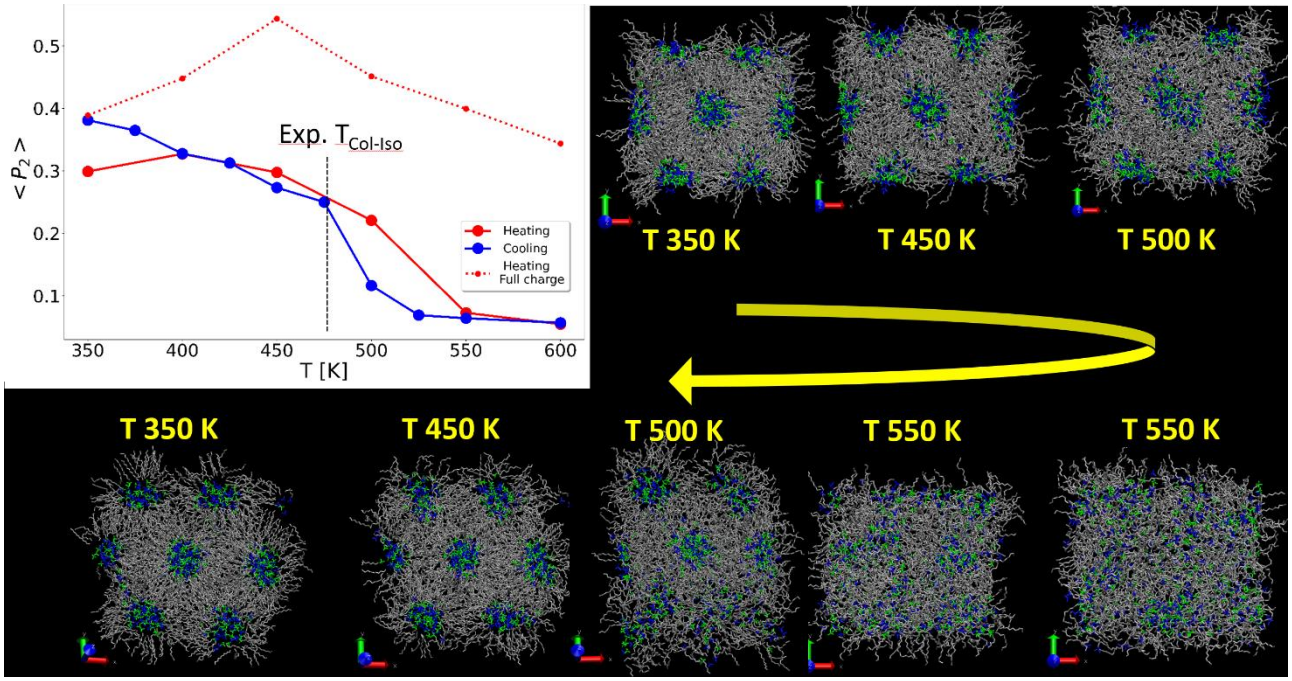
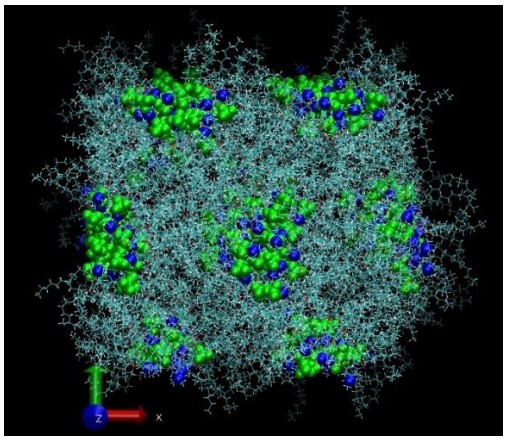
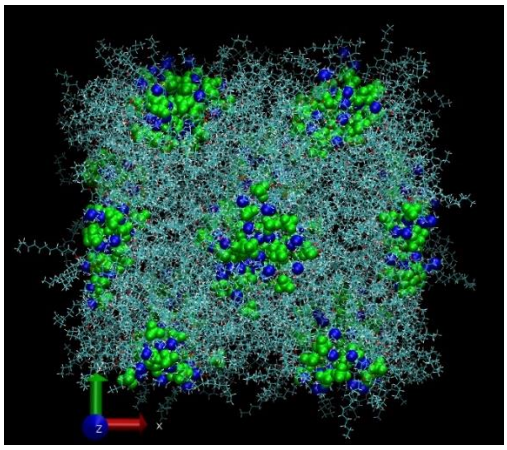


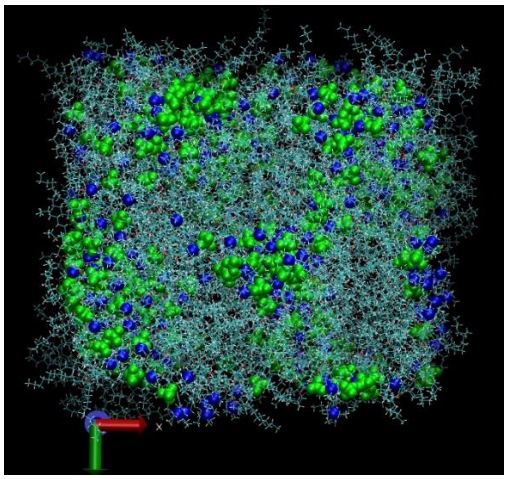
Figure S3. History of the thermal treatment of the small box (320 ion pairs) of **2[BF_4]**. The system is simulated for 100 ns at each temperature first in heating, up to 600 K, then in cooling, starting each simulation from the last configuration of the previous temperature run. The last 50 ns of each run are used to calculate the orientational order parameter, <P_2>, of the vector normal to the phenyl rings.



a)



b)



c)

Figure S4. Snapshots of the final configurations at 600 K of the heating runs using the full-charge Force Field and small boxes of 320 ion pairs. a) **1[BF_4]**; b) **2[BF_4]**; c) **3[BF_4]**. The hexagonal packing of the ionic moieties (tetrafluoroborate in green and the nitrogen of the ammonium group in blue) is clearly visible, indicating the lack of melting even at 600 K, although **3[BF_4]** appears less ordered than the other systems.