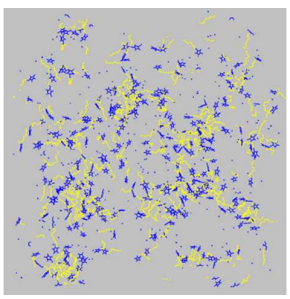
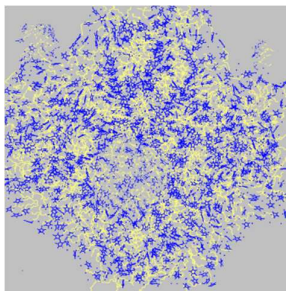
Supporting information

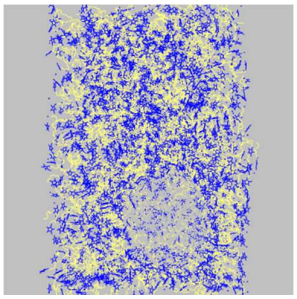
Unilamellar vesicle formation and microscopic structure of ionic liquids in aqueous solutions



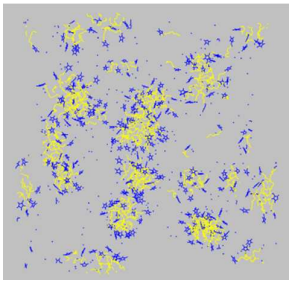
(a) C10-I



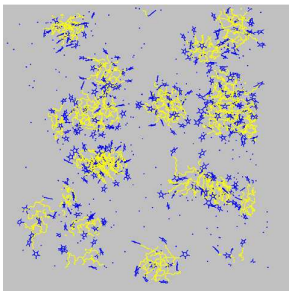
(b) C10-II



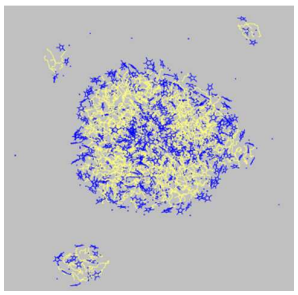
(c) C10-III



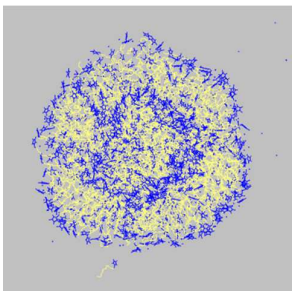
(a) C12-I



(d) C14-I

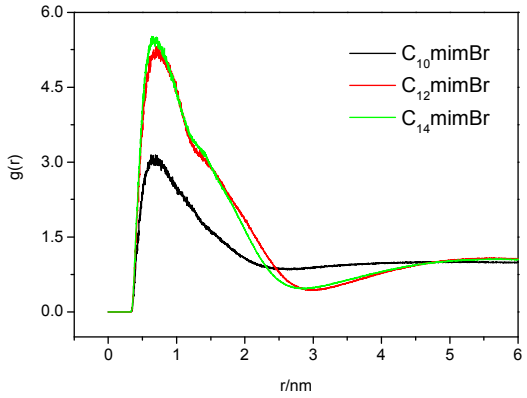


(e) C14-II

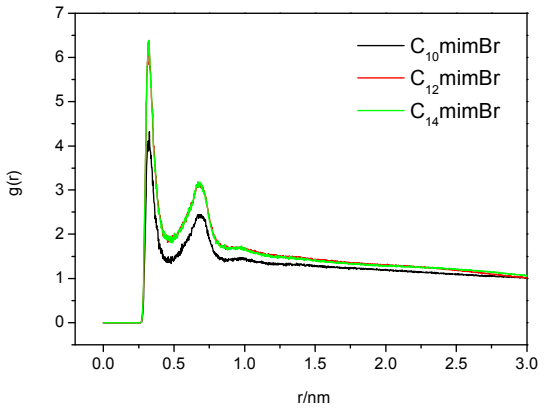


(f) C14-III

Figure S1. Cross-sectional views of the snapshots for cluster structures of $[C_x mim]Br$ (x=10, 12, 14) at different concentrations. Blue and yellow colors are used to depict the polar (imidazolium-ring, the connected CH_2 & CH_3, and anion) and nonpolar (alkyl chain in cation, from C2 to C12) part, respectively. Water is not shown.



(a)



(b)

Figure S2. Radial distribution functions between alkyl group of cations in C10-I, C12-I and C14-I systems. (a) chain terminal C with itself, (b) H5-Br

Table S1. Intermolecular energy for aqueous solution of [$C_n$mim]Br (n=10, 12, 14). (Ca: cation, An: anion, W: water)

a) C10-I system

	Electrostatic (kJ/mol)	Lennard-Jones (kJ/mol)	Intermolecular energy (kJ/mol)
Ca-Ca	113.22	-26.18	87.04
Ca-An	-225.10	-0.56	-225.66
An-An	52.38	-0.02	52.36
Ca-W	-280.84	-79.32	-360.16
An-W	-540.35	34.54	-505.81

b) C12-I system

	Electrostatic (kJ/mol)	Lennard-Jones (kJ/mol)	Intermolecular energy (kJ/mol)
Ca-Ca	150.11	-43.16	106.95
Ca-An	-271.03	-0.69	-271.72
An-An	58.20	-0.02	58.18
Ca-W	-333.36	-78.03	-411.39
An-W	-499.73	34.43	-465.30

c) C14-I system

	Electrostatic (kJ/mol)	Lennard-Jones (kJ/mol)	Intermolecular energy (kJ/mol)
Ca-Ca	170.56	-54.60	115.96
Ca-An	-285.76	-0.70	-286.46
An-An	60.11	-0.02	60.09
Ca-W	-369.09	-76.54	-445.63
An-W	-482.62	34.30	-448.32