Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Molecular Dynamics Study of The Effect of Alkyl Chain Length on Melting Points of $[C_nMIM][PF_6]$ Ionic Liquids

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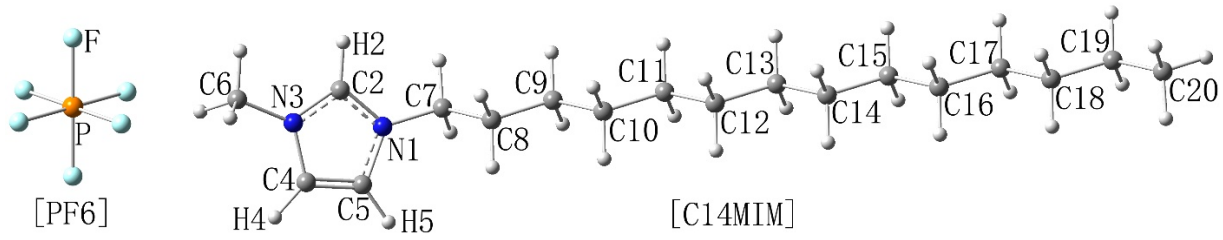

Figure S1: The labeling of heavy atoms in [C_{14}MIM][PF_6]. Hydrogen atoms are labeled after the C atoms they attach to. For example, H2 attaches to C2, H6 attaches to C6, and H7 attaches to C7, etc. Atoms in other molecules are labeled similarly.

Table S1: Derived partial charges of $[C_nMIM][PF_6]$ using AIMD simulation on the crystal phase.

n	**2**	**4**	**10**	**12**	**14**
P	0.482	0.807	1.751	1.945	2.130
F	-0.214	-0.268	-0.440	-0.474	-0.505
N1	0.172	0.146	0.168	0.195	0.198
C2	-0.119	-0.110	-0.079	-0.094	-0.095
N3	0.223	0.320	0.161	0.143	0.135
C4	-0.195	-0.198	-0.123	-0.107	-0.094
C5	-0.165	-0.194	-0.108	-0.113	-0.128
C6	-0.209	-0.325	-0.029	0.031	0.038
C7	0.006	-0.118	-0.050	-0.027	-0.014
C8	-0.278	-0.029	-0.031	-0.064	-0.066
C9		0.070	-0.011	-0.014	0.009
C10		-0.320	0.065	0.094	0.117
C11			-0.114	-0.090	-0.102
C12			0.133	0.101	0.127
C13			-0.134	-0.100	-0.068
C14			-0.026	0.093	0.051
C15			0.121	-0.130	-0.064
C16			-0.272	0.016	0.106
C17				0.098	-0.131
C18				-0.249	0.037
C19					0.108
C20					-0.237
H2	0.202	0.187	0.181	0.181	0.180
H4	0.195	0.202	0.149	0.142	0.135
H5	0.180	0.180	0.184	0.183	0.186
H6	0.114	0.134	0.069	0.055	0.054
H7	0.081	0.091	0.079	0.074	0.071
H8	0.095	0.052	0.047	0.049	0.046
H9		0.024	-0.003	-0.005	-0.013
H10		0.084	-0.002	-0.008	-0.016
H11			0.012	0.003	0.001
H12			-0.013	-0.011	-0.019
H13			0.025	0.015	0.006
H14			0.019	-0.007	-0.007
H15			-0.004	0.024	0.007
H16			0.060	0.009	-0.012
H17				-0.004	0.022
H18				0.055	0.001
H19					-0.009
H20					0.052

Table S2: Derived partial charges of $[C_nMIM][PF_6]$ using AIMD simulation with vdW correction on the crystal phase.

n	**2**	**4**	**10**	**12**	**14**
P	0.502	0.805	1.711	1.877	2.061
F	-0.218	-0.267	-0.427	-0.457	-0.487
N1	0.161	0.128	0.187	0.206	0.196
C2	-0.105	-0.103	-0.109	-0.097	-0.119
N3	0.220	0.335	0.206	0.178	0.202
C4	-0.199	-0.211	-0.151	-0.104	-0.119
C5	-0.163	-0.178	-0.121	-0.146	-0.132
C6	-0.226	-0.332	-0.121	-0.051	-0.080
C7	0.014	-0.104	-0.043	-0.048	-0.020
C8	-0.279	-0.051	-0.063	-0.030	-0.063
C9		0.090	0.015	-0.007	0.043
C10		-0.334	0.057	0.092	0.111
C11			-0.125	-0.099	-0.122
C12			0.176	0.114	0.194
C13			-0.177	-0.099	-0.121
C14			0.020	0.065	0.105
C15			0.123	-0.072	-0.099
C16			-0.294	-0.037	0.135
C17				0.147	-0.144
C18				-0.277	0.032
C19					0.135
C20					-0.286
H2	0.203	0.180	0.182	0.178	0.183
H4	0.197	0.202	0.153	0.143	0.141
H5	0.180	0.177	0.185	0.190	0.183
H6	0.119	0.137	0.088	0.070	0.076
H7	0.081	0.088	0.077	0.073	0.070
H8	0.095	0.056	0.050	0.038	0.038
H9		0.023	-0.008	-0.008	-0.021
H10		0.085	0.000	-0.010	-0.016
H11			0.011	0.003	0.001
H12			-0.019	-0.014	-0.030
H13			0.031	0.014	0.011
H14			0.008	-0.003	-0.017
H15			-0.006	0.014	0.013
H16			0.067	0.018	-0.017
H17				-0.013	0.024
H18				0.062	0.001
H19					-0.014
H20					0.065

Figure S3: Derived partial charges for each atom of $[C_2MIM][PF_6]$ using AIMD simulation on the crystal phase. The average value (Ave), standard deviation (SD) and the ratio of the two are also provided.

Atoms	**Mol1**	**Mol2**	**Mol3**	**Mol4**	**Ave**	**SD**	**(SD/Ave)%**
P	0.437	0.524	0.514	0.453	0.482	0.043	9.007
F	-0.246	-0.269	-0.256	-0.238	-0.252	0.013	-5.303
F	-0.190	-0.199	-0.197	-0.191	-0.194	0.004	-2.278
F	-0.221	-0.248	-0.261	-0.238	-0.242	0.017	-6.972
F	-0.182	-0.210	-0.213	-0.187	-0.198	0.016	-7.964
F	-0.184	-0.192	-0.183	-0.175	-0.184	0.007	-3.789
F	-0.216	-0.222	-0.210	-0.212	-0.215	0.005	-2.461
N1	0.157	0.154	0.178	0.197	0.172	0.020	11.705
C2	-0.192	-0.087	-0.045	-0.150	-0.119	0.065	-55.098
N3	0.252	0.242	0.189	0.208	0.223	0.029	13.172
C4	-0.210	-0.226	-0.179	-0.165	-0.195	0.028	-14.328
C5	-0.091	-0.168	-0.240	-0.162	-0.165	0.061	-36.841
C6	-0.243	-0.235	-0.177	-0.179	-0.209	0.035	-16.968
C7	0.044	0.037	-0.017	-0.040	0.006	0.041	683.807
C8	-0.296	-0.330	-0.257	-0.230	-0.278	0.044	-15.765
H2	0.235	0.183	0.170	0.219	0.202	0.030	15.042
H4	0.193	0.209	0.199	0.180	0.195	0.012	6.208
H5	0.150	0.187	0.210	0.173	0.180	0.025	13.974
H6	0.127	0.118	0.109	0.116	0.118	0.007	6.312
H6	0.122	0.117	0.096	0.098	0.108	0.013	12.171
H6	0.124	0.120	0.113	0.113	0.118	0.005	4.635
H7	0.070	0.072	0.077	0.084	0.076	0.006	8.235
H7	0.075	0.079	0.095	0.098	0.087	0.011	13.189
H8	0.118	0.126	0.112	0.111	0.117	0.007	5.908
H8	0.071	0.081	0.070	0.065	0.072	0.007	9.341
H8	0.104	0.109	0.089	0.087	0.097	0.011	11.213

Figure S4: Derived partial charges for each atom of $[C_4MIM][PF_6]$ using AIMD simulation on the crystal phase. The average value (Ave), standard deviation (SD) and the ratio of the two are also provided.

Atoms	**Mol1**	**Mol2**	**Ave**	**SD**	**(SD/Ave)%**
P	0.800	0.814	0.807	0.010	1.227
F	-0.245	-0.245	-0.245	0.000	0.000
F	-0.317	-0.314	-0.316	0.002	-0.672
F	-0.251	-0.261	-0.256	0.007	-2.762
F	-0.256	-0.257	-0.257	0.001	-0.276
F	-0.281	-0.283	-0.282	0.001	-0.501
F	-0.249	-0.256	-0.253	0.005	-1.960
N1	0.174	0.118	0.146	0.040	27.122
C2	-0.112	-0.107	-0.110	0.004	-3.229
N3	0.299	0.341	0.320	0.030	9.281
C4	-0.236	-0.159	-0.198	0.054	-27.568
C5	-0.153	-0.235	-0.194	0.058	-29.888
C6	-0.345	-0.304	-0.325	0.029	-8.934
C7	-0.082	-0.154	-0.118	0.051	-43.145
C8	-0.024	-0.034	-0.029	0.007	-24.383
C9	0.046	0.094	0.070	0.034	48.487
C10	-0.312	-0.328	-0.320	0.011	-3.536
H2	0.189	0.184	0.187	0.004	1.896
H4	0.213	0.191	0.202	0.016	7.701
H5	0.167	0.192	0.180	0.018	9.848
H6	0.128	0.116	0.122	0.008	6.955
H6	0.149	0.134	0.142	0.011	7.496
H6	0.140	0.139	0.140	0.001	0.507
H7	0.074	0.089	0.082	0.011	13.014
H7	0.088	0.114	0.101	0.018	18.203
H8	0.049	0.051	0.050	0.001	2.828
H8	0.051	0.055	0.053	0.003	5.337
H9	0.034	0.020	0.027	0.010	36.665
H9	0.025	0.016	0.021	0.006	31.044
H10	0.068	0.067	0.068	0.001	1.048
H10	0.095	0.090	0.093	0.004	3.822
H10	0.090	0.094	0.092	0.003	3.074

Figure S5: Derived partial charges for each atom of $[C_{10}MIM][PF_6]$ using AIMD simulation on the crystal phase. The average value (Ave), standard deviation (SD) and the ratio of the two are also provided.

Atoms	Mol1	Mol2	Mol3	Mol4	Ave	SD	(SD/Ave)%
P	1.779	1.703	1.746	1.769	1.749	0.034	1.932
F	-0.430	-0.412	-0.423	-0.434	-0.425	0.010	-2.269
F	-0.396	-0.385	-0.387	-0.386	-0.389	0.005	-1.304
F	-0.416	-0.400	-0.410	-0.417	-0.411	0.008	-1.900
F	-0.471	-0.460	-0.468	-0.478	-0.469	0.007	-1.589
F	-0.503	-0.479	-0.491	-0.499	-0.493	0.011	-2.147
F	-0.458	-0.447	-0.457	-0.455	-0.454	0.005	-1.099
N1	0.170	0.167	0.158	0.178	0.168	0.008	4.910
C2	-0.043	-0.065	-0.116	-0.092	-0.079	0.032	-40.228
N3	0.143	0.151	0.182	0.166	0.161	0.017	10.725
C4	-0.097	-0.139	-0.156	-0.101	-0.123	0.029	-23.444
C5	-0.161	-0.092	-0.059	-0.120	-0.108	0.043	-40.040
C6	-0.010	-0.004	-0.061	-0.040	-0.029	0.027	-92.697
C7	-0.067	-0.067	-0.027	-0.039	-0.050	0.020	-40.464
C8	-0.035	-0.031	-0.022	-0.034	-0.031	0.006	-19.397
C9	0.004	-0.011	-0.014	-0.023	-0.011	0.011	-102.045
C10	0.063	0.066	0.058	0.072	0.065	0.006	9.038
C11	-0.133	-0.122	-0.091	-0.111	-0.114	0.018	-15.680
C12	0.149	0.135	0.120	0.126	0.133	0.013	9.517
C13	-0.144	-0.132	-0.138	-0.120	-0.134	0.010	-7.676
C14	-0.028	-0.029	0.002	-0.049	-0.026	0.021	-80.861
C15	0.129	0.127	0.099	0.129	0.121	0.015	12.146
C16	-0.283	-0.271	-0.246	-0.288	-0.272	0.019	-6.891
H2	0.168	0.174	0.196	0.186	0.181	0.012	6.901
H4	0.139	0.156	0.162	0.138	0.149	0.012	8.130
H5	0.214	0.178	0.158	0.186	0.184	0.023	12.614
H6	0.073	0.073	0.092	0.087	0.081	0.010	11.991
H6	0.081	0.081	0.096	0.090	0.087	0.007	8.447
H6	0.036	0.034	0.049	0.037	0.039	0.007	17.391
H7	0.072	0.076	0.070	0.070	0.072	0.003	3.928
H7	0.095	0.092	0.076	0.077	0.085	0.010	11.646
H8	0.055	0.049	0.041	0.052	0.049	0.006	12.225
H8	0.047	0.045	0.039	0.045	0.044	0.003	7.873
H9	0.010	0.018	0.020	0.016	0.016	0.004	27.003
H9	-0.024	-0.020	-0.023	-0.020	-0.022	0.002	-9.478
H10	-0.004	-0.003	-0.003	-0.004	-0.004	0.001	-16.496
H10	-0.001	-0.003	0.001	0.002	0.000	0.002	-886.942
H11	0.003	0.001	-0.006	-0.003	-0.001	0.004	-322.490
H11	0.029	0.027	0.019	0.022	0.024	0.005	18.860
H12	-0.006	-0.004	-0.004	-0.004	-0.005	0.001	-22.222
H12	-0.025	-0.022	-0.019	-0.020	-0.022	0.003	-12.306
H13	0.017	0.012	0.013	0.012	0.014	0.002	17.633
H13	0.039	0.037	0.034	0.032	0.036	0.003	8.758
H14	0.014	0.015	0.006	0.018	0.013	0.005	38.668
H14	0.023	0.023	0.021	0.033	0.025	0.005	21.664
H15	-0.016	-0.017	-0.014	-0.016	-0.016	0.001	-7.989
H15	0.009	0.009	0.007	0.004	0.007	0.002	32.592
H16	0.074	0.072	0.066	0.077	0.072	0.005	6.430

H16	0.062	0.058	0.054	0.064	0.060	0.004	7.453
H16	0.052	0.047	0.043	0.055	0.049	0.005	10.792

Figure S6: Derived partial charges for each atom of $[C_{12}MIM][PF_6]$ using AIMD simulation on the crystal phase. The average value (Ave), standard deviation (SD) and the ratio of the two are also provided.

Atoms	Mol1	Mol2	Mol3	Mol4	Ave	SD	(SD/Ave)%
P	1.967	1.980	1.936	1.898	1.945	0.037	1.877
F	-0.481	-0.489	-0.482	-0.475	-0.482	0.006	-1.191
F	-0.540	-0.540	-0.524	-0.516	-0.530	0.012	-2.264
F	-0.424	-0.423	-0.424	-0.418	-0.422	0.003	-0.680
F	-0.469	-0.472	-0.458	-0.448	-0.462	0.011	-2.375
F	-0.512	-0.518	-0.506	-0.499	-0.509	0.008	-1.600
F	-0.448	-0.448	-0.440	-0.432	-0.442	0.008	-1.733
N1	0.197	0.214	0.190	0.180	0.195	0.014	7.332
C2	-0.094	-0.075	-0.079	-0.128	-0.094	0.024	-25.635
N3	0.144	0.141	0.132	0.156	0.143	0.010	6.919
C4	-0.080	-0.099	-0.119	-0.129	-0.107	0.022	-20.386
C5	-0.131	-0.153	-0.099	-0.067	-0.113	0.038	-33.397
C6	0.020	0.042	0.052	0.011	0.031	0.019	60.793
C7	-0.017	-0.058	-0.036	0.005	-0.027	0.027	-101.373
C8	-0.065	-0.061	-0.070	-0.061	-0.064	0.004	-6.649
C9	-0.026	-0.006	-0.011	-0.011	-0.014	0.009	-64.150
C10	0.102	0.094	0.092	0.089	0.094	0.006	5.899
C11	-0.090	-0.109	-0.090	-0.070	-0.090	0.016	-17.743
C12	0.098	0.116	0.101	0.090	0.101	0.011	10.740
C13	-0.088	-0.111	-0.109	-0.090	-0.100	0.012	-12.240
C14	0.087	0.097	0.101	0.087	0.093	0.007	7.654
C15	-0.122	-0.142	-0.141	-0.113	-0.130	0.014	-11.074
C16	0.008	0.025	0.025	0.006	0.016	0.010	65.152
C17	0.105	0.103	0.095	0.089	0.098	0.007	7.545
C18	-0.270	-0.261	-0.246	-0.217	-0.249	0.023	-9.343
H2	0.185	0.172	0.174	0.194	0.181	0.010	5.651
H4	0.129	0.136	0.149	0.152	0.142	0.011	7.666
H5	0.189	0.210	0.177	0.156	0.183	0.023	12.341
H6	0.075	0.067	0.067	0.078	0.072	0.006	7.833
H6	0.074	0.062	0.062	0.077	0.069	0.008	11.476
H6	0.024	0.023	0.022	0.034	0.026	0.006	21.593
H7	0.063	0.067	0.069	0.062	0.065	0.003	5.064
H7	0.075	0.094	0.089	0.071	0.082	0.011	13.369
H8	0.056	0.060	0.053	0.044	0.053	0.007	12.771
H8	0.046	0.045	0.047	0.041	0.045	0.003	5.877
H9	-0.022	-0.024	-0.023	-0.027	-0.024	0.002	-9.001
H9	0.014	0.008	0.015	0.017	0.014	0.004	28.689
H10	-0.002	-0.005	-0.007	-0.001	-0.004	0.003	-73.434
H10	-0.014	-0.012	-0.012	-0.012	-0.013	0.001	-8.000
H11	0.017	0.023	0.020	0.015	0.019	0.004	18.667
H11	-0.014	-0.008	-0.012	-0.019	-0.013	0.005	-34.517
H12	-0.005	-0.005	-0.002	-0.004	-0.004	0.001	-35.355
H12	-0.017	-0.021	-0.019	-0.015	-0.018	0.003	-14.344
H13	0.026	0.039	0.037	0.026	0.032	0.007	21.800
H13	-0.005	0.000	-0.001	-0.006	-0.003	0.003	-98.131
H14	-0.014	-0.012	-0.012	-0.013	-0.013	0.001	-7.509
H14	0.003	-0.004	-0.004	0.003	-0.001	0.004	-808.290
H15	0.034	0.042	0.041	0.032	0.037	0.005	13.400

H15	0.010	0.015	0.013	0.008	0.012	0.003	27.036
H16	0.006	0.002	0.001	0.004	0.003	0.002	68.226
H16	0.020	0.011	0.011	0.019	0.015	0.005	32.291
H17	-0.015	-0.015	-0.014	-0.014	-0.015	0.001	-3.982
H17	0.002	0.008	0.011	0.004	0.006	0.004	64.498
H18	0.074	0.069	0.066	0.059	0.067	0.006	9.361
H18	0.055	0.054	0.050	0.043	0.051	0.005	10.786
H18	0.056	0.050	0.044	0.040	0.048	0.007	14.737

Figure S7: Derived partial charges for each atom of [C_{14}MIM][PF_6] using AIMD simulation on the crystal phase. The average value (Ave), standard deviation (SD) and the ratio of the two are also provided.

Atoms	Mol1	Mol2	Mol3	Mol4	Ave	SD	(SD/Ave)%
P	2.152	2.086	2.119	2.161	2.130	0.034	1.604
F	-0.517	-0.506	-0.515	-0.519	-0.514	0.006	-1.116
F	-0.578	-0.555	-0.562	-0.579	-0.569	0.012	-2.094
F	-0.477	-0.464	-0.470	-0.476	-0.472	0.006	-1.276
F	-0.532	-0.521	-0.528	-0.540	-0.530	0.008	-1.496
F	-0.455	-0.453	-0.457	-0.456	-0.455	0.002	-0.375
F	-0.494	-0.472	-0.480	-0.499	-0.486	0.012	-2.560
N1	0.198	0.190	0.201	0.202	0.198	0.005	2.750
C2	-0.096	-0.138	-0.089	-0.056	-0.095	0.034	-35.566
N3	0.140	0.150	0.125	0.124	0.135	0.013	9.296
C4	-0.073	-0.117	-0.109	-0.076	-0.094	0.023	-24.000
C5	-0.139	-0.083	-0.113	-0.176	-0.128	0.039	-30.900
C6	0.020	0.020	0.067	0.045	0.038	0.023	59.585
C7	-0.005	0.021	-0.029	-0.044	-0.014	0.028	-199.754
C8	-0.060	-0.076	-0.074	-0.053	-0.066	0.011	-16.862
C9	-0.009	0.018	0.014	0.011	0.009	0.012	141.340
C10	0.131	0.111	0.116	0.110	0.117	0.010	8.287
C11	-0.109	-0.085	-0.106	-0.109	-0.102	0.012	-11.332
C12	0.130	0.111	0.126	0.140	0.127	0.012	9.498
C13	-0.059	-0.050	-0.062	-0.101	-0.068	0.023	-33.211
C14	0.040	0.031	0.032	0.101	0.051	0.034	65.835
C15	-0.050	-0.048	-0.058	-0.100	-0.064	0.024	-38.103
C16	0.102	0.100	0.107	0.114	0.106	0.006	5.899
C17	-0.129	-0.126	-0.135	-0.135	-0.131	0.005	-3.429
C18	0.039	0.038	0.039	0.033	0.037	0.003	7.711
C19	0.096	0.102	0.114	0.119	0.108	0.011	9.833
C20	-0.231	-0.221	-0.243	-0.253	-0.237	0.014	-5.887
H2	0.183	0.196	0.175	0.166	0.180	0.013	7.071
H4	0.125	0.146	0.142	0.128	0.135	0.010	7.621
H5	0.190	0.158	0.179	0.216	0.186	0.024	12.998
H6	0.073	0.074	0.056	0.060	0.066	0.009	13.849
H6	0.022	0.030	0.017	0.021	0.023	0.005	24.208
H6	0.078	0.079	0.067	0.071	0.074	0.006	7.779
H7	0.072	0.068	0.089	0.094	0.081	0.013	15.709
H7	0.059	0.058	0.066	0.064	0.062	0.004	6.255
H8	0.051	0.044	0.051	0.054	0.050	0.004	8.485
H8	0.041	0.040	0.044	0.040	0.041	0.002	4.589
H9	-0.029	-0.036	-0.032	-0.033	-0.033	0.003	-8.882
H9	0.008	0.009	0.008	0.003	0.007	0.003	38.686
H10	-0.025	-0.022	-0.021	-0.021	-0.022	0.002	-8.508
H10	-0.008	-0.006	-0.013	-0.010	-0.009	0.003	-32.282
H11	0.015	0.012	0.018	0.019	0.016	0.003	19.764
H11	-0.014	-0.018	-0.012	-0.011	-0.014	0.003	-22.514
H12	-0.014	-0.011	-0.012	-0.014	-0.013	0.002	-11.765
H12	-0.025	-0.020	-0.025	-0.029	-0.025	0.004	-14.891
H13	0.019	0.017	0.027	0.033	0.024	0.007	30.807
H13	-0.015	-0.015	-0.013	-0.007	-0.013	0.004	-30.288
H14	-0.015	-0.013	-0.009	-0.024	-0.015	0.006	-41.602

H14	0.005	0.006	0.003	-0.010	0.001	0.007	743.864
H15	0.020	0.020	0.028	0.035	0.026	0.007	28.072
H15	-0.014	-0.014	-0.012	-0.005	-0.011	0.004	-37.973
H16	-0.019	-0.018	-0.019	-0.020	-0.019	0.001	-4.297
H16	-0.004	-0.002	-0.008	-0.009	-0.006	0.003	-57.462
H17	0.010	0.008	0.009	0.011	0.010	0.001	13.589
H17	0.031	0.031	0.037	0.038	0.034	0.004	11.022
H18	-0.007	-0.009	-0.008	-0.005	-0.007	0.002	-23.556
H18	0.011	0.011	0.006	0.007	0.009	0.003	30.057
H19	0.000	0.000	0.004	0.003	0.002	0.002	117.803
H19	-0.018	-0.020	-0.021	-0.023	-0.021	0.002	-10.154
H20	0.062	0.058	0.062	0.065	0.062	0.003	4.651
H20	0.050	0.043	0.045	0.050	0.047	0.004	7.572
H20	0.044	0.042	0.047	0.050	0.046	0.004	7.650

Figure S8: Derived partial charges for each atom of $[C_2MIM][PF_6]$ using AIMD simulation with vdW correction on the crystal phase. The average value (Ave), standard deviation (SD) and the ratio of the two are also provided.

Atoms	**Mol1**	**Mol2**	**Mol3**	**Mol4**	**Ave**	**SD**	**(SD/Ave)%**
P	0.429	0.550	0.525	0.501	0.501	0.052	10.405
F	-0.246	-0.276	-0.259	-0.247	-0.257	0.014	-5.438
F	-0.184	-0.201	-0.198	-0.197	-0.195	0.008	-3.860
F	-0.218	-0.255	-0.265	-0.247	-0.246	0.020	-8.212
F	-0.184	-0.220	-0.217	-0.200	-0.205	0.017	-8.127
F	-0.185	-0.191	-0.179	-0.177	-0.183	0.006	-3.456
F	-0.218	-0.227	-0.214	-0.222	-0.220	0.006	-2.525
N1	0.149	0.149	0.161	0.183	0.161	0.016	9.988
C2	-0.186	-0.071	-0.029	-0.134	-0.105	0.069	-65.832
N3	0.258	0.234	0.183	0.203	0.220	0.033	15.103
C4	-0.230	-0.222	-0.180	-0.165	-0.199	0.032	-15.889
C5	-0.084	-0.172	-0.233	-0.163	-0.163	0.061	-37.522
C6	-0.257	-0.264	-0.194	-0.187	-0.226	0.041	-18.012
C7	0.045	0.037	-0.008	-0.018	0.014	0.032	225.802
C8	-0.299	-0.318	-0.257	-0.242	-0.279	0.035	-12.713
H2	0.238	0.183	0.171	0.221	0.203	0.031	15.488
H4	0.199	0.210	0.199	0.180	0.197	0.012	6.327
H5	0.149	0.187	0.209	0.175	0.180	0.025	13.893
H6	0.134	0.124	0.116	0.119	0.123	0.008	6.402
H6	0.124	0.126	0.099	0.099	0.112	0.015	13.423
H6	0.128	0.130	0.116	0.115	0.122	0.008	6.419
H7	0.069	0.073	0.076	0.080	0.075	0.005	6.248
H7	0.077	0.080	0.096	0.094	0.087	0.010	11.112
H8	0.118	0.123	0.113	0.113	0.117	0.005	4.100
H8	0.069	0.076	0.068	0.064	0.069	0.005	7.208
H8	0.106	0.105	0.092	0.087	0.098	0.009	9.712

Figure S9: Derived partial charges for each atom of $[C_4MIM][PF_6]$ using AIMD simulation with vdW correction on the crystal phase. The average value (Ave), standard deviation (SD) and the ratio of the two are also provided.

Atoms	**Mol1**	**Mol2**	**Ave**	**SD**	**(SD/Ave)%**
P	0.809	0.800	0.805	0.006	0.791
F	-0.250	-0.232	-0.241	0.013	-5.281
F	-0.317	-0.324	-0.321	0.005	-1.544
F	-0.244	-0.264	-0.254	0.014	-5.568
F	-0.263	-0.262	-0.263	0.001	-0.269
F	-0.288	-0.275	-0.282	0.009	-3.266
F	-0.244	-0.241	-0.243	0.002	-0.875
N1	0.083	0.173	0.128	0.064	49.718
C2	-0.094	-0.112	-0.103	0.013	-12.357
N3	0.348	0.321	0.335	0.019	5.708
C4	-0.238	-0.184	-0.211	0.038	-18.097
C5	-0.143	-0.213	-0.178	0.049	-27.808
C6	-0.360	-0.304	-0.332	0.040	-11.927
C7	-0.041	-0.166	-0.104	0.088	-85.399
C8	-0.068	-0.033	-0.051	0.025	-49.007
C9	0.080	0.100	0.090	0.014	15.713
C10	-0.328	-0.339	-0.334	0.008	-2.332
H2	0.179	0.180	0.180	0.001	0.394
H4	0.210	0.193	0.202	0.012	5.966
H5	0.167	0.187	0.177	0.014	7.990
H6	0.131	0.116	0.124	0.011	8.588
H6	0.158	0.138	0.148	0.014	9.555
H6	0.140	0.138	0.139	0.001	1.017
H7	0.069	0.090	0.080	0.015	18.678
H7	0.077	0.116	0.097	0.028	28.577
H8	0.060	0.051	0.056	0.006	11.467
H8	0.055	0.056	0.056	0.001	1.274
H9	0.036	0.020	0.028	0.011	40.406
H9	0.017	0.017	0.017	0.000	0.000
H10	0.075	0.072	0.074	0.002	2.886
H10	0.092	0.090	0.091	0.001	1.554
H10	0.090	0.093	0.092	0.002	2.318

Figure S10: Derived partial charges for each atom of $[C_{10}MIM][PF_6]$ using AIMD simulation with vdW correction on the crystal phase. The average value (Ave), standard deviation (SD) and the ratio of the two are also provided.

Atoms	Mol1	Mol2	Mol3	Mol4	Ave	SD	(SD/Ave)%
P	1.748	1.678	1.672	1.744	1.711	0.041	2.403
F	-0.404	-0.400	-0.381	-0.428	-0.403	0.019	-4.789
F	-0.396	-0.387	-0.389	-0.389	-0.390	0.004	-1.012
F	-0.402	-0.404	-0.408	-0.422	-0.409	0.009	-2.205
F	-0.436	-0.412	-0.410	-0.449	-0.427	0.019	-4.444
F	-0.505	-0.479	-0.496	-0.483	-0.491	0.012	-2.436
F	-0.453	-0.434	-0.436	-0.441	-0.441	0.009	-1.933
N1	0.182	0.173	0.177	0.214	0.187	0.019	10.026
C2	-0.077	-0.095	-0.137	-0.125	-0.109	0.027	-25.291
N3	0.210	0.189	0.222	0.203	0.206	0.014	6.691
C4	-0.146	-0.161	-0.175	-0.121	-0.151	0.023	-15.323
C5	-0.165	-0.101	-0.070	-0.146	-0.121	0.043	-35.730
C6	-0.118	-0.083	-0.168	-0.116	-0.121	0.035	-28.912
C7	-0.034	-0.034	-0.038	-0.067	-0.043	0.016	-36.868
C8	-0.087	-0.087	-0.045	-0.033	-0.063	0.028	-44.671
C9	0.051	0.009	0.027	-0.028	0.015	0.033	225.698
C10	0.035	0.087	0.020	0.087	0.057	0.035	60.950
C11	-0.117	-0.166	-0.081	-0.136	-0.125	0.036	-28.480
C12	0.161	0.233	0.111	0.199	0.176	0.052	29.756
C13	-0.170	-0.212	-0.141	-0.186	-0.177	0.030	-16.770
C14	0.022	0.045	-0.005	0.016	0.020	0.021	105.472
C15	0.117	0.120	0.104	0.149	0.123	0.019	15.496
C16	-0.296	-0.298	-0.251	-0.330	-0.294	0.032	-11.057
H2	0.172	0.178	0.192	0.185	0.182	0.009	4.762
H4	0.146	0.157	0.168	0.141	0.153	0.012	7.861
H5	0.216	0.178	0.161	0.186	0.185	0.023	12.415
H6	0.093	0.082	0.107	0.099	0.095	0.011	11.057
H6	0.098	0.098	0.121	0.117	0.109	0.012	11.275
H6	0.057	0.059	0.069	0.054	0.060	0.007	10.879
H7	0.067	0.071	0.072	0.071	0.070	0.002	3.156
H7	0.084	0.085	0.077	0.087	0.083	0.004	5.224
H8	0.059	0.055	0.044	0.045	0.051	0.007	14.602
H8	0.053	0.054	0.042	0.046	0.049	0.006	11.769
H9	0.000	0.014	0.014	0.021	0.012	0.009	71.903
H9	-0.035	-0.023	-0.034	-0.018	-0.028	0.008	-30.351
H10	0.003	-0.005	0.005	-0.009	-0.002	0.007	-440.538
H10	0.002	-0.008	0.012	0.000	0.002	0.008	548.398
H11	-0.001	0.004	-0.010	-0.003	-0.003	0.006	-232.092
H11	0.024	0.030	0.019	0.024	0.024	0.005	18.557
H12	-0.001	-0.017	0.003	-0.016	-0.008	0.010	-132.166
H12	-0.030	-0.042	-0.015	-0.035	-0.031	0.011	-37.526
H13	0.019	0.021	0.016	0.018	0.019	0.002	11.252
H13	0.049	0.048	0.040	0.040	0.044	0.005	11.129
H14	0.010	0.003	0.006	0.002	0.005	0.004	68.457
H14	0.008	0.003	0.017	0.011	0.010	0.006	60.024
H15	-0.019	-0.018	-0.013	-0.021	-0.018	0.003	-19.174

H15	0.013	0.009	0.005	-0.003	0.006	0.007	113.855
H16	0.079	0.074	0.070	0.090	0.078	0.009	11.061
H16	0.069	0.071	0.052	0.069	0.065	0.009	13.615
H16	0.058	0.060	0.047	0.062	0.057	0.007	11.810

Figure S11: Derived partial charges for each atom of [C_{12}MIM][PF_6] using AIMD simulation with vdW correction on the crystal phase. The average value (Ave), standard deviation (SD) and the ratio of the two are also provided.

Atoms	Mol1	Mol2	Mol3	Mol4	Ave	SD	(SD/Ave)%
P	1.950	1.896	1.818	1.845	1.877	0.058	3.105
F	-0.481	-0.467	-0.461	-0.471	-0.470	0.008	-1.789
F	-0.538	-0.527	-0.520	-0.509	-0.524	0.012	-2.326
F	-0.414	-0.407	-0.405	-0.411	-0.409	0.004	-0.985
F	-0.449	-0.441	-0.414	-0.432	-0.434	0.015	-3.464
F	-0.484	-0.487	-0.458	-0.462	-0.473	0.015	-3.144
F	-0.456	-0.442	-0.415	-0.427	-0.435	0.018	-4.099
N1	0.203	0.250	0.181	0.191	0.206	0.031	14.798
C2	-0.086	-0.097	-0.060	-0.146	-0.097	0.036	-37.031
N3	0.156	0.208	0.157	0.191	0.178	0.026	14.484
C4	-0.079	-0.092	-0.115	-0.128	-0.104	0.022	-21.351
C5	-0.157	-0.213	-0.123	-0.089	-0.146	0.053	-36.340
C6	-0.047	-0.057	-0.049	-0.050	-0.051	0.004	-8.570
C7	-0.037	-0.108	-0.029	-0.017	-0.048	0.041	-85.862
C8	-0.019	-0.017	-0.053	-0.029	-0.030	0.017	-56.009
C9	-0.056	0.031	-0.028	0.024	-0.007	0.042	-576.828
C10	0.168	0.040	0.133	0.027	0.092	0.069	75.270
C11	-0.164	-0.057	-0.150	-0.025	-0.099	0.068	-69.165
C12	0.223	0.027	0.206	-0.001	0.114	0.117	102.947
C13	-0.148	-0.051	-0.161	-0.035	-0.099	0.065	-65.744
C14	0.147	-0.009	0.143	-0.021	0.065	0.093	142.339
C15	-0.118	-0.030	-0.115	-0.026	-0.072	0.051	-70.777
C16	0.003	-0.075	0.001	-0.077	-0.037	0.045	-121.752
C17	0.145	0.172	0.134	0.138	0.147	0.017	11.623
C18	-0.315	-0.277	-0.283	-0.232	-0.277	0.034	-12.350
H2	0.177	0.170	0.170	0.195	0.178	0.012	6.631
H4	0.131	0.137	0.149	0.154	0.143	0.011	7.422
H5	0.194	0.219	0.180	0.165	0.190	0.023	12.114
H6	0.087	0.081	0.045	0.085	0.075	0.020	26.610
H6	0.092	0.079	0.091	0.091	0.088	0.006	7.008
H6	0.032	0.039	0.081	0.037	0.047	0.023	48.025
H7	0.059	0.074	0.058	0.068	0.065	0.008	11.787
H7	0.075	0.101	0.085	0.063	0.081	0.016	19.856
H8	0.031	0.045	0.040	0.031	0.037	0.007	18.901
H8	0.043	0.036	0.046	0.032	0.039	0.006	16.297
H9	-0.015	-0.033	-0.017	-0.031	-0.024	0.009	-38.790
H9	0.016	-0.004	0.017	0.005	0.009	0.010	117.057
H10	-0.021	0.006	-0.018	0.015	-0.005	0.018	-394.405
H10	-0.030	-0.004	-0.024	0.000	-0.015	0.015	-101.593
H11	0.020	0.010	0.021	0.006	0.014	0.007	52.004
H11	-0.005	-0.009	-0.003	-0.015	-0.008	0.005	-66.144
H12	-0.029	0.022	-0.022	0.026	-0.001	0.029	-3835.700
H12	-0.054	-0.004	-0.050	0.002	-0.027	0.030	-111.667
H13	0.024	0.024	0.030	0.016	0.024	0.006	24.445
H13	0.002	0.006	0.008	0.003	0.005	0.003	57.974
H14	-0.028	0.028	-0.024	0.030	0.002	0.032	2120.447

H14	-0.025	0.005	-0.024	0.011	-0.008	0.019	-229.424
H15	0.025	0.016	0.027	0.012	0.020	0.007	35.824
H15	0.007	0.007	0.008	0.008	0.008	0.001	7.698
H16	0.015	0.035	0.014	0.034	0.025	0.012	47.190
H16	0.003	0.016	0.002	0.021	0.011	0.009	90.183
H17	-0.024	-0.021	-0.018	-0.012	-0.019	0.005	-27.325
H17	-0.006	-0.012	0.002	-0.012	-0.007	0.007	-94.761
H18	0.080	0.070	0.068	0.058	0.069	0.009	13.070
H18	0.076	0.068	0.070	0.057	0.068	0.008	11.708
H18	0.058	0.049	0.048	0.041	0.049	0.007	14.237

Figure S12: Derived partial charges for each atom of $[C_{14}MIM][PF_6]$ using AIMD simulation with vdW correction on the crystal phase. The average value (Ave), standard deviation (SD) and the ratio of the two are also provided.

Atoms	Mol1	Mol2	Mol3	Mol4	Ave	SD	(SD/Ave)%
P	2.039	2.088	1.989	2.123	2.060	0.058	2.836
F	-0.513	-0.491	-0.497	-0.497	-0.500	0.009	-1.889
F	-0.574	-0.534	-0.553	-0.557	-0.555	0.016	-2.962
F	-0.461	-0.457	-0.464	-0.488	-0.468	0.014	-2.987
F	-0.465	-0.514	-0.475	-0.516	-0.493	0.026	-5.343
F	-0.459	-0.466	-0.446	-0.460	-0.458	0.008	-1.840
F	-0.435	-0.471	-0.398	-0.500	-0.451	0.044	-9.805
N1	0.186	0.208	0.201	0.188	0.196	0.011	5.380
C2	-0.109	-0.170	-0.124	-0.072	-0.119	0.041	-34.154
N3	0.171	0.268	0.162	0.207	0.202	0.048	23.814
C4	-0.107	-0.166	-0.125	-0.079	-0.119	0.036	-30.577
C5	-0.136	-0.089	-0.134	-0.170	-0.132	0.033	-25.127
C6	-0.008	-0.182	0.029	-0.157	-0.080	0.106	-132.717
C7	-0.012	-0.025	-0.008	-0.033	-0.020	0.012	-59.289
C8	-0.074	-0.041	-0.068	-0.067	-0.063	0.015	-23.461
C9	0.053	0.015	0.051	0.051	0.043	0.018	43.194
C10	0.131	0.135	0.081	0.098	0.111	0.026	23.467
C11	-0.149	-0.117	-0.100	-0.123	-0.122	0.020	-16.622
C12	0.188	0.232	0.119	0.238	0.194	0.055	28.261
C13	-0.089	-0.136	-0.083	-0.177	-0.121	0.044	-36.353
C14	0.067	0.117	0.065	0.169	0.105	0.049	47.150
C15	-0.072	-0.064	-0.120	-0.140	-0.099	0.037	-37.232
C16	0.116	0.096	0.163	0.166	0.135	0.035	25.708
C17	-0.129	-0.108	-0.181	-0.159	-0.144	0.032	-22.338
C18	0.025	0.019	0.046	0.037	0.032	0.012	38.089
C19	0.134	0.128	0.140	0.139	0.135	0.006	4.067
C20	-0.277	-0.268	-0.296	-0.302	-0.286	0.016	-5.573
H2	0.181	0.203	0.176	0.173	0.183	0.014	7.407
H4	0.127	0.160	0.145	0.131	0.141	0.015	10.639
H5	0.192	0.156	0.178	0.207	0.183	0.022	11.834
H6	0.066	0.099	0.058	0.094	0.079	0.020	25.599
H6	0.025	0.062	0.033	0.069	0.047	0.022	45.535
H6	0.106	0.120	0.087	0.094	0.102	0.014	14.228
H7	0.073	0.081	0.069	0.083	0.077	0.007	8.638
H7	0.064	0.060	0.066	0.063	0.063	0.003	3.953
H8	0.039	0.027	0.037	0.040	0.036	0.006	16.686
H8	0.039	0.034	0.045	0.043	0.040	0.005	12.065
H9	-0.047	-0.034	-0.044	-0.039	-0.041	0.006	-13.940
H9	-0.002	0.003	0.000	-0.008	-0.002	0.005	-265.474
H10	-0.012	-0.033	-0.009	-0.022	-0.019	0.011	-57.173
H10	-0.013	-0.018	-0.005	-0.014	-0.013	0.005	-43.574
H11	0.020	0.011	0.016	0.016	0.016	0.004	23.400
H11	-0.012	-0.020	-0.012	-0.015	-0.015	0.004	-25.593
H12	-0.021	-0.032	-0.001	-0.027	-0.020	0.014	-67.153
H12	-0.040	-0.047	-0.025	-0.050	-0.041	0.011	-27.532
H13	0.021	0.023	0.031	0.038	0.028	0.008	27.628

H13	-0.013	-0.011	-0.006	0.001	-0.007	0.006	-86.046
H14	-0.016	-0.028	-0.004	-0.032	-0.020	0.013	-63.246
H14	-0.007	-0.013	-0.008	-0.027	-0.014	0.009	-67.018
H15	0.023	0.020	0.040	0.037	0.030	0.010	33.222
H15	-0.005	-0.016	0.005	0.000	-0.004	0.009	-224.537
H16	-0.017	-0.015	-0.019	-0.026	-0.019	0.005	-24.868
H16	-0.013	-0.006	-0.021	-0.021	-0.015	0.007	-47.399
H17	0.014	0.004	0.018	0.013	0.012	0.006	48.237
H17	0.030	0.027	0.048	0.037	0.036	0.009	26.274
H18	-0.001	-0.003	-0.002	-0.003	-0.002	0.001	-42.552
H18	0.005	0.009	0.001	0.001	0.004	0.004	95.743
H19	-0.008	-0.001	0.003	-0.001	-0.002	0.005	-261.341
H19	-0.022	-0.026	-0.025	-0.028	-0.025	0.003	-9.901
H20	0.077	0.070	0.075	0.074	0.074	0.003	3.978
H20	0.059	0.060	0.065	0.069	0.063	0.005	7.345
H20	0.056	0.052	0.060	0.065	0.058	0.006	9.546