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

Supplementary Information

Why is the electroanalytical performance of carbon paste electrodes involving ionic liquid binder higher than paraffinic binders? a simulation investigation

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Table S1. Atomic charges calculation by using the GAUSSIAN 03 at the B3LYP/6-311G for $[C_4mim]PF_6$.

atom	charge	atom	charge
N_1	-0.357	H_2	0.203
C_2	0.327	H_4	0.204
N_3	-0.355	H_5	0.277
C_4	-0.019	H_6	0.225
C_5	-0.017	H_7	0.227
C_6	-0.357	H_8	0.237
C_7	-0.157	H_9	0.182
C_8	-0.399	H_{10}	0.201
C_9	-0.381	P	2.554
C_{10}	-0.569	F	-0.587

Table S2. Atomic charges calculations by using the GAUSSIAN 03 at the B3LYP/6-311G for $C_{20}H_{42}$.

atom	charge	atom	charge
C_{P1}	-0.658	H_1	0.137
C_{P2}	-0.217	H_2	0.127
C_{P3}	-0.278	H_3	0.118
C_{P4}	-0.128	H_4	0.121
C_{P5}	-0.066	H_5	0.123
C_{P6}	-0.183	H_6	0.124
C_{P7}	-0.345	H_7	0.125
C_{P8}	-0.322	H_8	0.125
C_{P9}	-0.273	H_9	0.124
C_{P10}	-0.164	H_{10}	0.124

Table S3. The distance of closest approach (Å): $[C_4mim]PF_6$ intercalated between graphite charged plates.

atoms of ionic liquid	distance of closet approach			
	C_1	C_106	C_512	C_556
N_1	4.85	5.55	5.95	6.25
C_2	4.65	5.25	5.65	6.85
N_3	4.55	5.45	4.85	7.45
C_4	3.55	4.75	5.05	7.75
C_5	3.95	4.45	5.65	6.85
C_6	3.85	5.25	4.65	7.95
C_7	6.35	5.05	6.85	5.25
C_{10}	4.25	4.55	7.45	4.55
P	4.45	4.55	4.75	6.05
F	3.25	3.55	3.45	5.05

Table S4. The distance of closest approach (Å): *n*-$C_{20}H_{42}$ atoms intercalated between graphite charged plates.

atoms of paraffin	distance of closest approach			
	C_1	C_106	C_512	C_556
C_{P1}	3.25	3.25	3.45	3.35
C_{P10}	3.55	3.55	3.65	3.75

Table S5. The distance of closest approach (Å): $[C_4mim]PF_6$ placed on graphite uncharged plates.

IL atoms	graphite atoms			
	C_1	C_106	C_512	C_556
N_1	4.35	6.35	6.75	5.75
C_2	4.65	5.75	6.65	7.05
N_3	5.35	4.55	7.05	7.55
C_4	5.45	4.35	6.25	8.05
C_5	4.55	5.45	5.75	5.65
C_6	4.75	3.75	7.55	8.05
C_7	3.75	7.05	6.95	5.25
C_{10}	3.45	8.35	6.45	3.75
P	4.35	4.95	8.35	7.75
F	3.35	3.65	6.85	6.65

Table S6. The distance of closest approach (Å): $[C_4mim]PF_6$ intercalated between graphite uncharged plates.

atoms of ionic liquid	distance of closet approach			
	C_1	C_106	C_512	C_556
N_1	6.35	3.85	6.35	6.55
C_2	6.85	4.25	6.75	6.35
N_3	6.25	3.85	7.75	6.65
C_4	5.05	3.45	7.95	8.25
C_5	5.05	3.45	7.95	8.25
C_6	5.45	4.75	8.45	6.15
C_7	5.35	4.75	5.05	5.65
C_{10}	5.65	4.05	4.05	3.75
P	4.55	5.25	5.85	5.85
F	3.25	4.05	4.65	4.45

Table S7. The distance of closest approach (Å): *n*-$C_{20}H_{42}$ placed on graphite uncharged plates.

atoms of paraffin	distance of closest approach			
	C_1	C_106	C_512	C_556
C_{P1}	3.35	3.45	3.55	3.55
C_{P10}	6.65	3.55	3.65	7.65

Table S8. The distance of closest approach (Å): *n*-$C_{20}H_{42}$ atoms intercalated between graphite uncharged plates.

atoms of paraffin	distance of closest approach			
	C_1	C_106	C_512	C_556
C_{P1}	3.45	3.45	3.55	3.55
C_{P10}	3.55	3.55	3.25	3.55

IL on Graphite Charged Plates: Figures S1-S8

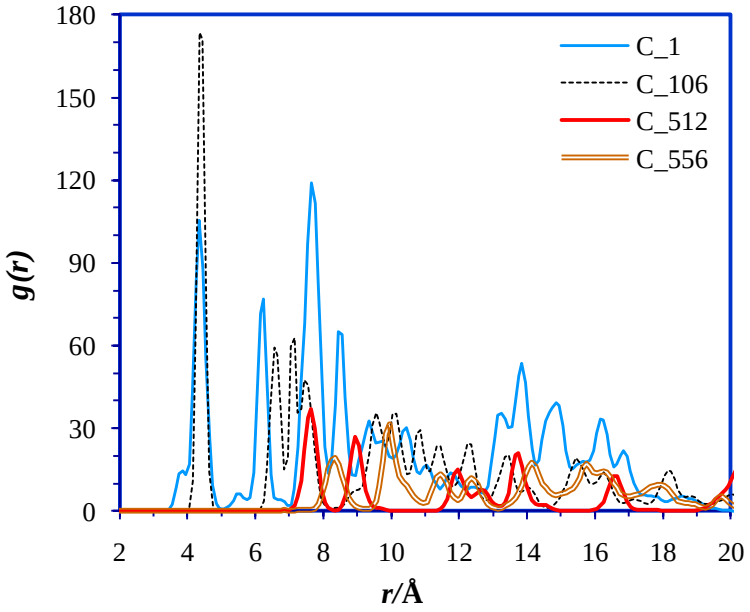

Figure S1. Pair correlation functions (at 323 K) between C_2 atom of IL monolayer and carbon atoms at different locations on double-C_{600} graphite charged plates.

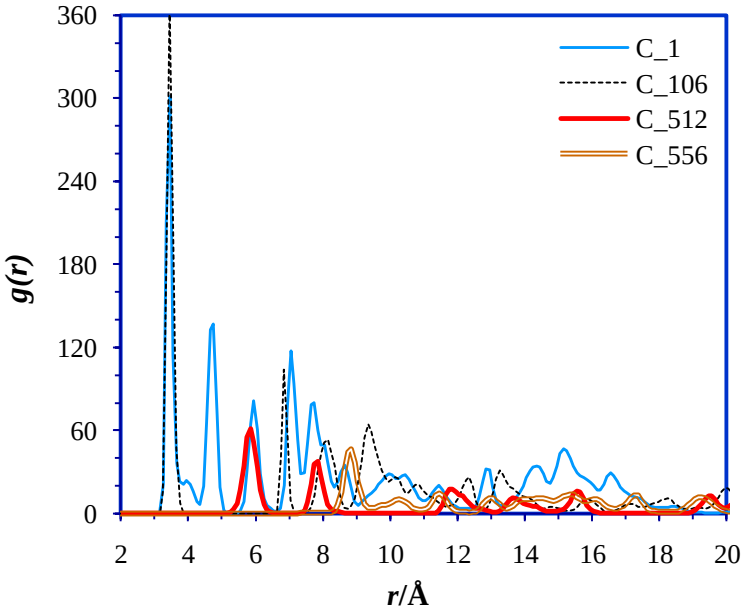

Figure S2. The same as Figure S1, but for C_4 atom.

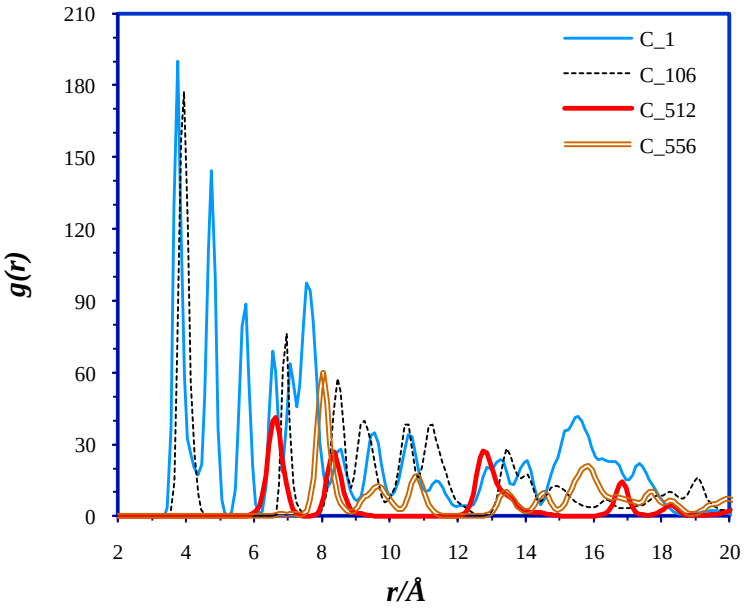

Figure S3. The same as Figure S1, but for C_5 atom.

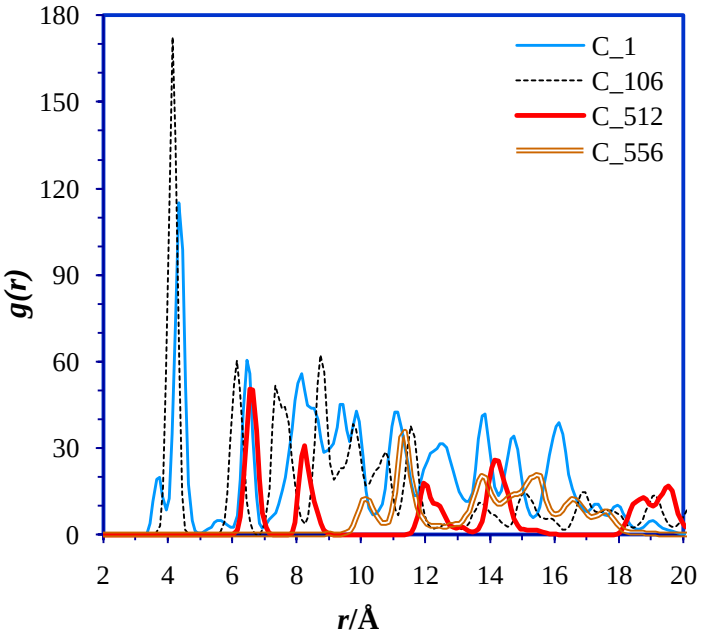

Figure S4. The same as Figure S1, but for C_6 atom.

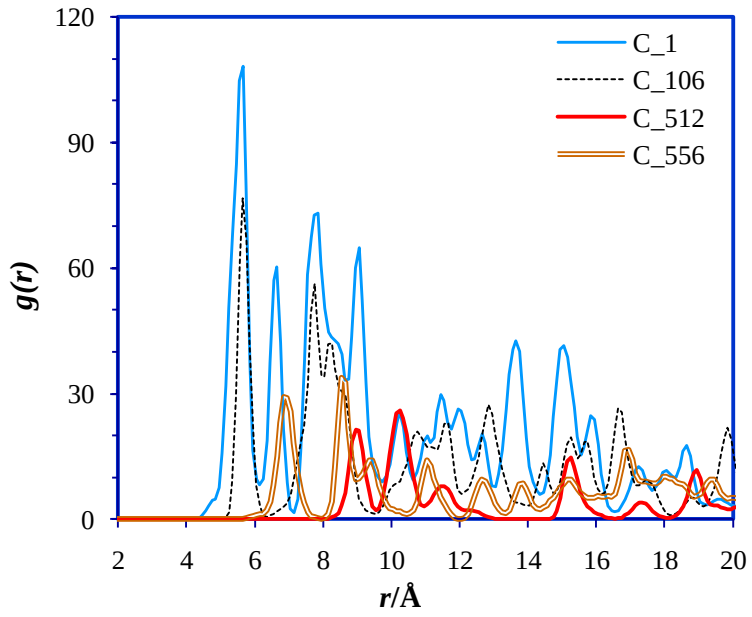

Figure S5. The same as Figure S1, but for C_7 atom.

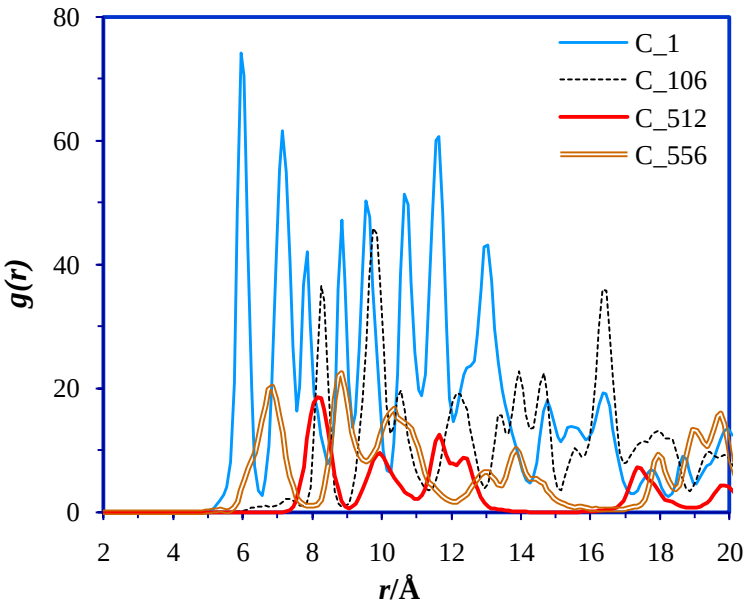

Figure S6. The same as Figure S1, but for C_{10} atom.

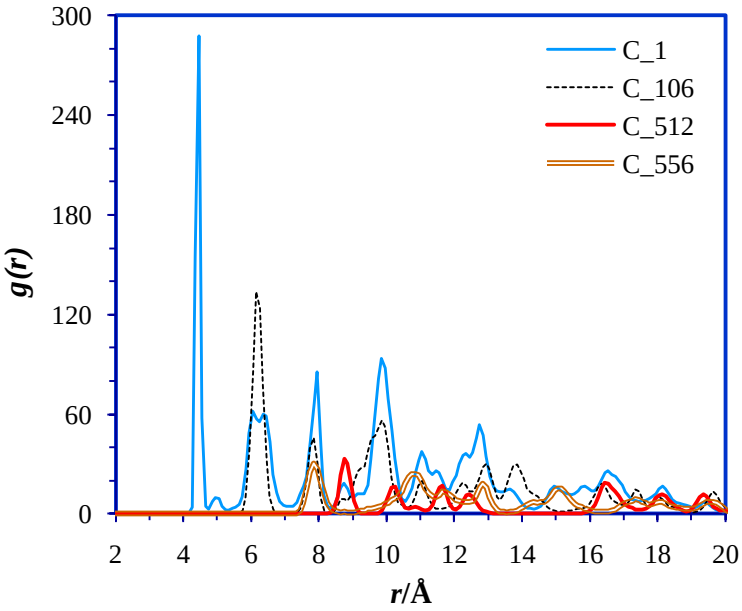

Figure S7. The same as Figure S1, but for P atom.

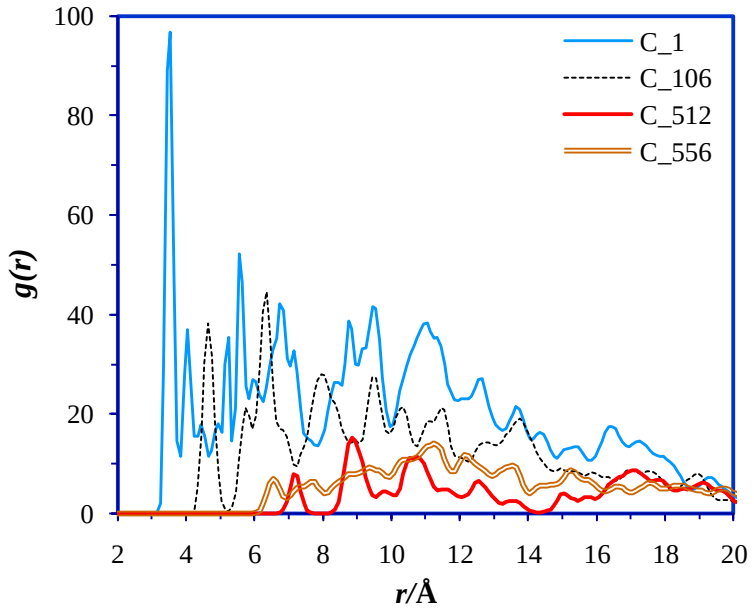

Figure S8. The same as Figure S1, but for F atom.

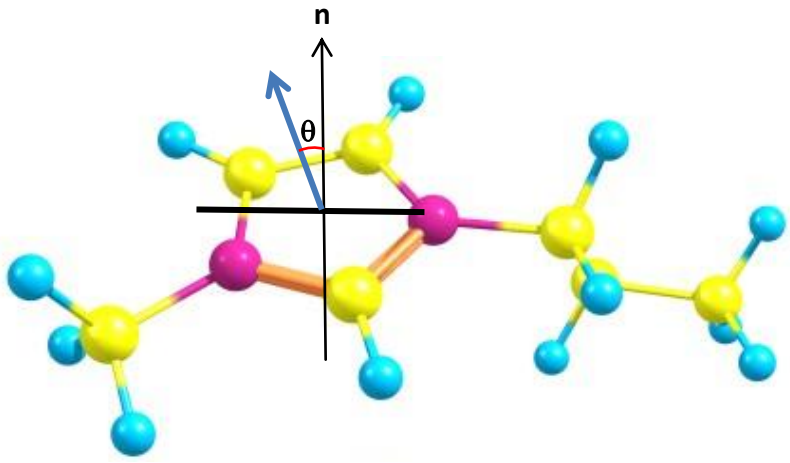

Figure S9. The average orientation of the imidazolium ring plane with to respect to graphite surface (of the double-C_{600}). (***Θ***) is the angle between normal of charged graphite plate (**n**) and normal of the imidazolium ring plane.

IL Intercalated between Graphite Charged Plates: Figures S10-S19

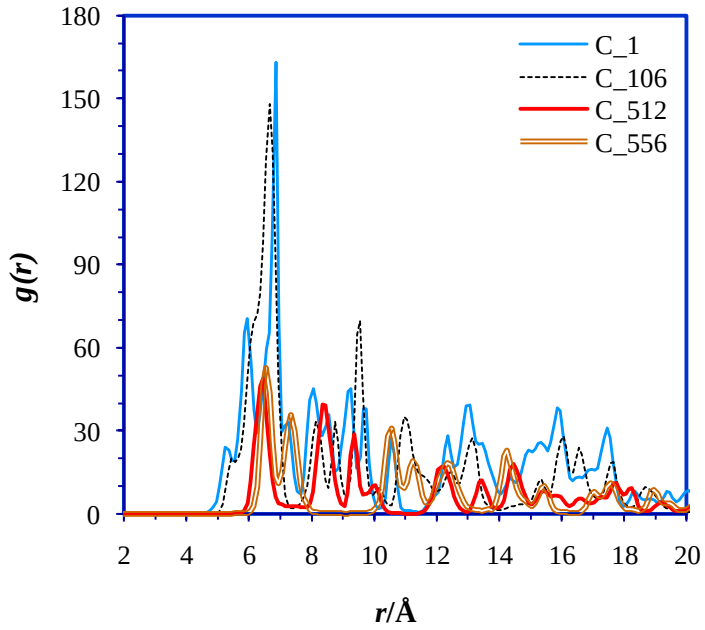

Figure S10. Pair correlation functions (at 323 K) between N_1 atom of IL monolayer and carbon atoms at different locations in between double-C_{600} graphite charged plates.

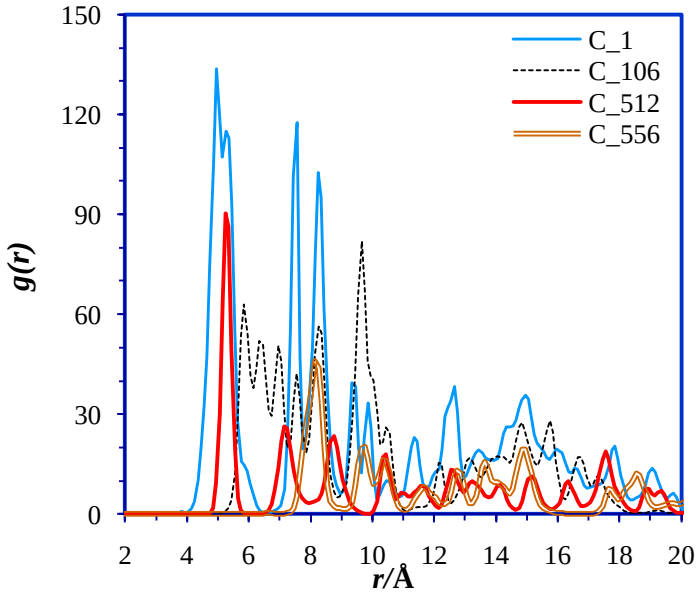

Figure S11. The same as Figure S10, but for N_3.

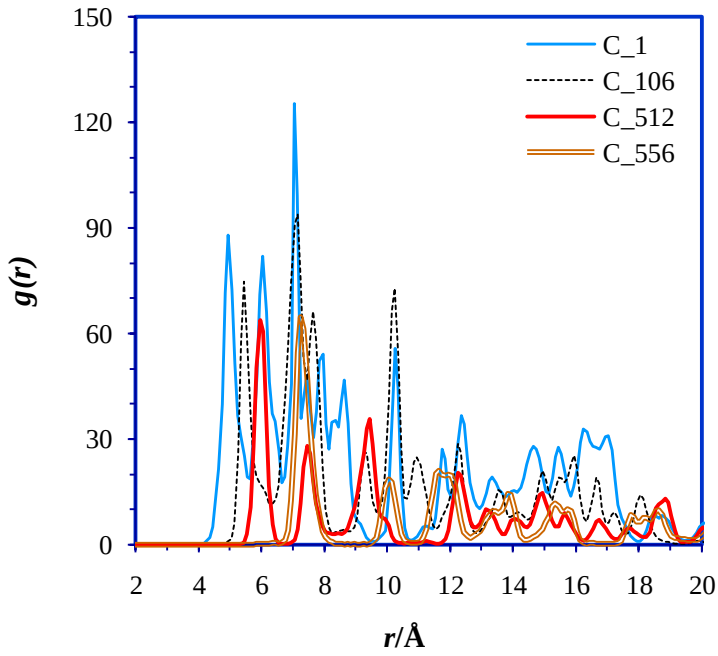

Figure S12. The same as Figure S10, but for C_2.

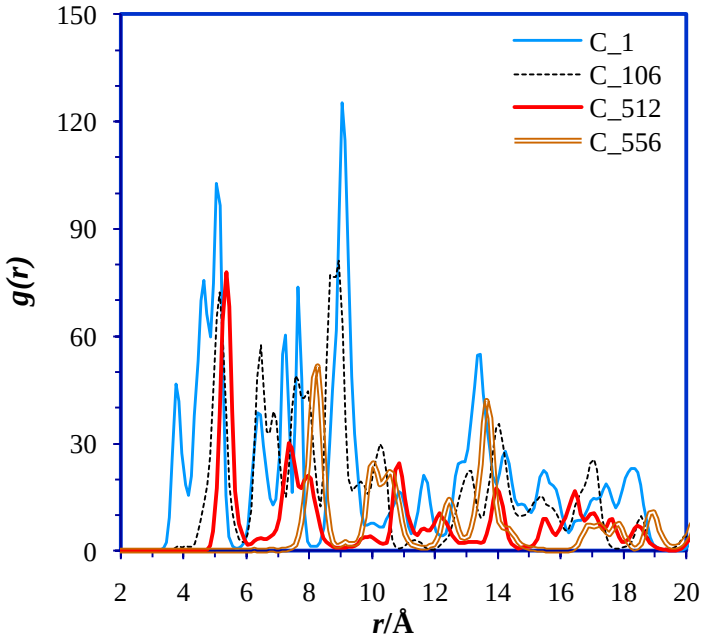

Figure S13. The same as Figure S10, but for C_4.

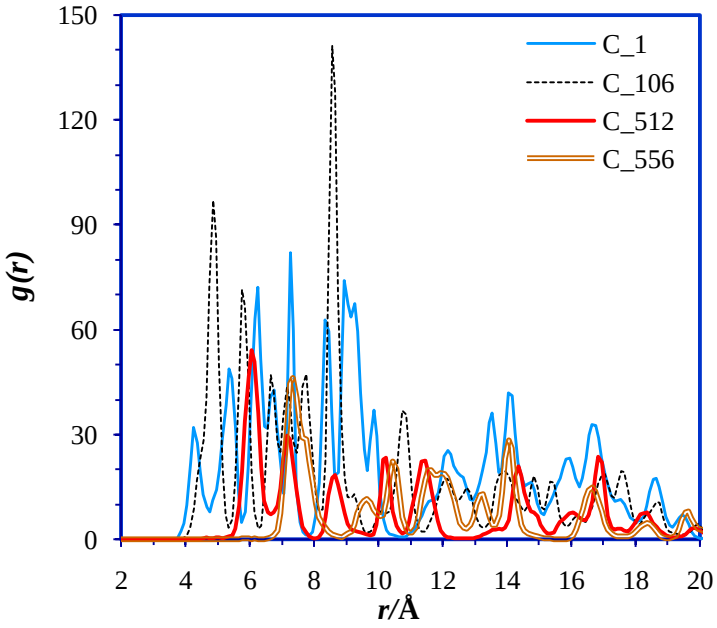

Figure S14. The same as Figure S10, but for C_5.

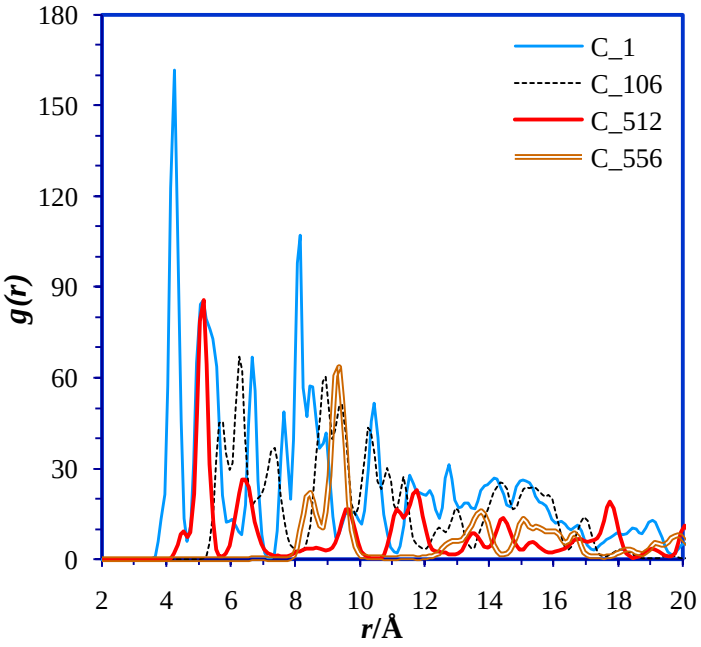

Figure S15. The same as Figure S10, but for C_6.

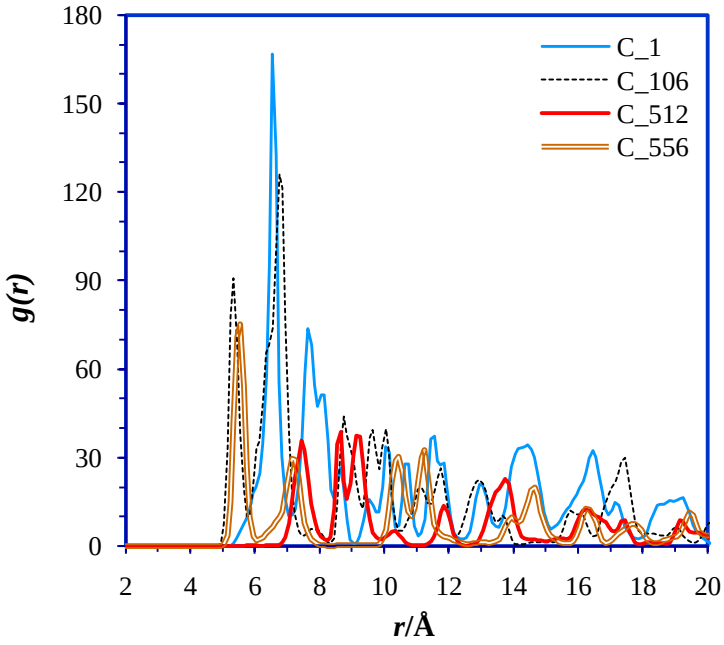

Figure S16. The same as Figure S10, but for C_7.

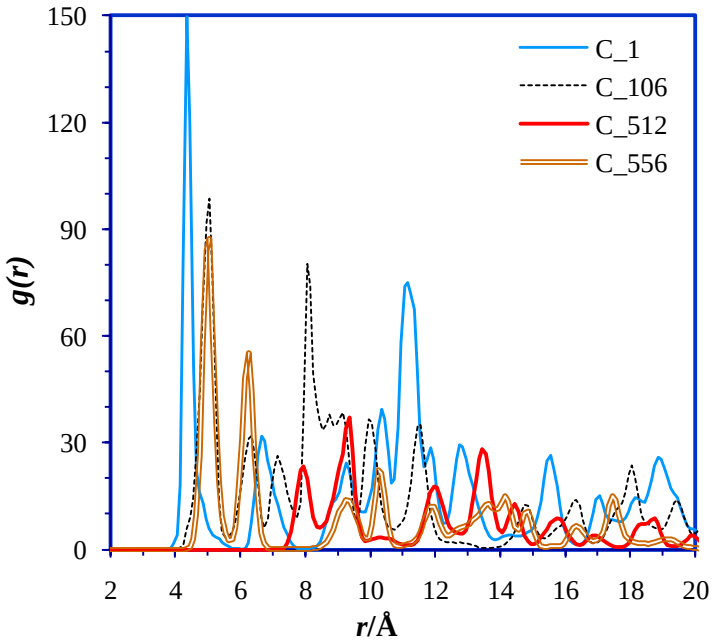

Figure S17. The same as Figure S10, but for C_{10}.

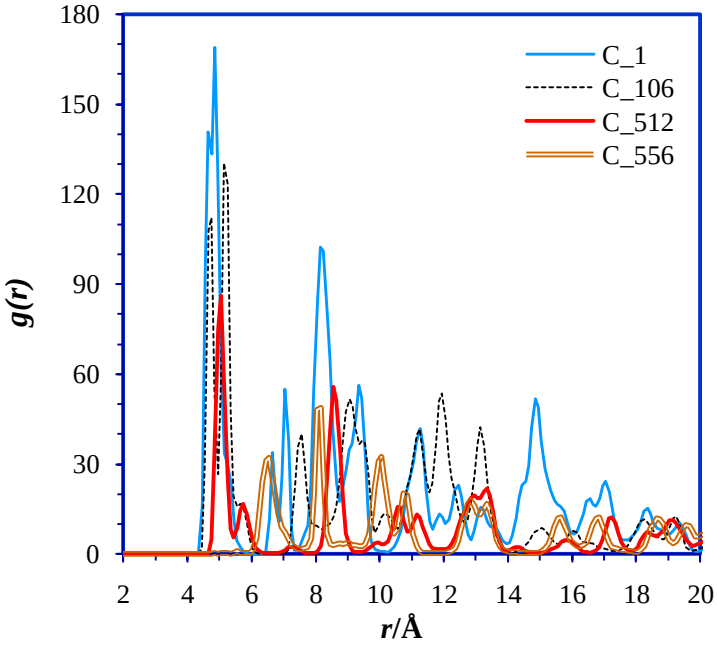

Figure S18. The same as Figure S10, but for P.

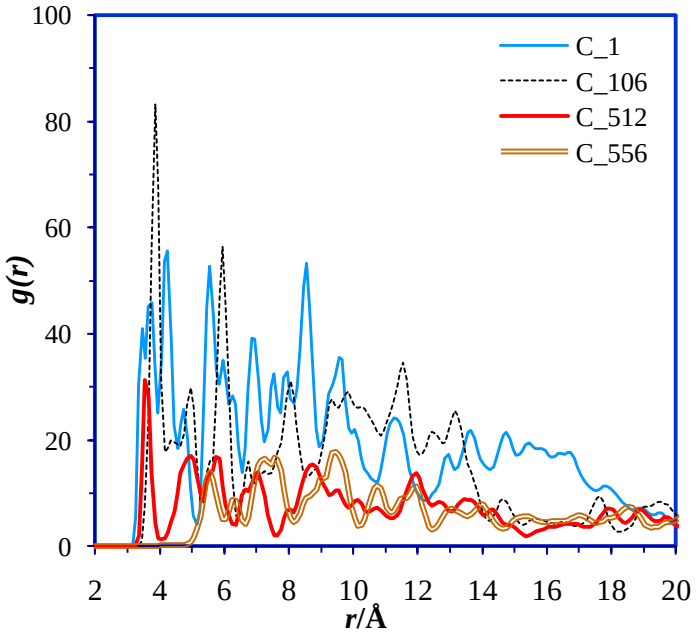

Figure S19. The same as Figure S10, but for F.

Paraffin Intercalated between Graphite Charged Plates: Figures S20 and S21

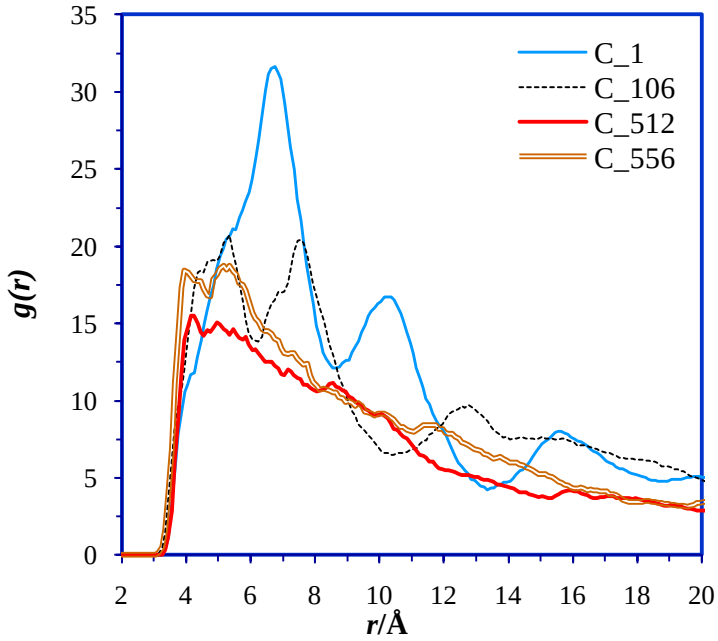

Figure S20. Pair correlation functions (at 323 K) between C_{P1} atom of paraffine and carbon atoms at different locations in between double-C_{600} graphite charged plates.

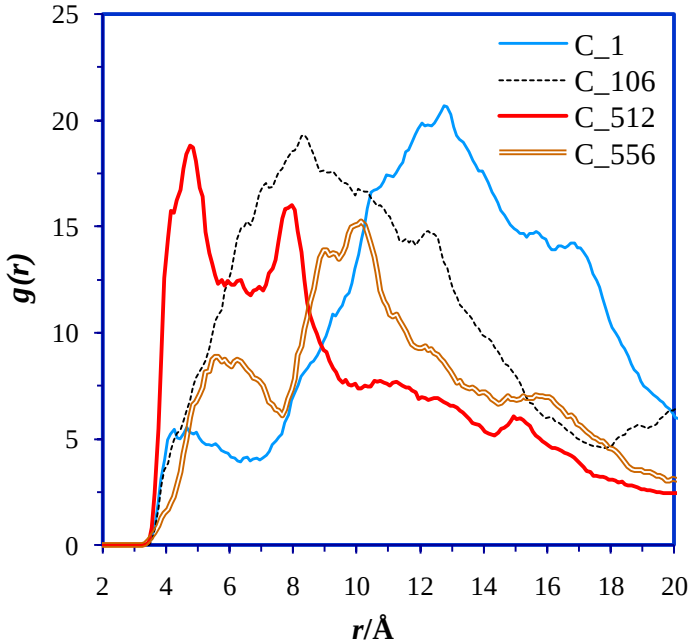

Figure S21. The same as Figure S20, but for C_{P10}.

IL on Graphite Uncharged Plates: Figures 22-31

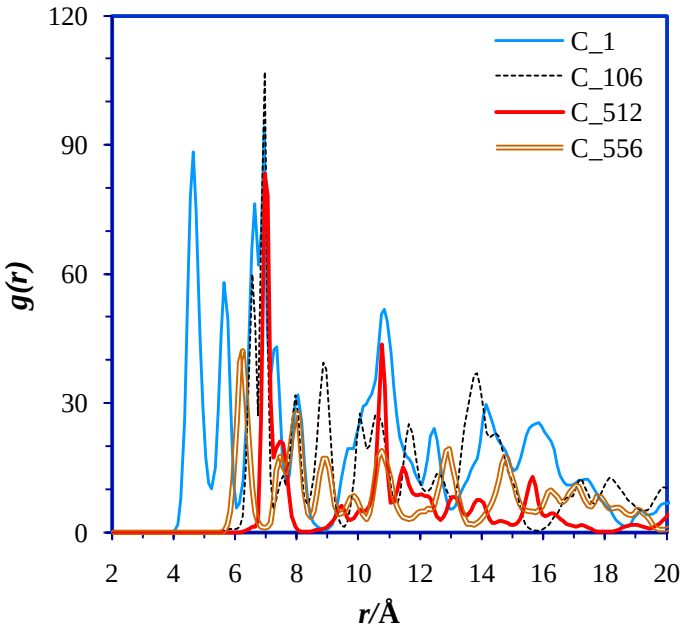

Figure S22. Pair correlation functions (at 323 K) between N_1 atom of monolayer IL and carbon atoms at different locations on double-C_{600} graphite uncharged plates.

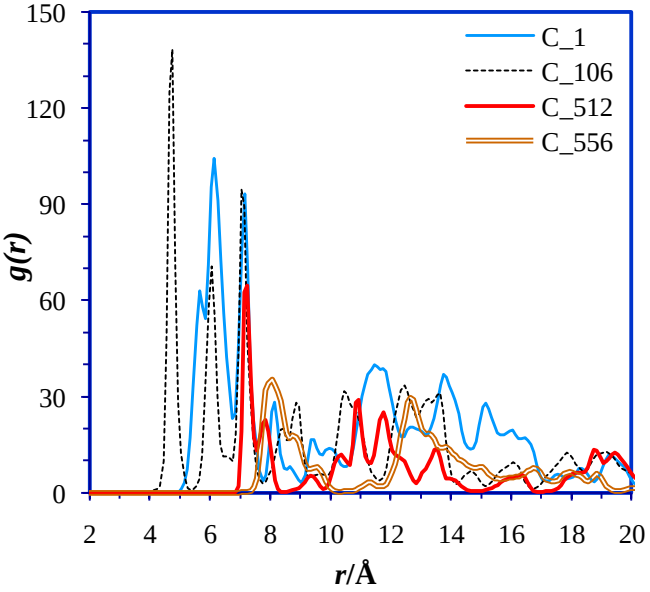

Figure S23. The same as Figure S22, but for N_3.

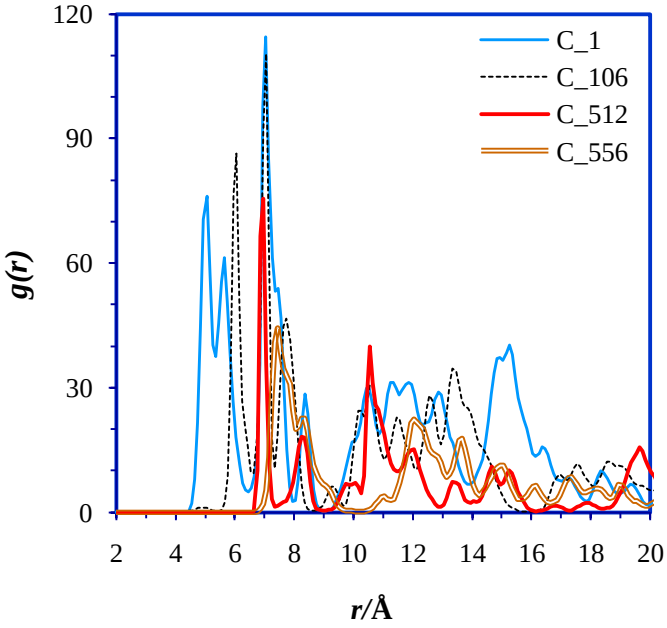

Figure S24. The same as Figure S22, but for C_2.

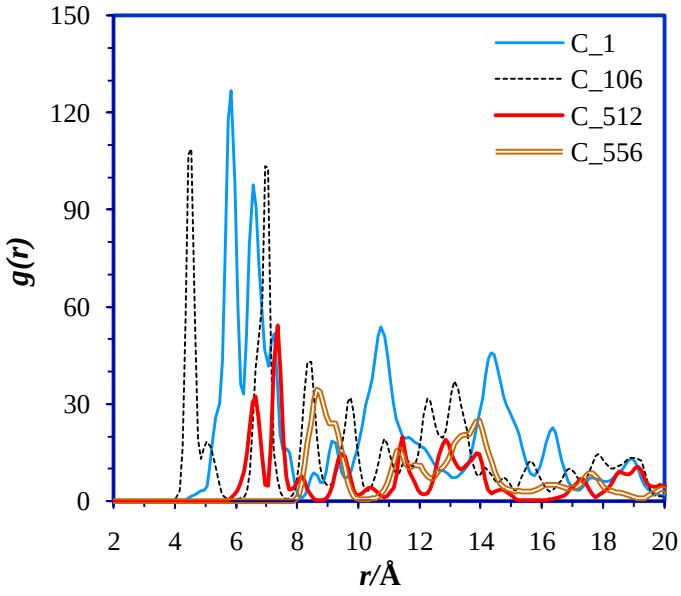

Figure S25. The same as Figure S22, but for C_4.

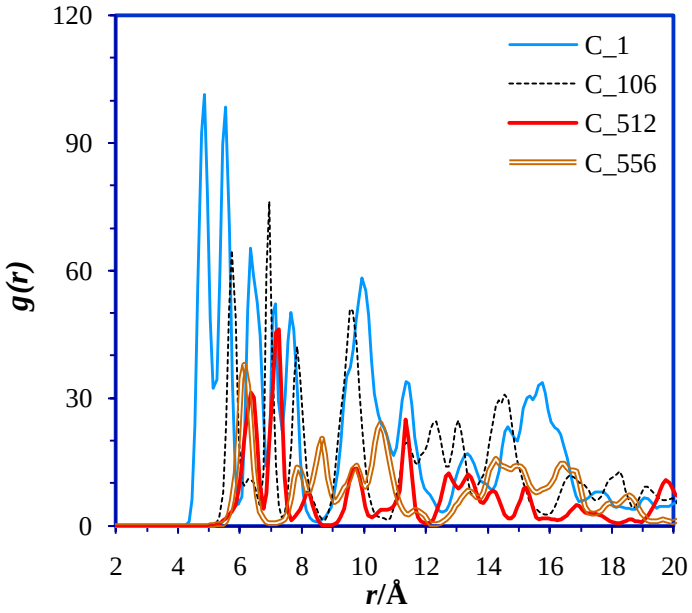

Figure S26. The same as Figure S22, but for C_5.

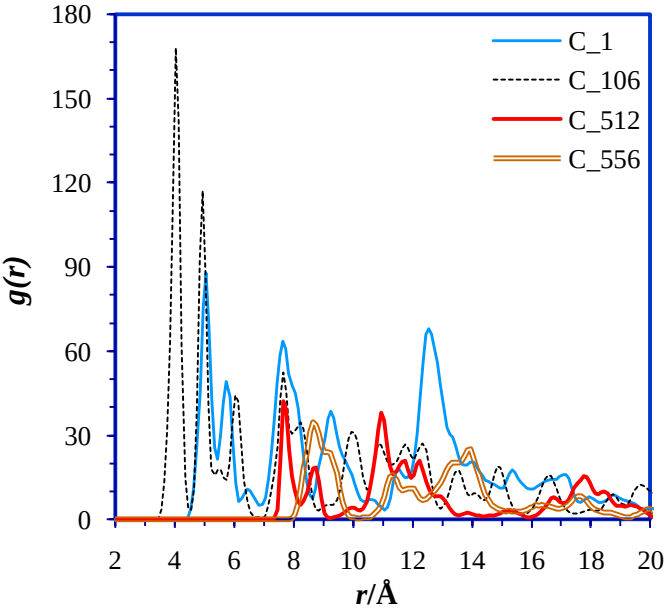

Figure S27. The same as Figure S22, but for C_6.

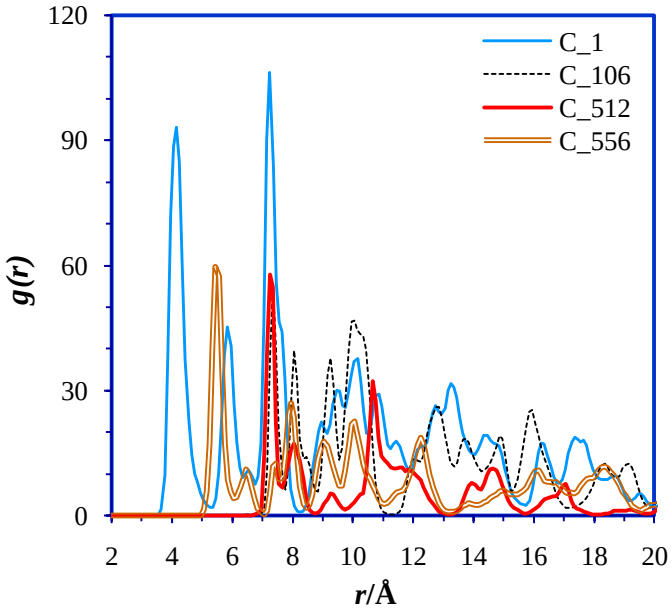

Figure S28. The same as Figure S22, but for C_7.

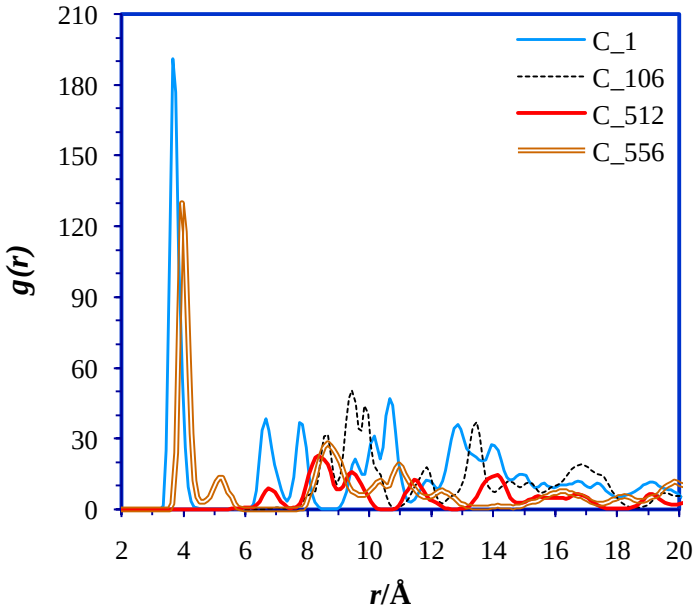

Figure S29. The same as Figure S22, but for C_{10}.

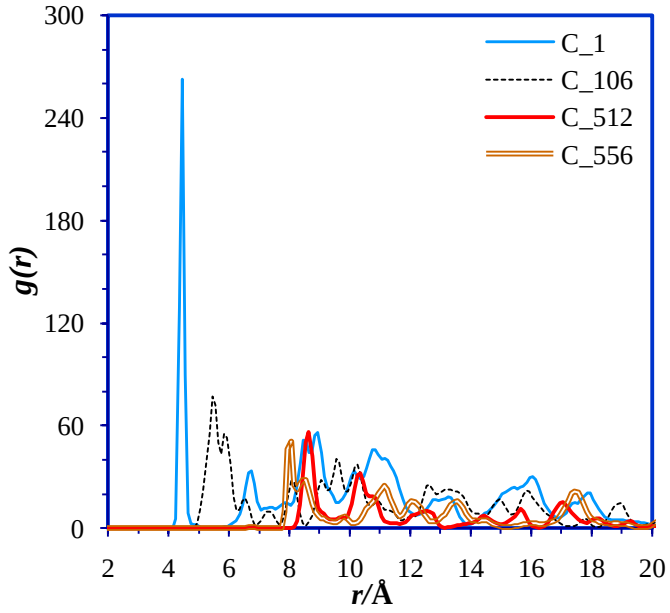

Figure S30. The same as Figure S22, but for P.

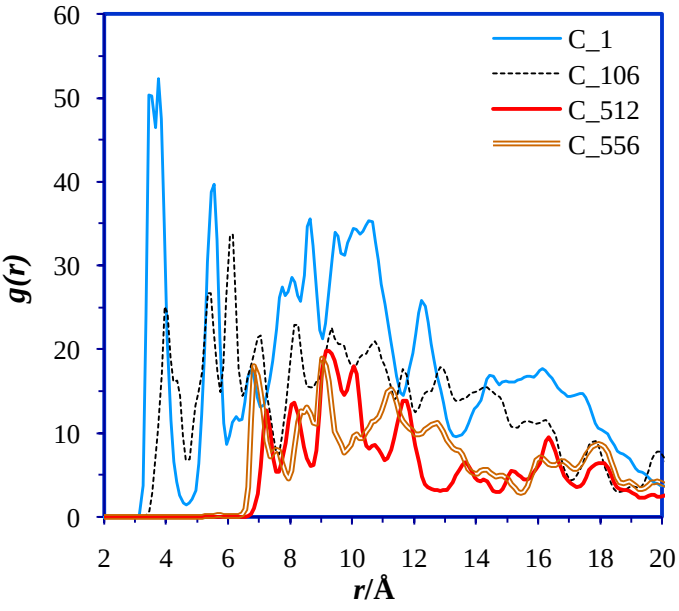

Figure S31. The same as Figure S22, but for F.

IL Intercalated between Graphite Uncharged Plates: Figures S32-S41

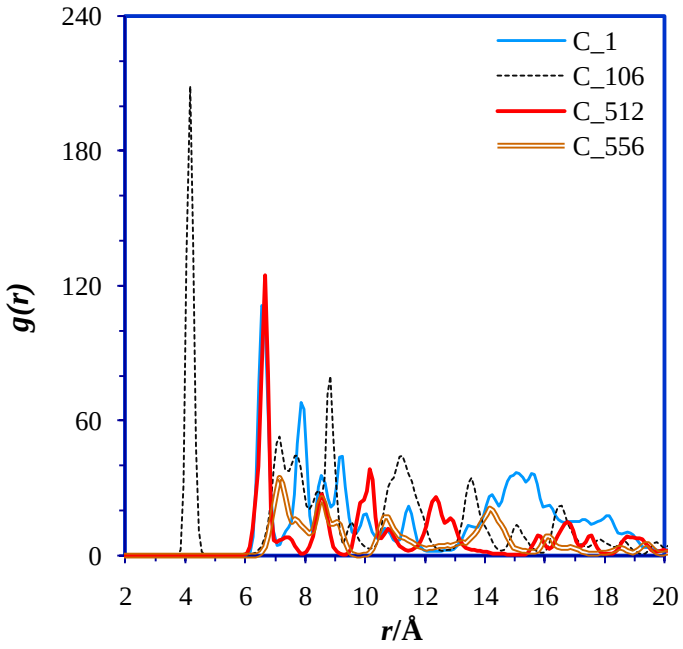

Figure S32. Pair correlation functions (at 323 K) between N_1 atom of monolayer IL and carbon atoms at different locations in between double-C_{600} graphite uncharged plates.

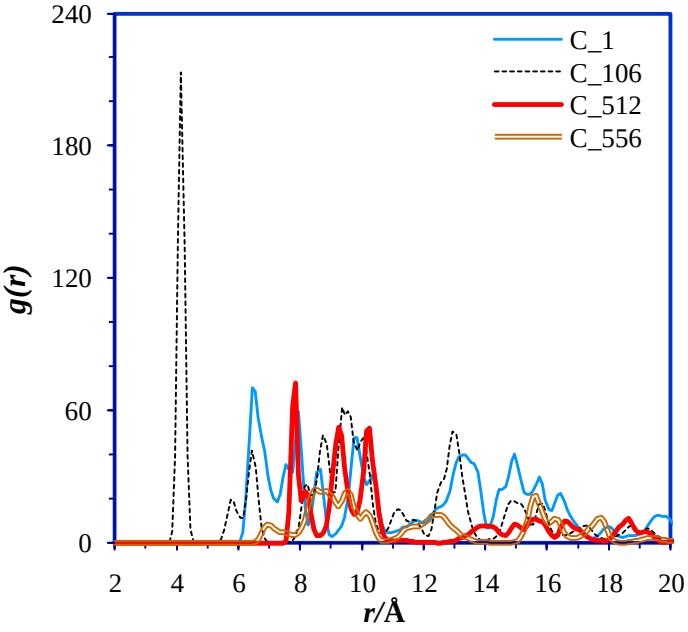

Figure S33. The same as Figure S32, but for N_3.

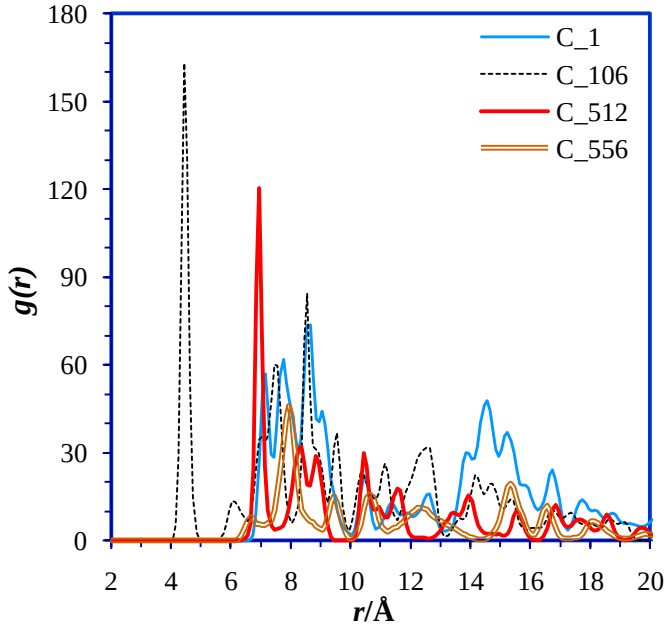

Figure S34. The same as Figure S32, but for C_2.

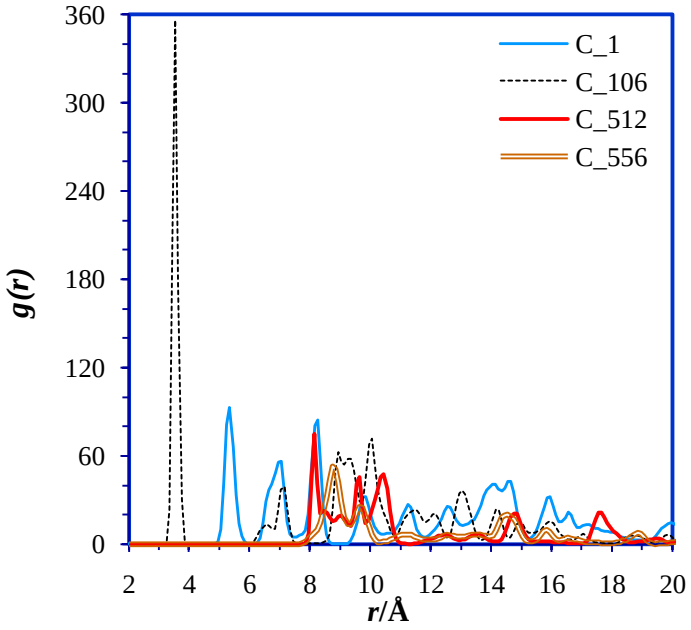

Figure S35. The same as Figure S32, but for C_4.

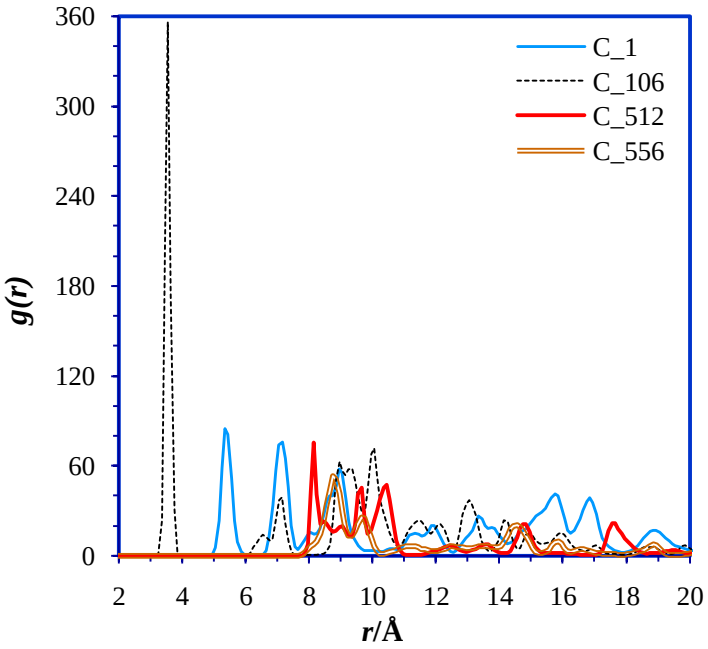

Figure S36. The same as Figure S32, but for C_5.

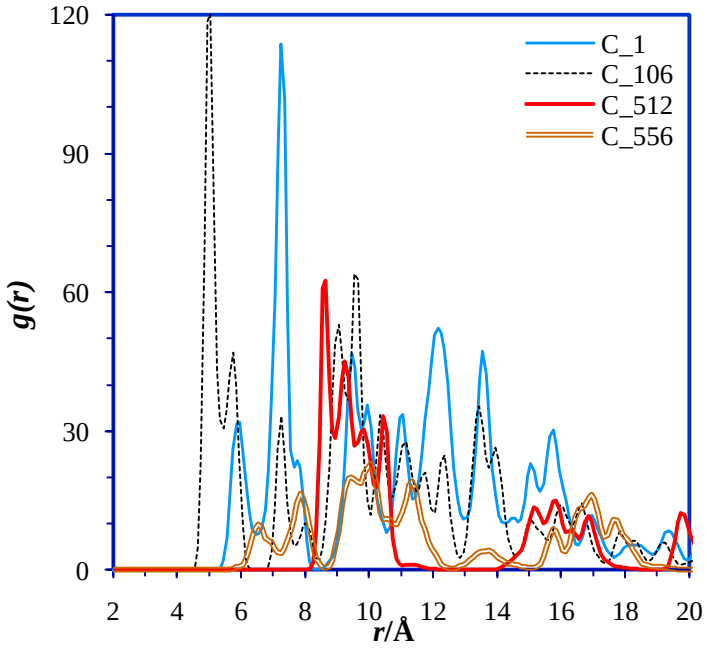

Figure S37. The same as Figure S32, but for C_6.

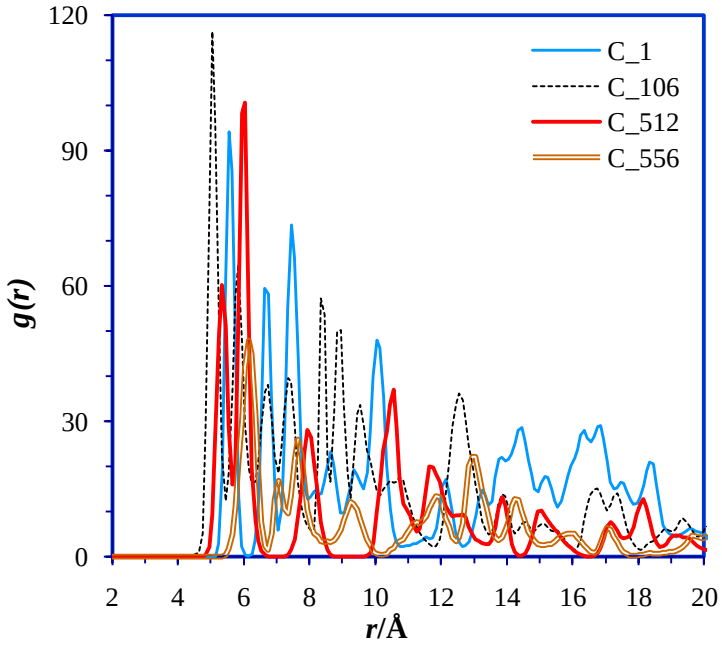

Figure S38. The same as Figure S32, but for C_7.

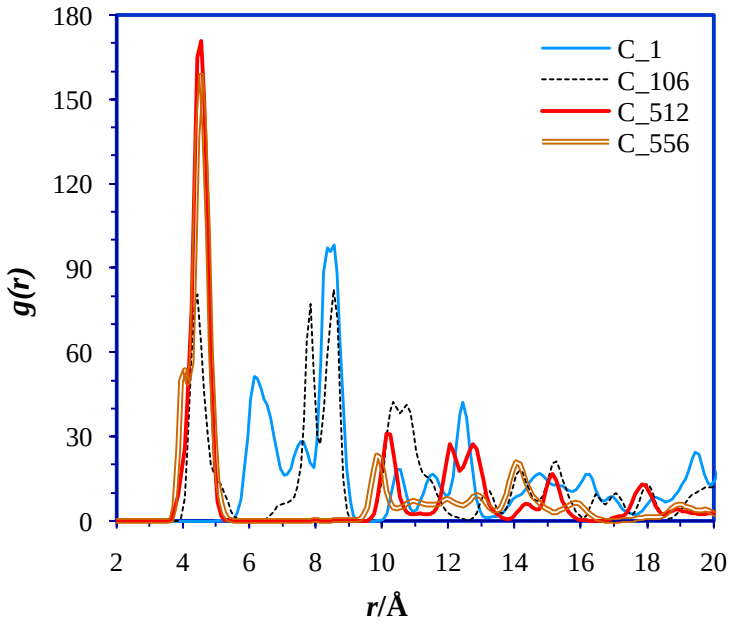

Figure S39. The same as Figure S32, but for C_{10}.

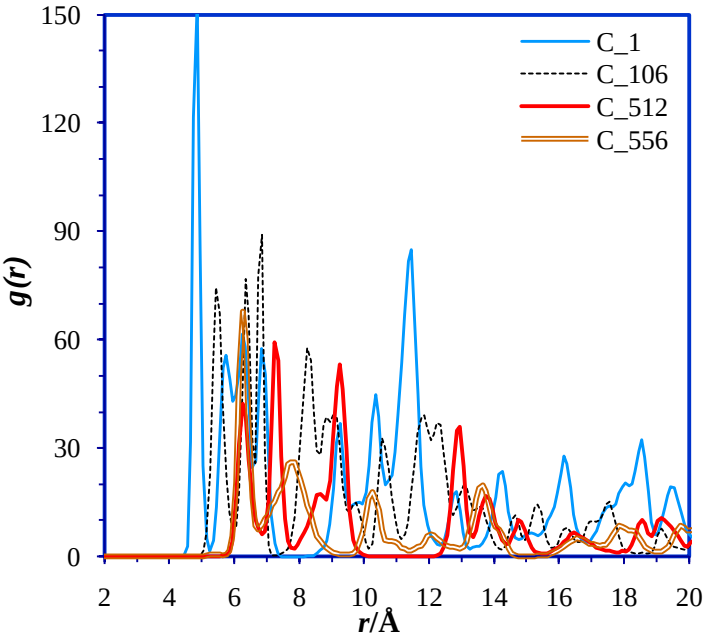

Figure S40. The same as Figure S32, but for P.

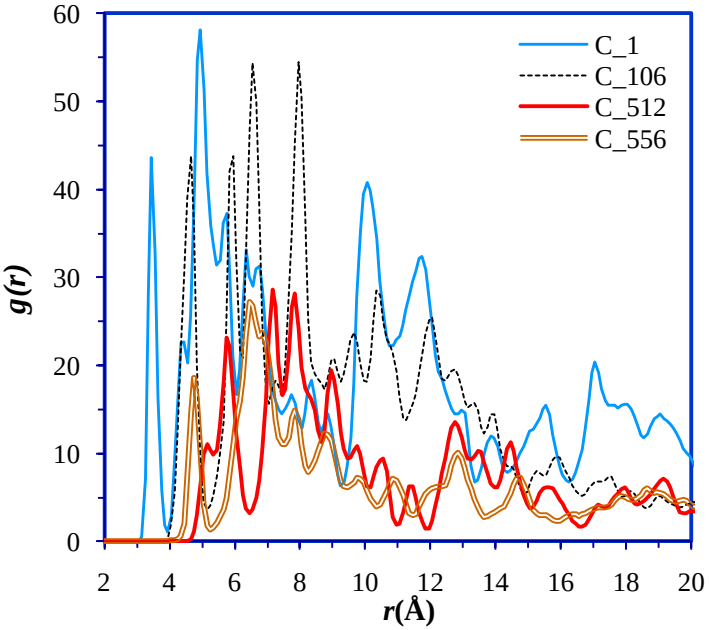

Figure S41. The same as Figure S32, but for F.

Paraffin on Graphite Uncharged Plates: Figures 42 and 43

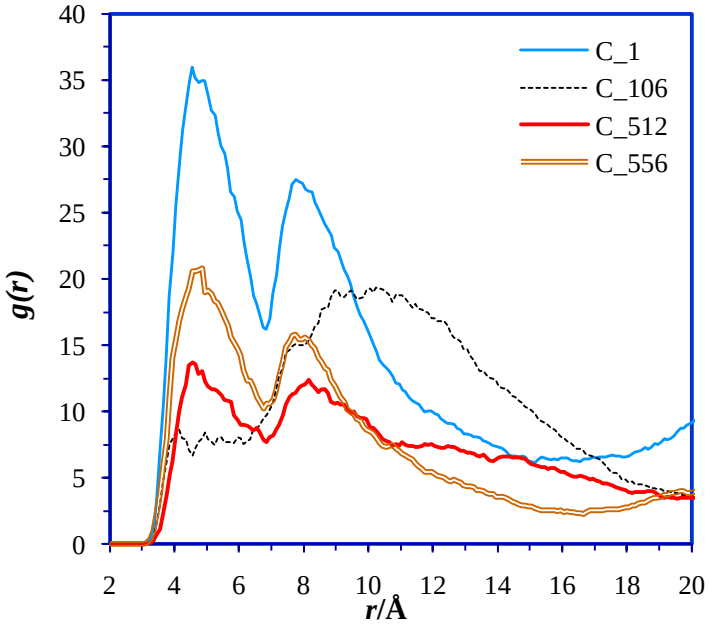

Figure S42. Pair correlation functions (at 323 K) between C_{P1} atom of monolayer IL and carbon atoms at different locations on double-C_{600} graphite uncharged plates.

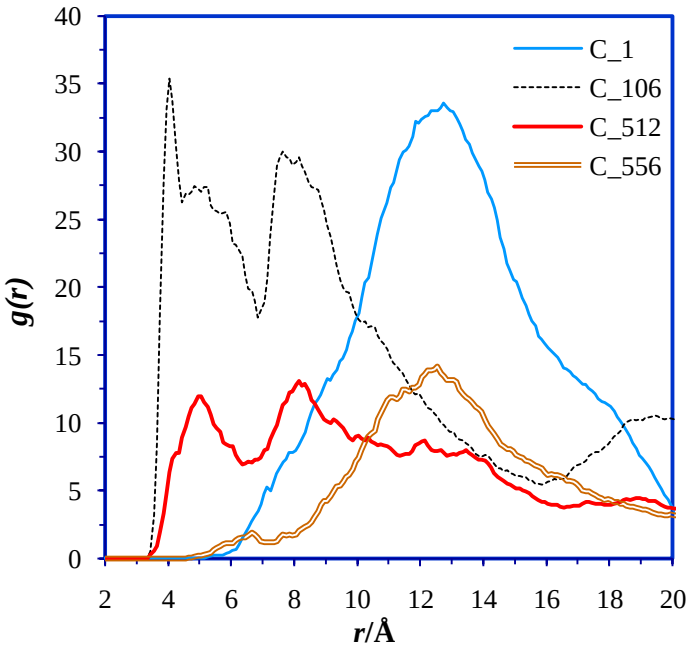

Figure S43. The same as Figure S42 but for C_{P10}.

Paraffin Intercalated between Graphite Uncharged Plates: Figures 44 and 45

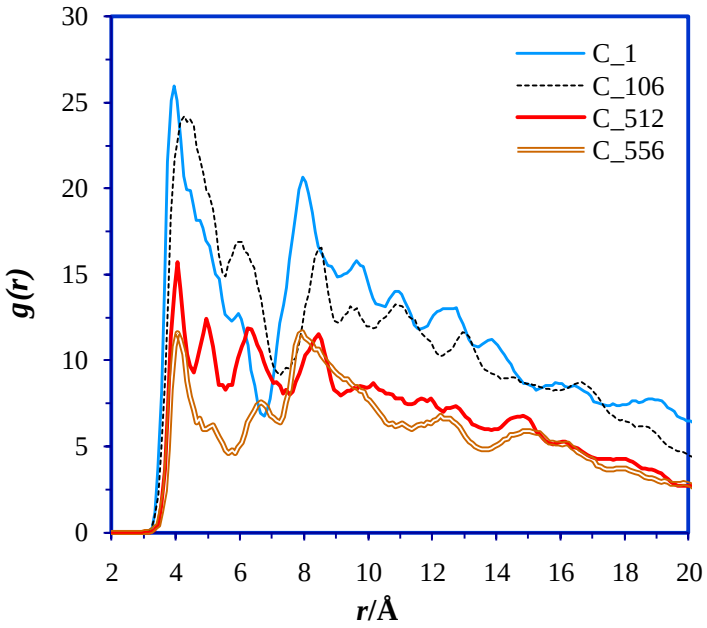

Figure S44. Pair correlation functions (at 323 K) between C_{P1} atom of monolayer IL and carbon atoms at different locations in between double-C_{600} graphite uncharged plates.

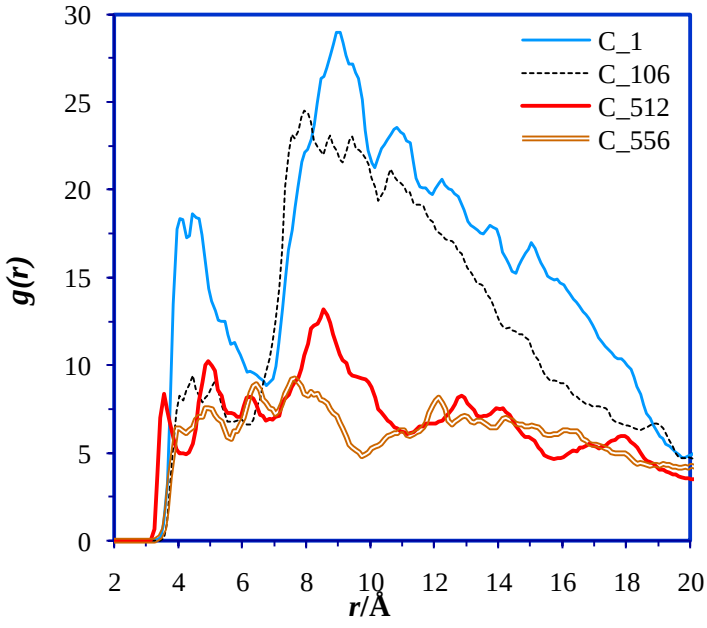

Figure S45. The same as Figure S44 but for C_{P10}.