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Insight into Structure-Antibacterial Activity of Amino Cation-based and Acetate Anion-based Ionic Liquids from the Computational Interaction with POPC Phospholipid Bilayer

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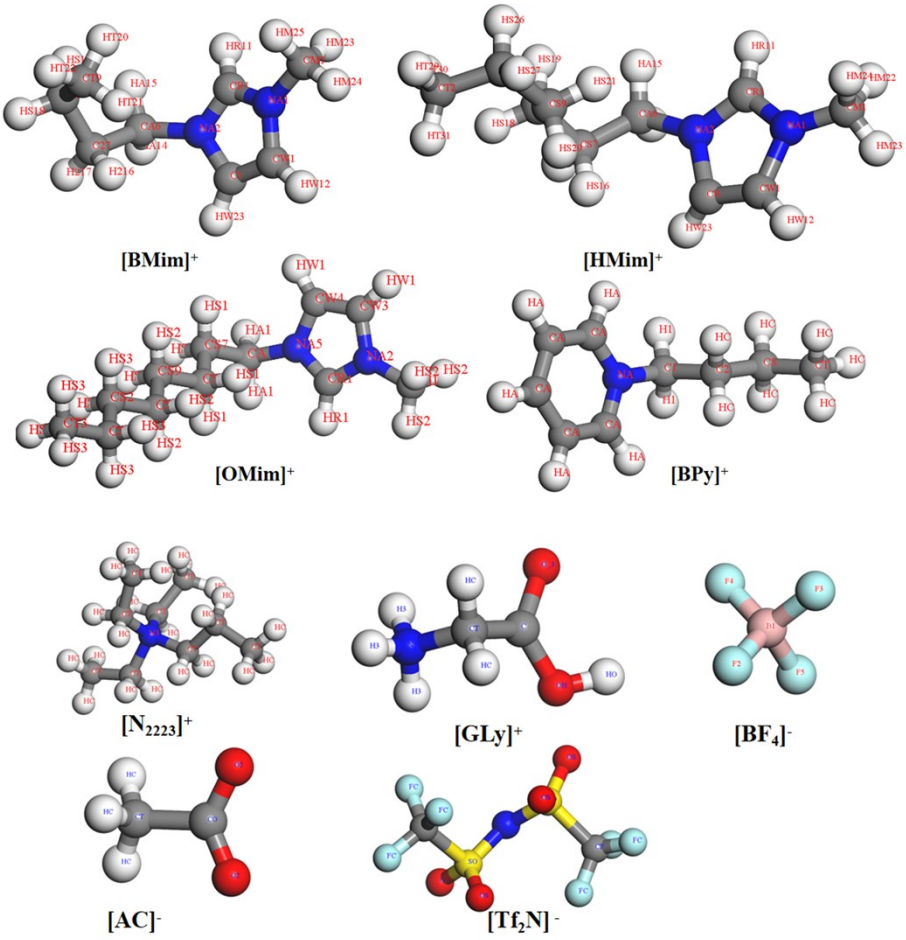

Figure S1. The atom labels and series of cations and anions in this work.

Table S1. The L-J potential of the BMIM, HMIM, and OMIM cations.

Atom name	C6	C12
N	3.35e-03	3.95e-06
CR	3.34e-03	4.69e-06
CW	3.34e-03	4.69e-06
CM	2.03e-03	3.73e-06
CA	2.03e-03	3.73e-06
CS	2.03e-03	3.73e-06
CT	2.03e-03	3.73e-06
HR	1.30e-05	3.37e-10
HW	1.30e-05	3.37e-10
HA	2.52e-05	1.26e-09
HS	2.52e-05	1.26e-09
HT	2.52e-05	1.26e-09

Table S2. Charge of the BMIM, HMIM, and OMIM cations.

$[BMIM]^+$		$[HMIM]^+$		$[OMIM]^+$	
Atom	charge	Atom	charge	Atom	charge
CR1	-0.11	CR11	-0.09	CR11	-0.09
NA1	0.24	NA12	0.22	NA12	0.22
CW1	-0.26	CW13	-0.24	CW13	-0.24
CW2	-0.24	CW24	-0.24	CW24	-0.24
NA2	0.27	NA25	0.22	NA25	0.22
CA6	-0.29	CAL6	-0.17	CA6	-0.17
CS7	0.10	CSL7	-0.12	CS7	-0.12
CS8	0.14	CSL8	-0.12	CS8	-0.12
CT9	-0.32	CSL9	-0.12	CS9	-0.12
CM10	-0.36	CM10	-0.35	CM10	-0.35
HR11	0.21	HR11	0.21	HR11	0.21
HW12	0.27	HW12	0.27	HW12	0.27
HW23	0.27	HW13	0.27	HW13	0.27
HA14	0.15	HA14	0.18	HA14	0.18
HA15	0.15	HA15	0.18	HA15	0.18
HS16	0.02	HS16	0.06	HS16	0.06
HS17	0.02	HS17	0.06	HS17	0.06
HS18	-0.01	HS18	0.06	HS18	0.06
HS19	-0.01	HS19	0.06	HS19	0.06
HT20	0.10	HS20	0.06	HS20	0.06
HT21	0.10	HS21	0.06	HS21	0.06
HT22	0.10	HM22	0.18	HM22	0.18
HM23	0.16	HM23	0.18	HM23	0.18
HM24	0.16	HM24	0.18	HM24	0.18
HM25	0.16	CSL25	-0.12	CS25	-0.12
		HS26	0.06	HS26	0.06
		HS27	0.06	HS27	0.06
		CT28	-0.24	CS28	-0.12
		HT29	0.08	HS29	0.06
		HT30	0.08	HS30	0.06
		HT31	0.08	CS31	-0.12

	HS32	0.06
	HS33	0.06
	CT34	-0.24
	HT35	0.08
	HT36	0.08
	HT37	0.08

Table S3. The L-J potential and charge of the $[BPy]^+$ cation.

Atom name	C6	C12	charge
C1	2.03e-03	3.73e-06	0.2444
C2	2.03e-03	3.73e-06	-0.1600
CS	2.03e-03	3.73e-06	-0.2417
CT1	2.03e-03	3.73e-06	-0.3599
CA	2.77e-03	6.55e-06	0.1013
HA	1.01e-04	2.03e-08	0.2095
HC	1.23e-04	2.99e-08	0.2665
H1	1.23e-04	2.99e-08	0.2703
NA	4.80e-03	8.09e-06	0.1567

Table S4. The L-J potential and charge of the $[N_{2223}]^+$ cation

Atom name	C6	C12	charge
N3	3.35e-03	3.95e-06	0
CT1	2.03E-03	3.73e-06	-0.18
CT2	2.03e-03	3.73e-06	-0.12
HC	1.23e-04	2.99e-08	0.06

Table S5. The L-J potential and charge of the $[GLy]^+$ cation

Atom name	C6	C12	charge
HC	1.23e-04	2.99e-08	0.12
C	4.89e-03	1.36e-05	0.66
OH	2.07e-03	1.51e-06	-0.60
O_3	2.36e-03	1.59e-06	-0.44
HO	0	0	0.48
N3	3.35e-03	3.95e-06	-0.32
H3	1.23e-04	2.99e-08	0.33
CT	1.23e-04	2.99e-08	-0.01

Table S6. The L-J potential and charge of the $[OAc]^-$ anion

Atom name	C6	C12	charge
CT	1.25e-02	1.15e-04	-0.253
CO	2.95e-03	6.40e-06	1.027
HC	8.53e-08	6.86e-15	0.002
O2	5.45e-01	2.51e-01	-0.890

Table S7. The L-J potential and charge of the $[BF_4]^-$ anion

Atom name	C6	C12	charge
B	3.35e-03	7.05e-06	0.96
F	9.42e-04	8.69e-07	1.027

Table S8. The L-J potential and charge of the $[OAc]^-$ anion

Atom name	C6	C12	charge
SO	8.37E-03	1.68E-05	1.02
OS	2.36E-03	1.59E-06	-0.53
FC	5.85E-04	3.85E-07	-0.16
CF	2.03E-03	3.73E-06	0.35
NI	3.35E-03	3.95E-06	-0.66

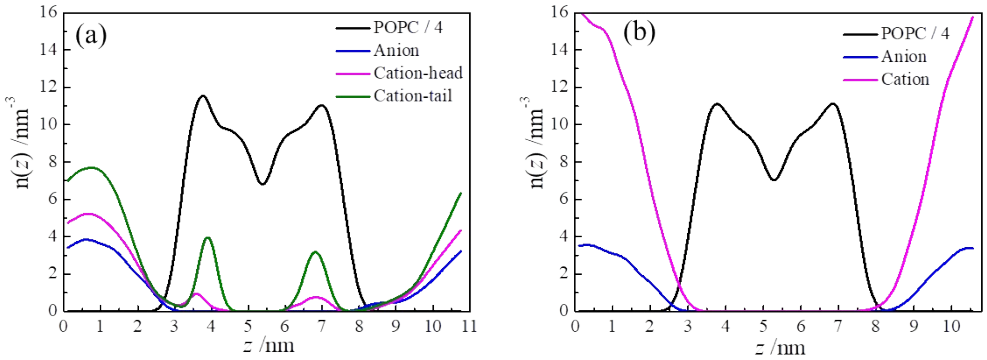

Figure S2. Number density profiles of the POPC bilayer with water solution in presence of ILs with different alkyl chain length of cations. (a) [BPy][OAc] and (b) [N_{2223}][OAc].

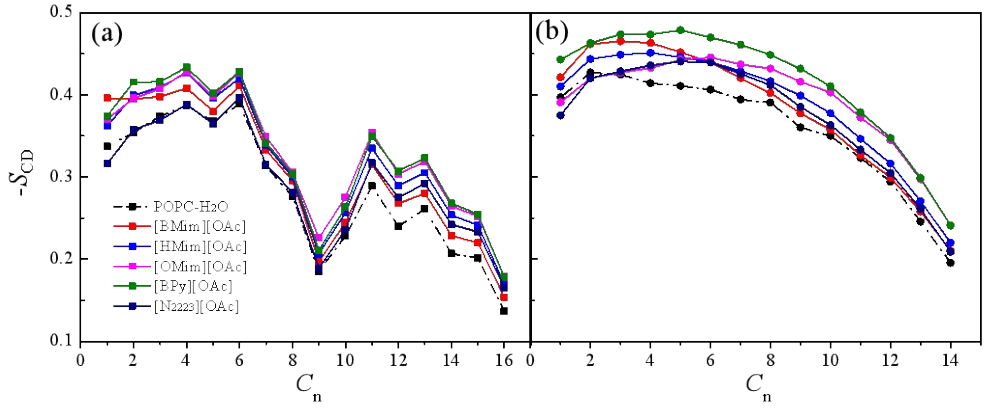

Figure S3. Deuterium order parameters for the *sn*-1 (a, oleoyl chain) and *sn*-2 (b, palmitoyl chain) tails for the hydrated POPC bilayer in contact with ILs.

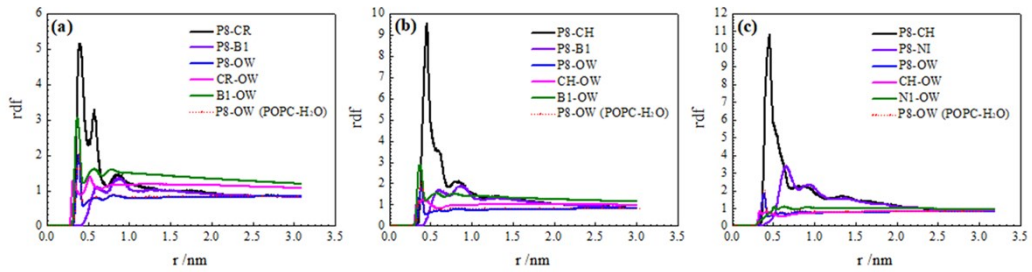

Figure S4. Radial pair distribution functions (rdf) for selected atomic pairs in POPC-H2O and POPC-IL-H2O systems. Atom names: (P8) phosphorus atom in POPC, (CR) carbon atom between two N atoms in alkyl chain imidazole, (B1) boron atom in tetrafluoroborate anions, (OW) oxygen atom in

H2O, (NI) nitrogen atom in bis(trifluoromethanesulfonyl)imide anions, (CH) carbon atom in amino acid cations.

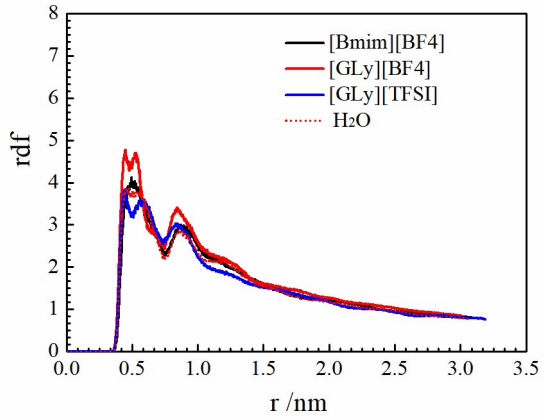

Figure S5. Radial pair distribution functions (rdf) for P8-P8 atom pairs in POPC-H_2O and POPC-IL-H_2O systems.