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

SUPPORTING INFORMATION
PCCP

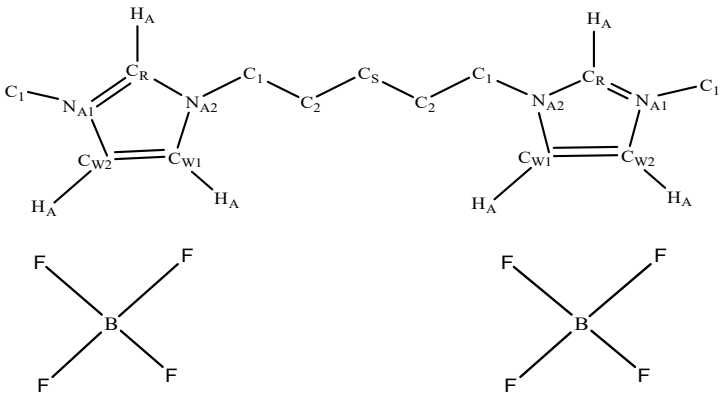
Extension of Transferable Coarse-Grained Models to Dicationic Ionic Liquids

Majid Moosavi*, Zahra Ostadsharif Memar

Department of Chemistry, University of Isfahan, Isfahan 81746-73441, Iran

*Corresponding author. Tel.: +98-313-7934942; Fax: +98-313-668-9732
E-mail: m.mousavi@sci.ui.ac.ir

Table S1 Force field parameters for $[C_5(mim)_2][BF_4]_2$ DIL and also for $[C_n(mim)_2][BF_4]_2$ (with n=3,6,9,12) DILs in the AA model



Lennard-Jones parameters

Atom	ε/kcal.mol^{-1}	σ/Å
C_1	0.066	3.50
C_2	0.066	3.50
C_C	0.066	3.50
C_R	0.070	3.55
C_W	0.070	3.55
H_A	0.030	2.42
H_C	0.030	2.50
H_1	0.030	2.50
N_A	0.170	3.25
B	0.095	3.58
F	0.061	3.12

Bond parameters

Atom	Atom	ε/kcal.mol^{-1}	σ/Å
C_W	H_A	183.500	1.08
C_1	H_1	170.000	1.09
C_2	H_C	170.000	1.09
C_S	H_C	170.000	1.09
C_R	N_A	238.528	1.32
C_{W1}	C_{W2}	260.038	1.34
C_1	NA	168.499	1.47
C_1	C_2	133.963	1.53
C_2	C_S	133.963	1.53
C_W	N_A	213.552	1.38
B	F	290.000	1.39

Angle parameters

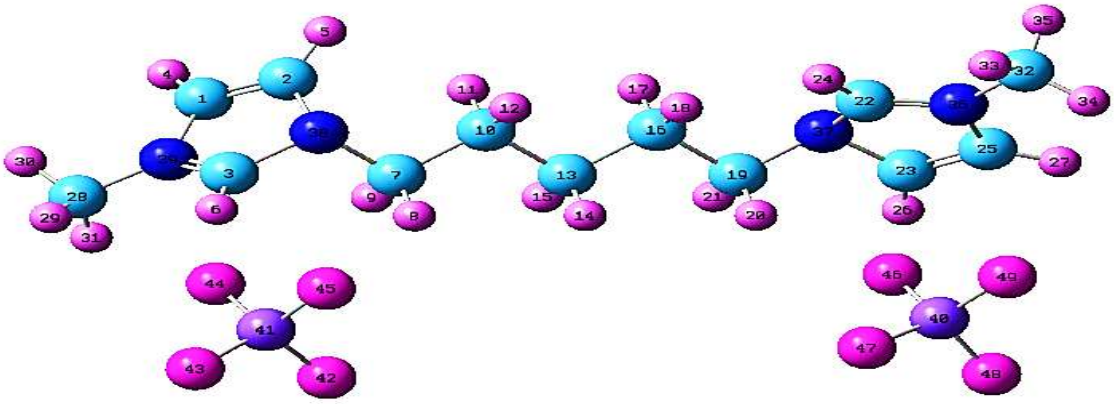
Atom	Atom	Atom	k_θ / kcal.mol^{-1}.rad^{-2}	θeq / deg
C_R	N_A	C_W	34.967	108.00
C_W	N_A	C_1	34.967	125.60
C_R	N_A	C_1	34.967	126.40
N_A	C_R	H_A	17.483	125.10
N_A	C_R	N_A	34.967	109.80
N_A	C_W	C_W	34.967	107.10
N_A	C_W	H_A	17.483	122.00
C_W	C_W	H_A	17.483	130.90
N_A	C_1	H_1	37.429	110.70
C_1	C_2	H_C	37.429	110.70
C_2	C_1	H_1	37.429	110.70
C_S	C_2	H_C	37.429	110.70
C_2	C_S	H_C	37.429	110.70
C_1	C_2	C_S	50.000	112.70
C_2	C_S	C_2	50.000	112.70
N_A	C_1	C_2	50.000	112.70
H_1	C_1	H_1	32.995	107.80
H_C	C_2	H_C	32.995	107.80
H_C	C_S	H_C	32.995	107.80

Proper dihedral parameters

Atom	Atom	Atom	Atom	kϕ,1/kcal.mol^{-1}	kϕ,2/kcal.mol^{-1}	kϕ,3/kcal.mol^{-1}	kϕ,4/kcal.mol^{-1}
X	C_R	N_A	X	0.00	4.65	0.00	0.00
X	C_W	C_W	X	0.00	10.75	0.00	0.00
X	C_W	N_A	X	0.00	2.30	0.00	0.00
C_W	N_A	C_1	H_1	0.00	0.00	0.13	0.00
C_R	N_A	C_1	H_1	0.00	0.00	0.00	0.00
C_W	N_A	C_1	C_2	-1.38	1.06	0.21	0.00
C_R	N_A	C_1	C_2	-0.77	0.00	0.00	0.00
N_A	C_1	C_2	C_S	0.18	-0.16	0.24	0.00
N_A	C_1	C_2	H_C	0.00	0.00	0.00	0.00
C_1	C_2	C_S	H_C	0.00	0.00	0.37	0.00
C_2	C_S	C_2	H_C	0.00	0.00	0.37	0.00
H_C	C_2	C_1	H_1	0.00	0.00	0.32	0.00
H_C	C_2	C_S	H_C	0.00	0.00	0.32	0.00

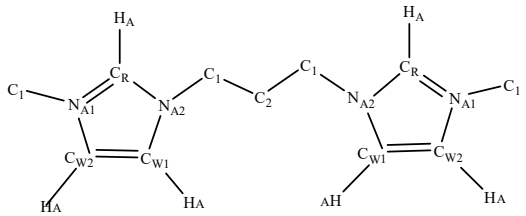
Improper dihedral parameters

Atom	Atom	Atom	Atom	K_ϕ / kcal.mol^{-1}	d	n
X	N_A	**X**	**X**	1.00	-1.00	2.00
X	C_W	**X**	**X**	1.10	-1.00	2.00
X	C_R	**X**	**X**	1.10	-1.00	2.00

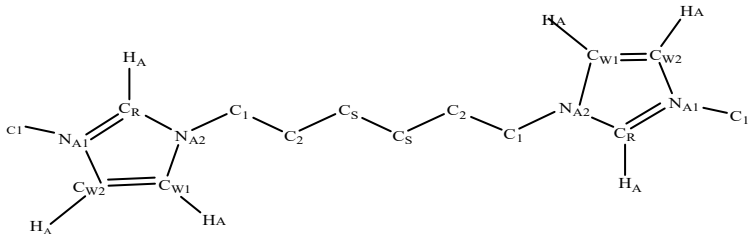


Partial charges in CHELPG method

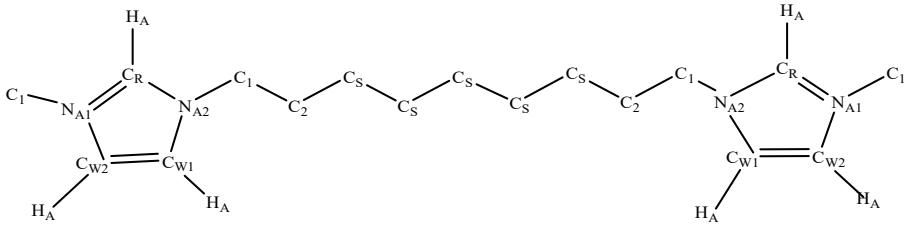
$[C_5(mim)_2]^{+2}$				$[BF_4]^-$	
Atom	q / e	Atom	q / e	Atom	q / e
C_1	-0.1703	H_{17}	0.1857	B_1	1.1453
C_2	-0.1307	C_{12}	-0.1684	F_1	-0.5250
C_3	-0.0581	H_{18}	0.1913	F_2	-0.5236
H_1	0.1765	H_{19}	0.1808	F_3	-0.4818
H_2	0.1708	C_{13}	-0.1841	F_4	-0.4962
H_3	0.2102	H_{20}	0.1717	B_1	1.0887
C_4	0.0962	H_{21}	0.0789	F_5	-0.5154
H_4	0.0783	H_{22}	0.1146	F_6	-0.5047
H_5	0.0868	N_1	0.1729	F_7	-0.4680
C_5	-0.1104	N_2	0.0972	F_8	-0.5045
H_6	0.0259	N_3	0.0843	Total charge	-1.785
H_7	0.0279	N_4	0.1773		
C_6	-0.0628	C_9	-0.1304		
H_8	0.0451	H_{14}	0.0990		
H_9	-0.0091	H_{15}	0.1457		
C_7	0.3504	H_{16}	0.0668		
H_{10}	-0.0785	C_{10}	-0.0105		
H_{11}	-0.0065	C_{11}	-0.1522		
C_8	-0.1208	H_{13}	0.0570		
H_{12}	0.0872				
Total charge		1.785			



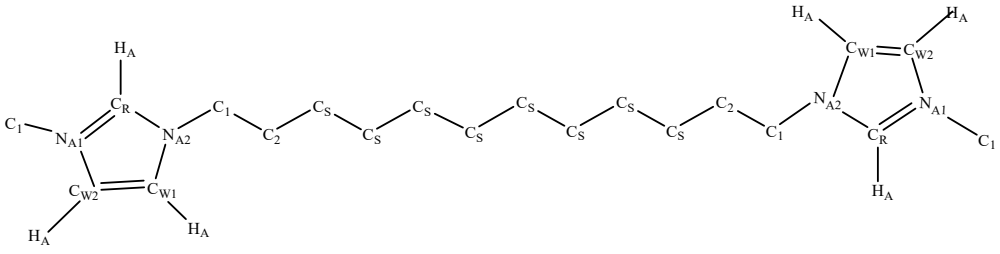
$[C_3(mim)_2]^{2+}$



$[C_6(mim)_2]^{2+}$



$[C_9(mim)_2]^{2+}$



$[C_{12}(mim)_2]^{2+}$

Lennard-Jones parameters

Atom	ε/kcal.mol^{-1}	σ/Å
$[C_3(mim)_2]^{2+}$		
C_1	0.066	3.50
C_2	0.066	3.50
C_R	0.070	3.55
C_W	0.070	3.55
H_A	0.030	2.42
H_C	0.030	2.50
H_1	0.030	2.50
N_A	0.170	3.25
$[C_6(mim)_2]^{2+}$		
C_1	0.066	3.50
C_2	0.066	3.50
C_S	0.066	3.50
C_R	0.070	3.55
C_W	0.070	3.55
H_A	0.030	2.42
H_C	0.030	2.50
H_1	0.030	2.50
N_A	0.170	3.25
$[C_9(mim)_2]^{2+}$		
C_1	0.066	3.50
C_2	0.066	3.50
C_S	0.066	3.50
C_R	0.070	3.55
C_W	0.070	3.55
H_A	0.030	2.42
H_C	0.030	2.50
H_1	0.030	2.50
N_A	0.170	3.25
$[C_{12}(mim)_2]^{2+}$		
C_1	0.066	3.50
C_2	0.066	3.50
C_S	0.066	3.50
C_R	0.070	3.55
C_W	0.070	3.55
H_A	0.030	2.42
H_C	0.030	2.50
H_1	0.030	2.50
N_A	0.170	3.25

Bond parameters

Atom	Atom	ε/kcal.mol^{-1}	σ/Å
$[C_3(mim)_2]^{2+}$			
C_W	H_A	183.500	1.08
C_R	H_A	183.500	1.08
C_1	H_1	170.000	1.09
C_2	H_C	170.000	1.09
C_R	N_A	238.528	1.32
C_{W1}	C_{W2}	260.038	1.34
C_1	N_A	168.499	1.47
C_1	C_2	133.963	1.53
C_W	N_A	213.552	1.38
$[C_6(mim)_2]^{2+}$			
C_W	H_A	183.500	1.08
C_R	H_A	183.500	1.08
C_1	H_1	170.000	1.09
C_2	H_C	170.000	1.09
C_S	H_C	170.000	1.09
C_R	N_A	238.528	1.32
C_{W1}	C_{W2}	260.038	1.34
C_1	N_A	168.499	1.47
C_1	C_2	133.963	1.53
C_2	C_S	133.963	1.53
C_S	C_S	133.963	1.53
C_W	N_A	213.552	1.38
$[C_9(mim)_2]^{2+}$			
C_W	H_A	183.500	1.08
C_R	H_A	183.500	1.08
C_1	H_1	170.000	1.09
C_2	H_C	170.000	1.09
C_S	H_S	170.000	1.09
C_R	N_A	238.528	1.32
C_{W1}	C_{W2}	260.038	1.34
C_1	N_A	168.499	1.47
C_1	C_2	133.963	1.53
C_2	C_S	133.963	1.53
C_S	C_S	133.963	1.53
C_W	N_A	213.552	1.38

Atom	Atom	ε/kcal.mol^{-1}	σ/Å
$[C_{12}(mim)_2]^{2+}$			
C_W	H_A	183.500	1.08
C_R	H_A	183.500	1.08
C_1	H_1	170.000	1.09
C_2	H_C	170.000	1.09
C_S	H_C	170.000	1.09
C_R	N_A	238.528	1.32
C_{W1}	C_{W2}	260.038	1.34
C_1	N_A	168.499	1.47
C_1	C_2	133.963	1.53
C_2	C_S	133.963	1.53
C_S	C_S	133.963	1.53
C_W	N_A	213.552	1.38

Angle parameters

Atom	Atom	Atom	k_θ / kcal.mol^{-1}.rad^{-2}	θ_{eq} / deg
$[C_3(mim)_2]^{2+}$				
C_R	N_A	C_W	34.967	108.00
C_W	N_A	C_1	34.967	125.60
C_R	N_A	C_1	34.967	126.40
N_A	C_R	H_A	17.483	125.10
N_A	C_R	N_A	34.967	109.80
N_A	C_W	C_W	34.967	107.10
N_A	C_W	H_A	17.483	122.00
C_W	C_W	H_A	17.483	130.90
N_A	C_1	H_1	37.429	110.70
C_1	C_2	H_C	37.429	110.70
C_2	C_1	H_1	37.429	110.70
C_1	C_2	C_1	50.000	112.70
N_A	C_1	C_2	50.000	112.70
H_1	C_1	H_1	32.995	107.80
H_C	C_2	H_C	32.995	107.80
$[C_6(mim)_2]^{2+}$				
C_R	N_A	C_W	34.967	108.00
C_W	N_A	C_1	34.967	125.60
C_R	N_A	C_1	34.967	126.40
N_A	C_R	H_A	17.483	125.10
N_A	C_R	N_A	34.967	109.80
N_A	C_W	C_W	34.967	107.10
N_A	C_W	H_A	17.483	122.00
C_W	C_W	H_A	17.483	130.90
N_A	C_1	H_1	37.429	110.70
C_1	C_2	H_C	37.429	110.70
C_2	C_1	H_1	37.429	110.70
C_S	C_2	H_C	37.429	110.70
C_2	C_S	H_C	37.429	110.70
C_S	C_S	H_C	37.429	110.70
C_1	C_2	C_S	50.000	112.70
C_2	C_S	C_S	50.000	112.70
N_A	C_1	C_2	50.000	112.70
H_1	C_1	H_1	32.995	107.80
H_C	C_2	H_C	32.995	107.80
H_C	C_S	H_C	32.995	107.80

Angle parameters

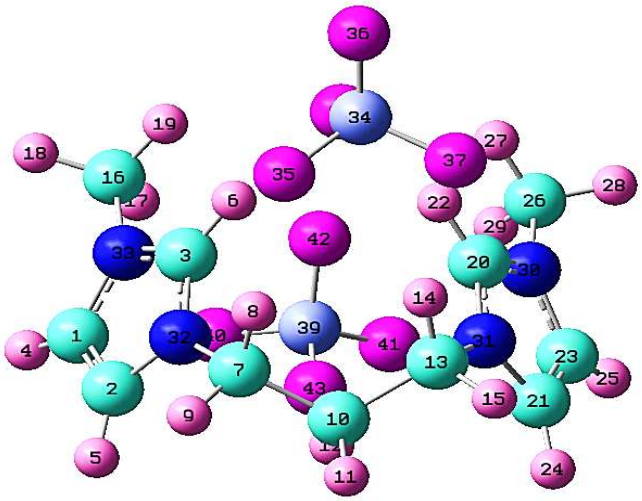
Atom	Atom	Atom	k_θ / kcal.mol^{-1}.rad^{-2}	θ_{eq} / deg
$[C_9(mim)_2]^{2+}$				
C_R	N_A	C_W	34.967	108.00
C_W	N_A	C_1	34.967	125.60
C_R	N_A	C_1	34.967	126.40
N_A	C_R	H_A	17.483	125.10
N_A	C_R	N_A	34.967	109.80
N_A	C_W	C_W	34.967	107.10
N_A	C_W	H_A	17.483	122.00
C_W	C_W	H_A	17.483	130.90
N_A	C_1	H_1	37.429	110.70
C_1	C_2	H_C	37.429	110.70
C_2	C_1	H_1	37.429	110.70
C_S	C_2	H_C	37.429	110.70
C_2	C_S	H_C	37.429	110.70
C_S	C_S	H_C	37.429	110.70
C_1	C_2	C_S	50.000	112.70
C_2	C_S	C_S	50.000	112.70
C_S	C_S	C_S	50.000	112.70
N_A	C_1	C_2	50.000	112.70
H_1	C_1	H_1	32.995	107.80
H_C	C_2	H_C	32.995	107.80
H_C	C_S	H_C	32.995	107.80
$[C_{12}(mim)_2]^{2+}$				
C_R	N_A	C_W	34.967	108.00
C_W	N_A	C_1	34.967	125.60
C_R	N_A	C_1	34.967	126.40
N_A	C_R	H_A	17.483	125.10
N_A	C_R	N_A	34.967	109.80
N_A	C_W	C_W	34.967	107.10
N_A	C_W	H_A	17.483	122.00
C_W	C_W	H_A	17.483	130.90
N_A	C_1	H_1	37.429	110.70
C_1	C_2	H_C	37.429	110.70
C_2	C_1	H_1	37.429	110.70
C_S	C_2	H_C	37.429	110.70
C_2	C_S	H_C	37.429	110.70
C_S	C_S	H_C	37.429	110.70
C_1	C_2	C_S	50.000	112.70
C_2	C_S	C_S	50.000	112.70
C_S	C_S	C_S	50.000	112.70
N_A	C_1	C_2	50.000	112.70
H_1	C_1	H_1	32.995	107.80
H_C	C_2	H_C	32.995	107.80
H_C	C_S	H_C	32.995	107.80

Proper dihedral parameters

Atom	Atom	Atom	Atom	$k_{\phi,1}$/kcal.mol^{-1}	$k_{\phi,2}$/kcal.mol^{-1}	$k_{\phi,3}$/kcal.mol^{-1}	$k_{\phi,4}$/kcal.mol^{-1}
$[C_3(mim)_2]^{2+}$							
X	C_R	N_A	X	0.00	4.65	0.00	0.00
X	C_W	C_W	X	0.00	10.75	0.00	0.00
X	C_W	N_A	X	0.00	2.30	0.00	0.00
C_W	N_A	C_1	H_1	0.00	0.00	0.13	0.00
C_R	N_A	C_1	H_1	0.00	0.00	0.00	0.00
C_W	N_A	C_1	C_2	-1.38	1.06	0.21	0.00
C_R	N_A	C_1	C_2	-0.77	0.00	0.00	0.00
N_A	C_1	C_2	C_1	0.18	-0.16	0.24	0.00
N_A	C_1	C_2	H_C	0.00	0.00	0.00	0.00
C_1	C_2	C_1	H_1	0.00	0.00	0.37	0.00
H_C	C_2	C_1	H_C	0.00	0.00	0.32	0.00
$[C_6(mim)_2]^{2+}$							
X	C_R	N_A	X	0.00	4.65	0.00	0.00
X	C_W	C_W	X	0.00	10.75	0.00	0.00
X	C_W	N_A	X	0.00	2.30	0.00	0.00
C_W	N_A	C_1	H_1	0.00	0.00	0.13	0.00
C_R	N_A	C_1	H_1	0.00	0.00	0.00	0.00
C_W	N_A	C_1	C_2	-1.38	1.06	0.21	0.00
C_R	N_A	C_1	C_2	-0.77	0.00	0.00	0.00
N_A	C_1	C_2	C_S	0.18	-0.16	0.24	0.00
N_A	C_1	C_2	H_C	0.00	0.00	0.00	0.00
C_1	C_2	C_S	H_C	0.00	0.00	0.37	0.00
C_2	C_S	C_S	H_C	0.00	0.00	0.37	0.00
C_S	C_S	C_2	H_C	0.00	0.00	0.37	0.00
H_C	C_2	C_1	H_1	0.00	0.00	0.32	0.00
H_C	C_2	C_S	H_C	0.00	0.00	0.32	0.00
H_C	C_S	C_S	H_C	0.00	0.00	0.32	0.00

Proper dihedral parameters

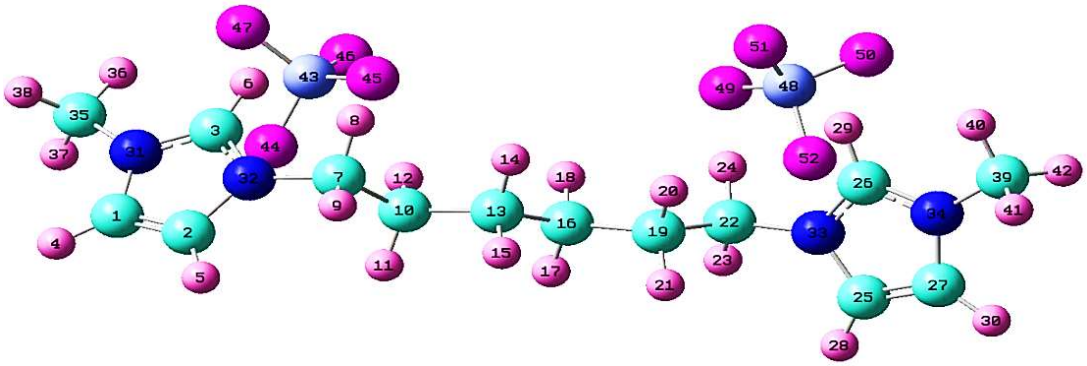
Atom	Atom	Atom	Atom	$k_{\phi,1}$/kcal.mol^{-1}	$k_{\phi,2}$/kcal.mol^{-1}	$k_{\phi,3}$/kcal.mol^{-1}	$k_{\phi,4}$/kcal.mol^{-1}
$[C_9(mim)_2]^{2+}$							
X	C_R	N_A	X	0.00	4.65	0.00	0.00
X	C_W	C_W	X	0.00	10.75	0.00	0.00
X	C_W	N_A	X	0.00	2.30	0.00	0.00
C_W	N_A	C_1	H_1	0.00	0.00	0.13	0.00
C_R	N_A	C_1	H_1	0.00	0.00	0.00	0.00
C_W	N_A	C_1	C_2	-1.38	1.06	0.21	0.00
C_R	N_A	C_1	C_2	-0.77	0.00	0.00	0.00
N_A	C_1	C_2	C_S	0.18	-0.16	0.24	0.00
N_A	C_1	C_2	H_C	0.00	0.00	0.00	0.00
C_1	C_2	C_S	H_C	0.00	0.00	0.37	0.00
C_2	C_S	C_S	H_C	0.00	0.00	0.37	0.00
C_S	C_S	C_2	H_C	0.00	0.00	0.37	0.00
C_S	C_S	C_S	H_C	0.00	0.00	0.37	0.00
H_C	C_2	C_1	H_1	0.00	0.00	0.32	0.00
H_C	C_2	C_S	H_C	0.00	0.00	0.32	0.00
H_C	C_S	C_S	H_C	0.00	0.00	0.32	0.00
$[C_{12}(mim)_2]^{2+}$							
X	C_R	N_A	X	0.00	4.65	0.00	0.00
X	C_W	C_W	X	0.00	10.75	0.00	0.00
X	C_W	N_A	X	0.00	2.30	0.00	0.00
C_W	N_A	C_1	H_1	0.00	0.00	0.13	0.00
C_R	N_A	C_1	H_1	0.00	0.00	0.00	0.00
C_W	N_A	C_1	C_2	-1.38	1.06	0.21	0.00
C_R	N_A	C_1	C_2	-0.77	0.00	0.00	0.00
N_A	C_1	C_2	C_S	0.18	-0.16	0.24	0.00
N_A	C_1	C_2	H_C	0.00	0.00	0.00	0.00
C_1	C_2	C_S	H_C	0.00	0.00	0.37	0.00
C_2	C_S	C_S	H_C	0.00	0.00	0.37	0.00
C_S	C_S	C_2	H_C	0.00	0.00	0.37	0.00
C_S	C_S	C_S	H_C	0.00	0.00	0.37	0.00
H_C	C_2	C_1	H_1	0.00	0.00	0.32	0.00
H_C	C_2	C_S	H_C	0.00	0.00	0.32	0.00
H_C	C_S	C_S	H_{CC}	0.00	0.00	0.32	0.00



$[C_3(mim)_2][BF_4]_2$

Partial charges in CHELPG method

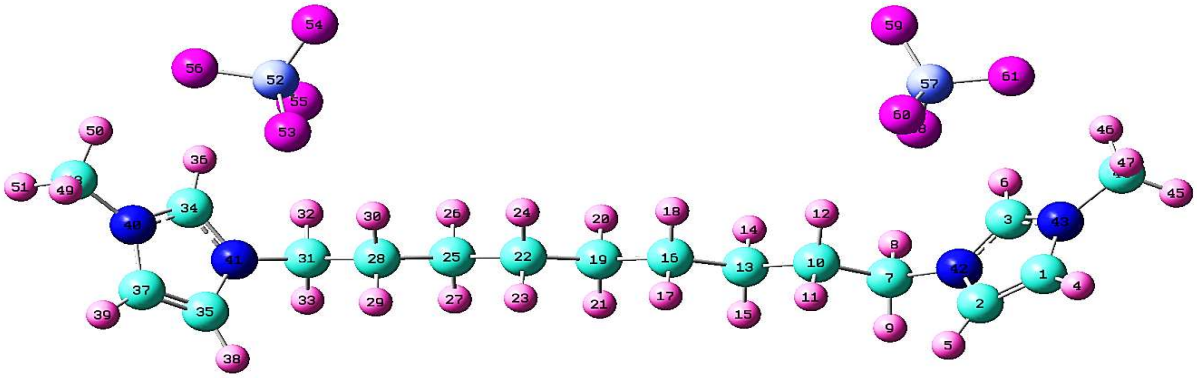
$[C_3(mim)_2]^{+2}$				$[BF_4]^-$	
Atom	**q / e**	**Atom**	**q / e**	**Atom**	**q / e**
C_1	-0.1226	H_{18}	0.0790	B_{34}	0.7217
C_2	-0.1629	H_{19}	0.1231	F_{35}	-0.3809
C_3	0.0114	C_{20}	-0.0337	F_{36}	-0.3535
H_4	0.1985	C_{21}	-0.1602	F_{37}	-0.3913
H_5	0.1804	H_{22}	0.2140	F_{38}	-0.3803
H_6	0.1750	C_{23}	-0.1213	F_{39}	0.6565
C_7	0.0617	H_{24}	0.1734	B_{40}	-0.3653
H_8	0.0411	H_{25}	0.1919	F_{41}	-0.3676
H_9	0.0307	C_{26}	-0.1508	F_{42}	-0.3709
C_{10}	0.1547	H_{27}	0.1140	F_{43}	-0.3474
H_{11}	-0.0310	H_{28}	0.0761	Total charge	-1.579
H_{12}	-0.0081	H_{29}	0.1318		
C_{13}	0.0480	N_{30}	0.1041		
H_{14}	0.0562	N_{31}	0.0691		
H_{15}	0.0322	N_{32}	0.0406		
C_{16}	-0.1564	N_{33}	0.0891		
H_{17}	0.1301				
Total charge		1.579			



$[C_6(mim)_2][BF_4]_2$

Partial charges in CHELPG method

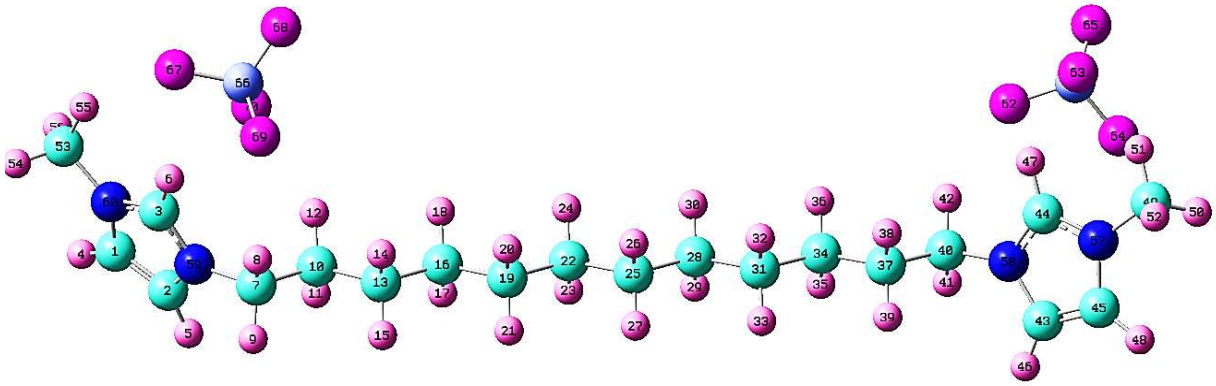
$[C_6(mim)_2]^{+2}$				$[BF_4]^-$	
Atom	**q / e**	**Atom**	**q / e**	**Atom**	**q / e**
C_1	-0.1288	C_{22}	-0.0848	B_{43}	1.0951
C_2	-0.1623	H_{23}	0.0462	F_{44}	-0.5151
C_3	-0.0037	H_{24}	0.0734	F_{45}	-0.4817
H_4	0.1662	C_{25}	-0.1662	F_{46}	-0.4730
H_5	0.1863	C_{26}	-0.0028	F_{47}	-0.5066
H_6	0.1934	C_{27}	-0.1255	B_{48}	1.0946
C_7	-0.0829	H_{28}	0.1874	F_{49}	-0.4816
H_8	0.0729	H_{29}	0.1930	F_{50}	-0.5064
H_9	0.0456	H_{30}	0.1655	F_{51}	-0.4729
C_{10}	0.3808	N_{31}	0.1468	F_{52}	-0.5148
H_{11}	-0.0770	N_{32}	0.0683	Total charge	-1.763
H_{12}	-0.0413	N_{33}	0.0700		
C_{13}	-0.1018	N_{34}	0.1448		
H_{14}	0.0420	C_{35}	-0.1415		
H_{15}	-0.0119	H_{36}	0.1532		
C_{16}	-0.1008	H_{37}	0.1155		
H_{17}	-0.0120	H_{38}	0.0614		
H_{18}	0.0418	C_{39}	-0.1407		
C_{19}	0.3804	H_{40}	0.1532		
H_{20}	-0.0412	H_{41}	0.1153		
H_{21}	-0.0768	H_{42}	0.0613		
Total charge		1.763			



$[C_9(mim)_2][BF_4]_2$

Partial charges in CHELPG method

$[C_9(mim)_2]^{+2}$				$[BF_4]^-$	
Atom	q / e	Atom	q / e	Atom	q / e
C_1	-0.1534	H_{27}	-0.0066	B_{52}	1.0953
C_2	-0.1558	C_{28}	0.3231	F_{53}	-0.4991
C_3	0.0230	H_{29}	-0.0769	F_{54}	-0.4675
H_4	0.1738	H_{30}	-0.0220	F_{55}	-0.4832
H_5	0.1879	C_{31}	-0.0341	F_{56}	-0.5163
H_6	0.1718	H_{32}	0.0767	B_{57}	1.0591
C_7	0.0038	H_{33}	0.0259	F_{58}	-0.4755
H_8	0.0661	C_{34}	0.0002	F_{59}	-0.4602
H_9	0.0161	C_{35}	-0.1431	F_{60}	-0.4794
C_{10}	0.2907	H_{36}	0.1851	F_{61}	-0.5049
H_{11}	-0.0804	C_{37}	-0.1564	Total charge	-1.732
H_{12}	-0.0198	H_{38}	0.1844		
C_{13}	-0.0612	H_{39}	0.1722		
H_{14}	0.0118	N_{40}	0.1514		
H_{15}	-0.0097	N_{41}	0.0448		
C_{16}	-0.0372	N_{42}	0.0482		
H_{17}	-0.0140	N_{43}	0.1348		
H_{18}	0.0109	C_{44}	-0.1197		
C_{19}	0.203	H_{45}	0.0625		
H_{20}	-0.0354	H_{46}	0.1465		
H_{21}	-0.0592	H_{47}	0.0992		
C_{22}	0.0084	C_{48}	-0.1333		
H_{23}	-0.0246	H_{49}	0.1024		
H_{24}	0.0020	H_{50}	0.1552		
C_{25}	-0.1077	H_{51}	0.0623		
H_{26}	0.0277				
Total charge		1.732			



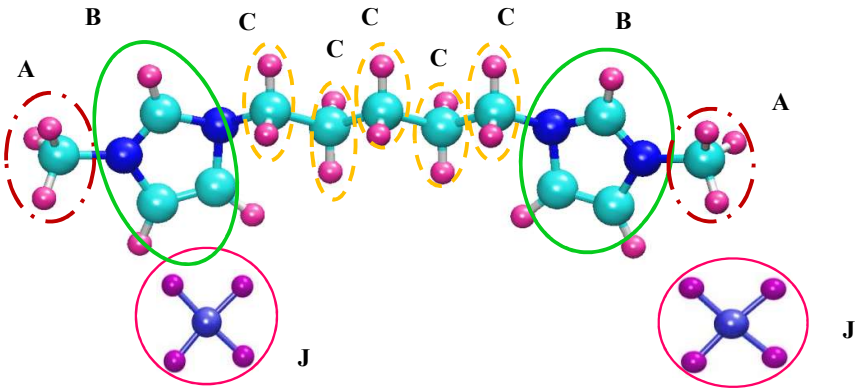
$[C_{12}(mim)_2][BF_4]_2$

Partial charges in CHELPG method

$[C_{12}(mim)_2]^{+2}$						$[BF_4]^-$	
Atom	**q / e**	**Atom**	**q / e**	**Atom**	**q / e**	**Atom**	**q / e**
C_1	-0.1422	H_{21}	-0.0401	H_{41}	0.0680	B_{61}	1.0711
C_2	-0.1729	C_{22}	0.0124	H_{42}	0.1117	F_{62}	-0.4966
C_3	-0.0111	H_{23}	-0.0233	C_{43}	-0.2051	F_{63}	-0.4949
H_4	0.1696	H_{24}	-0.0233	C_{44}	-0.0475	F_{64}	-0.5016
H_5	0.1927	C_{25}	0.1008	C_{45}	-0.1255	F_{65}	-0.4643
H_6	0.1818	H_{26}	-0.0348	H_{46}	0.1982	B_{66}	1.0777
C_7	-0.0655	H_{27}	-0.0432	H_{47}	0.2107	F_{67}	-0.5099
H_8	0.0806	C_{28}	0.0442	H_{48}	0.1664	F_{68}	-0.4651
H_9	0.0298	H_{29}	-0.0249	C_{49}	-0.1024	F_{69}	-0.4793
C_{10}	0.3291	H_{30}	-0.0187	H_{50}	0.1126	F_{70}	-0.4902
H_{11}	-0.0825	C_{31}	-0.0182	H_{51}	0.1312	Total charge	-1.753
H_{12}	-0.0290	H_{32}	-0.0012	H_{52}	0.0502		
C_{13}	-0.0828	H_{33}	-0.0097	C_{53}	-0.1342		
H_{14}	0.0231	C_{34}	0.1793	H_{54}	0.0629		
H_{15}	-0.0069	H_{35}	-0.0506	H_{55}	0.1533		
C_{16}	0.0224	H_{36}	-0.0281	H_{56}	0.1029		
H_{17}	-0.0251	C_{37}	0.0573	N_{57}	0.1331		
H_{18}	-0.0023	H_{38}	-0.0269	N_{58}	0.1780		
C_{19}	0.1164	H_{39}	-0.0407	N_{59}	0.0884		
H_{20}	-0.0282	C_{40}	-0.0737	N_{60}	0.1535		
Total charge			1.753				

Table S2 Force field parameters for $[C_5(mim)_2][BF_4]_2$ DIL in the three mapping schemes of CG model. The similar parameters have been used for $[C_n(mim)_2][BF_4]_2$ (with n=3,6,9,12) in the CG-1 model.

Force-field parameters for CG (scheme-1)



Lennard-Jones parameters

Bead	Bead	Potential Type	ε/kcal.mol^{-1}	σ/Å
A	A	lj12-6	0.086	3.41
A	B	lj12-6	0.229	3.90
A	C	lj12-6	0.089	3.68
A	J	lj12-6	0.258	4.11
B	B	lj12-6	0.612	4.38
B	C	lj12-6	0.236	4.17
B	J	lj12-6	0.688	4.59
C	C	lj12-6	0.091	3.95
C	J	lj12-6	0.266	4.38
J	J	lj12-6	0.774	4.80

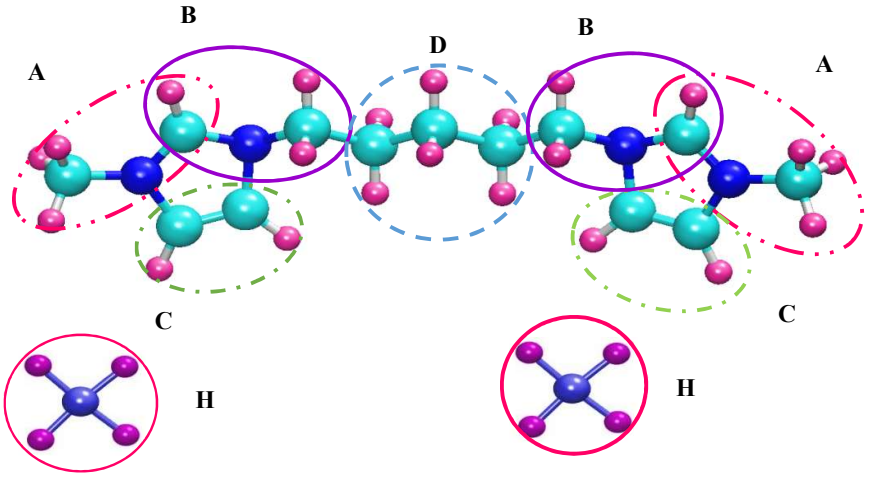
Bond parameters

Bead	Bead	k_b / kcal.mol^{-1}.Å^{-2}	r_{eq} / Å
A	B	210.792	2.71
B	C	219.647	2.69
C	C	297.635	1.66

Angle parameters

Bead	Bead	Bead	k_Θ / kcal.mol^{-1}.rad^{-2}	Θ_{eq} / deg
A	B	C	138.983	142.38
B	C	C	68.269	109.45
C	C	C	62.049	114.00

Force-field parameters for CG (scheme-2)



Lennard-Jones parameters

Bead	Bead	Potential Type	ε/kcal.mol^{-1}	σ/Å
A	A	lj9-6	0.376	4.10
A	B	lj9-6	0.360	4.05
A	C	lj9-6	0.274	4.05
A	D	lj9-6	0.348	4.30
A	H	lj12-6	0.539	4.45
B	B	lj9-6	0.346	4.10
B	C	lj9-6	0.263	4.05
B	D	lj9-6	0.334	4.30
B	H	lj12-6	0.517	4.45
C	C	lj9-6	0.200	3.60
C	D	lj9-6	0.254	3.76
C	H	lj12-6	0.393	4.20
D	D	lj9-6	0.420	4.51
D	H	lj12-6	0.570	4.65

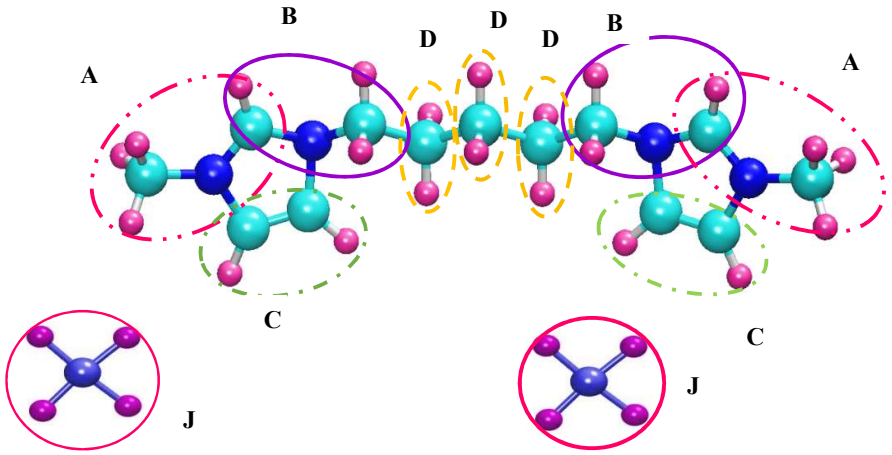
Bond parameters

Bead	Bead	k_b / kcal.mol^{-1}.Å^{-2}	r_{eq} / Å
A	B	179.540	2.97
A	C	223.750	2.30
B	C	230.650	2.27
B	D	7.980	3.23

Angle parameters

Bead	Bead	Bead	k_θ / kcal.mol^{-1}.rad^{-2}	Θ_{eq} / deg
A	B	C	932.500	51.22
A	C	B	433.260	81.88
C	A	B	748.700	50.39
A	B	D	4.910	143.82
C	B	D	1.400	147.83

Force-field parameters for CG (scheme-3)



Lennard-Jones parameters

Bead	Bead	Potential Type	ε/kcal.mol^{-1}	σ/Å
A	A	lj9-6	0.376	4.10
A	B	lj9-6	0.360	4.05
A	C	lj9-6	0.274	4.05
A	D	lj12_6	0.185	4.03
A	J	lj12_6	0.539	4.45
B	B	lj9_6	0.346	4.10
B	C	lj9_6	0.263	4.05
B	D	lj12_6	0.178	4.03
B	J	lj12_6	0.517	4.45
C	C	lj9_6	0.200	3.60
C	D	lj12_6	0.135	3.78
C	J	lj12_6	0.393	4.20
D	D	lj12_6	0.091	3.95
D	J	lj12_6	0.266	4.38
J	J	lj12_6	0.774	4.80

Bond parameters

Bead	Bead	k_b / kcal.mol^{-1}.Å^{-2}	r_{eq} / Å
A	B	179.540	2.97
A	C	223.750	2.30
B	C	230.650	2.27
B	D	7.980	3.23
D	D	297.635	1.66

Angle parameters

Bead	Bead	Bead	k_θ / kcal.mol^{-1}.rad^{-2}	Θ_{eq} / deg
A	B	C	932.500	51.22
A	C	B	433.260	81.88
C	A	B	748.700	50.39
A	B	D	4.910	143.82
C	B	D	1.400	147.83
D	D	D	62.049	114.00
B	D	D	68.269	109.45

Table S3 Diffusion coefficients for the studied DILs in both CG and AA models obtained from the simulations and corrected for system-size dependences (Yeh-Hummer correlation) at 500 K and at 1 atm with confidence intervals expressed as ±σ.

	D_{cation} (10^{-11} $m^2.s^{-1}$)		D_{anion} (10^{-11} $m^2.s^{-1}$)	
	D_{PBC}	D_0	D_{PBC}	D_0
		$[C_3(mim)_2][BF_4]_2$		
CG (1)	201.37±0.7492	247.19±0.7492	253.39±0.6577	284.55±0.6577
AA	46.36±0.4824	55.22±0.4824	69.09±0.2826	76.33±0.2826
		$[C_6(mim)_2][BF_4]_2$		
CG (1)	155.98±0.5886	192.25±0.5886	234.05±0.4385	262.35±0.4385
AA	33.18±0.2236	39.33±0.2236	46.60±0.2147	51.18±0.2147
		$[C_9(mim)_2][BF_4]_2$		
CG (1)	184.75±1.4868	227.52±1.4868	327.25±0.5111	363.04±0.5111
AA	30.35±0.3543	36.21±0.3543	45.23±0.2716	49.42±0.7492
		$[C_{12}(mim)_2][BF_4]_2$		
CG (1)	143.08±2.5839	174.40±2.5839	305.41±1.8920	336.72±1.8920
AA	19.20±0.1293	22.79±0.1293	45.68±0.1823	49.74±0.1823

Table S4 The fitting parameters of VFT equation for $[C_{12}(mim)_2][BF_4]_2$ in both AA and CG models.

	All-Atom		Coarse-Grained	
	Cation	Anion	Cation	Anion
		D_{PBC}		
$D' / 10^{-11}$ $m^2.s^{-1}$	0.0002	0.0003	0.0001	0.0004
B' / K	-7154.8	-5846.9	-10793.6	-10256.1
T_0 / K	1113	984	1265	1252
R^2	0.9723	0.9921	0.9776	0.9819
		D_0		
$D'/ 10^{-11}$ $m^2.s^{-1}$	0.0002	0.0002	0.0005	0.0003
B' / K	-6981.0	-6166.7	-8912.2	-10727.4
T_0 / K	1105	998	1192	1270
R^2	0.9720	0.9922	0.9768	0.9820

Table S5 Diffusion coefficients of $[C_{12}(mim)_2][BF_4]_2$ in both CG and AA models in the temperature range of 350-500 K and at 1 atm obtained from the simulations and corrected for system-size dependences (Yeh-Hummer correlation) with confidence intervals expressed as $\pm\sigma$.

	Diffusion Coefficient of Cation (10^{-11} $m^2.s^{-1}$)		Diffusion Coefficient of Anion (10^{-11} $m^2.s^{-1}$)	
	D_{PBC}	D_0	D_{PBC}	D_0
		T (350K)		
CG (1)	2.25±0.0277	2.74±0.0277	6.69±0.0465	7.38±0.0465
AA	0.29±0.0076	0.35±0.0076	0.43±0.0155	0.47±0.0155
		T (400K)		
CG (1)	25.64±0.1485	31.25±0.1485	61.65±0.1333	67.97±0.1333
AA	3.13±0.0219	3.73±0.0219	4.56±0.0113	4.98±0.0113
		T (450K)		
CG (1)	71.03±0.8100	86.58±0.8100	148.58±0.5479	163.81±0.5479
AA	9.67±0.1235	11.51±0.1235	16.67±0.1774	18.17±0.1774
		T (500K)		
CG (1)	143.08±2.5839	174.40±2.5839	305.41±1.8920	336.72±1.8920
AA	19.20±0.1293	22.79±0.1293	45.68±0.1823	49.74±0.1823

Table S6 The hydrodynamic radii of the cations and anions of the studied DILs.

	Hydrodynamic Radii R / Å	
ILs	Cation	Anion
$[C_3(mim)_2][BF_4]_2$	4.18	2.47
$[C_5(mim)_2][BF_4]_2$	4.37	2.47
$[C_6(mim)_2][BF_4]_2$	4.32	2.47
$[C_9(mim)_2][BF_4]_2$	4.71	2.47
$[C_{12}(mim)_2][BF_4]_2$	4.77	2.47

Table S7 Electrical conductivity of $[C_{12}(mim)_2][BF_4]_2$ in both CG and AA models in the temperature range of 350-500 K and at 1 atm with confidence intervals expressed as ±σ.

T (K)	CG (1)	AA
	σ (mS.cm^{-1})	
350	$2.45 \times 10^{-6} \pm 2.4967 \times 10^{-7}$	$2.04 \times 10^{-7} \pm 3.9232 \times 10^{-8}$
400	$2.05 \times 10^{-5} \pm 1.6532 \times 10^{-6}$	$1.82 \times 10^{-6} \pm 1.1954 \times 10^{-7}$
450	$4.40 \times 10^{-5} \pm 4.6099 \times 10^{-6}$	$5.35 \times 10^{-6} \pm 5.1905 \times 10^{-7}$
500	$1.58 \times 10^{-4} \pm 9.9291 \times 10^{-6}$	$1.15 \times 10^{-5} \pm 6.3096 \times 10^{-7}$

Table S8 Transference numbers for the studied DILs in Both CG and AA models at 500 K and at 1 atm with confidence intervals expressed as ±σ.

	t_+	t_-
	$[C_3(mim)_2][BF_4]_2$	
CG (1)	0.61±0.0043	0.39±0.0023
AA	0.57±0.0104	0.43±0.0050
	$[C_6(mim)_2][BF_4]_2$	
CG (1)	0.57±0.0039	0.42±0.0021
AA	0.59±0.0074	0.41±0.0043
	$[C_9(mim)_2][BF_4]_2$	
CG (1)	0.53±0.0069	0.45±0.0031
AA	0.57±0.0120	0.43±0.0065
	$[C_{12}(mim)_2][BF_4]_2$	
CG (1)	0.48±0.0145	0.52±0.0088
AA	0.46±0.0055	0.54±0.0050

Figure Captions

Fig. S1 Temperature-dependent density for $[C_3(mim)_2][BF_4]_2$ and $[C_{12}(mim)_2][BF_4]_2$ in both CG and AA models at different temperatures and at 1 atm with confidence intervals expressed as ±σ.

Fig. S2 Isobaric expansion coefficients for the studied DILs with increasing linkage alkyl chain for both CG and AA models at 1 atm with confidence intervals expressed as ±σ.

Fig. S3 Temperature-dependent isobaric expansion coefficients for $[C_3(mim)_2][BF_4]_2$ and $[C_{12}(mim)_2][BF_4]_2$ in both CG and AA models at different temperatures and at 1 atm. The error bars are smaller than the symbols.

Fig. S4 Snapshots of the simulation boxes of the studied DILs in both CG and AA models at 400 K and at 1 atm. The polar (depicted in pink) and nonpolar (depicted in blue) domains have been also shown in the figure.

Fig. S5 Comparison of anion-anion RDFs of $[C_6(mim)_2][BF_4]_2$ in systems containing 252, 512 and 1000 DIL molecules in both CG and AA models.

Fig. S6 Mean square displacement (MSD) plots of cation and anion of the studied DILs at 500 K and at 1 atm in coarse-grained model. The evolution of β parameter with time has been also shown in each plot.

Fig. S7 Mean square displacement (MSD) plots of cation and anion of the studied DILs at 500 K and at 1 atm in all-atom model. The evolution of β parameter with time has been also shown in each plot.

Fig. S8 Mean square displacement (MSD) plots of cation and anion of $[C_{12}(mim)_2][BF_4]_2$ in coarse-grained model in the temperature range of 350-500 K and at 1 atm. The evolution of β parameter with time has been also shown in each plot.

Fig. S9 Mean square displacement (MSD) plots of cation and anion of $[C_{12}(mim)_2][BF_4]_2$ in all-atom model in the temperature range of 350-500 K and at 1 atm. The evolution of β parameter with time has been also shown in each plot.

Fig. S1

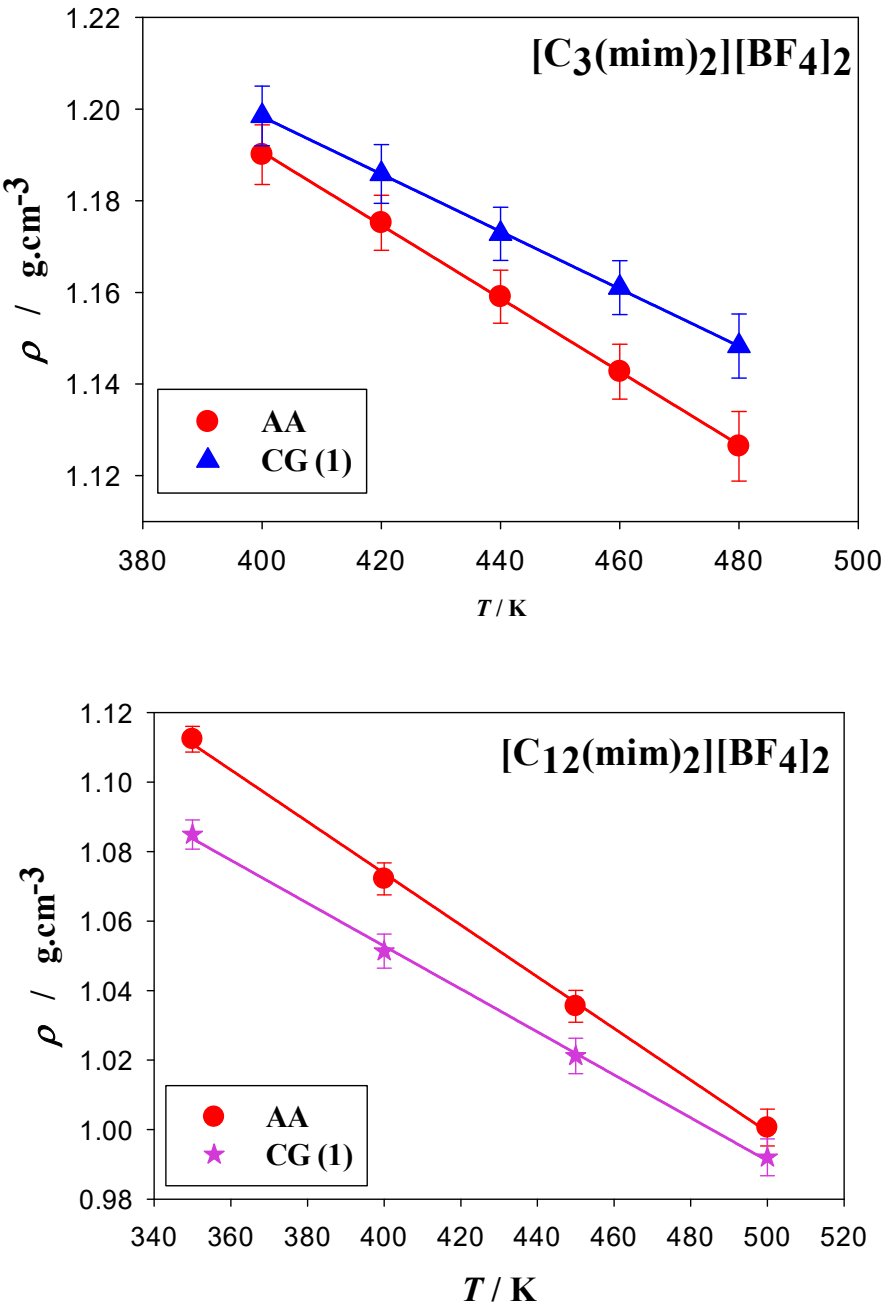


Fig. S2

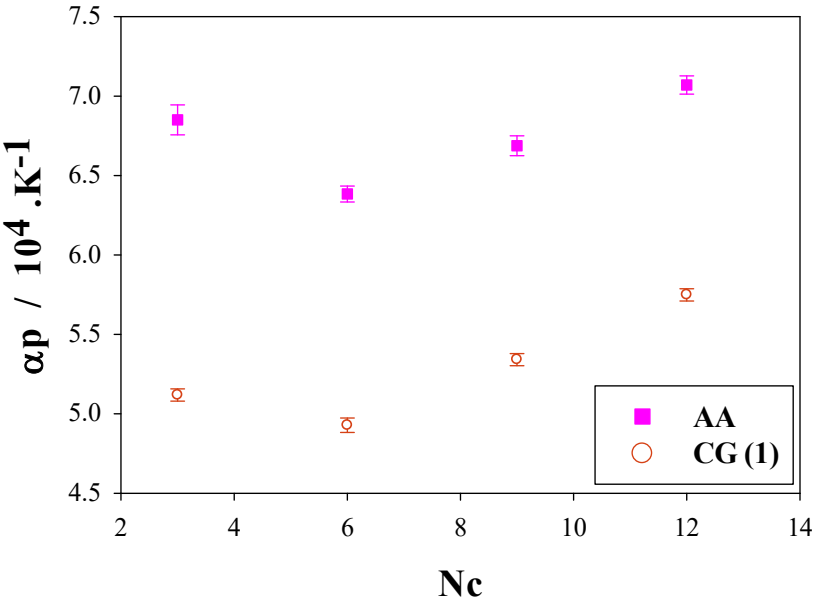
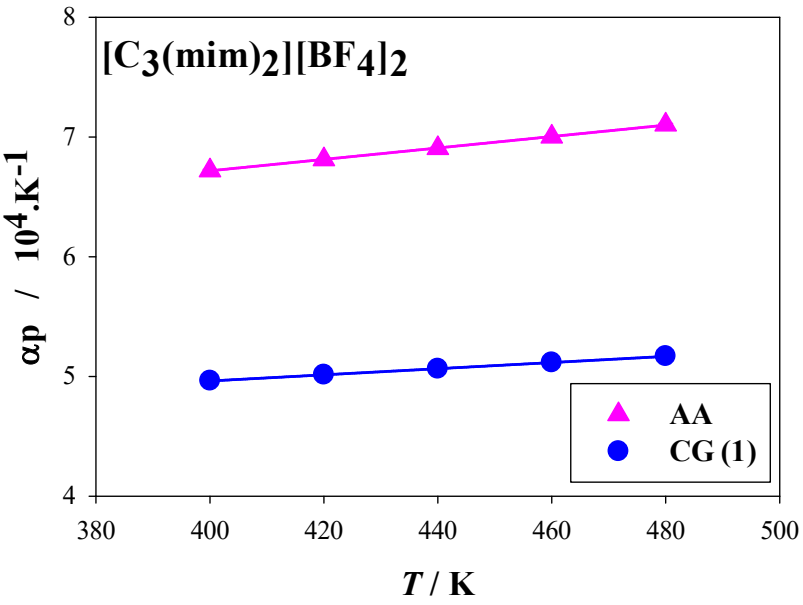


Fig. S3


[C3(mim)2][BF4]2
αp / 10^4.K^-1
T / K
AA
CG (1)
8
7
6
5
4
380
400
420
440
460
480
500

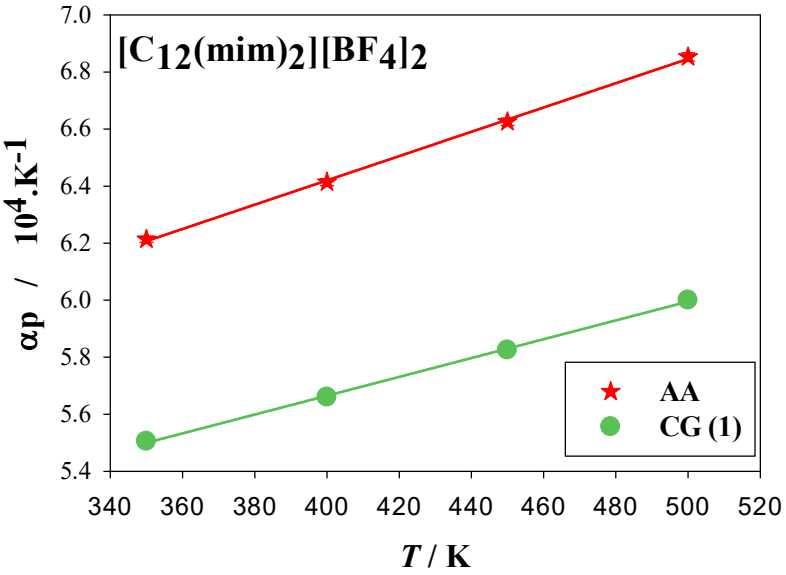
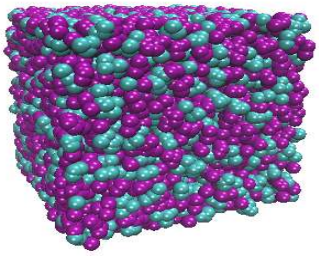
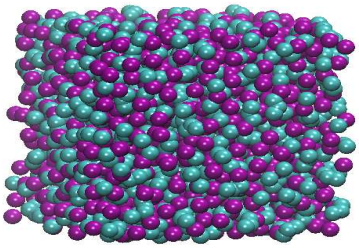

[C12(mim)2][BF4]2
αp / 10^4.K^-1
T / K
AA
CG (1)
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
340
360
380
400
420
440
460
480
500
520

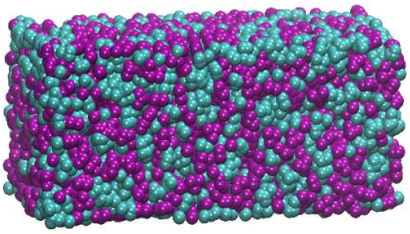
Fig. S4



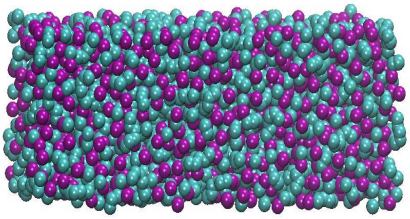
$[C_3(mim)_2][BF_4]_2$ (AA)



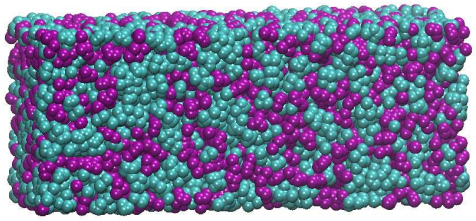
$[C_3(mim)_2][BF_4]_2$ (CG (1))



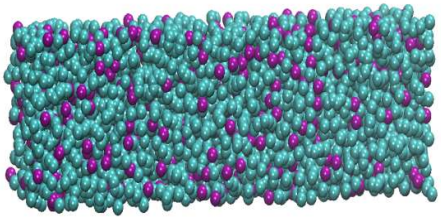
$[C_6(mim)_2][BF_4]_2$ (AA)



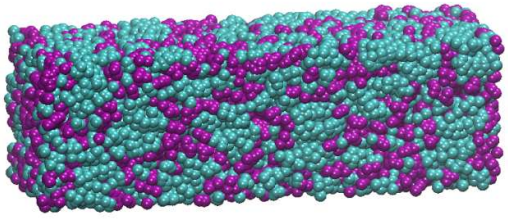
$[C_6(mim)_2][BF_4]_2$ (CG (1))



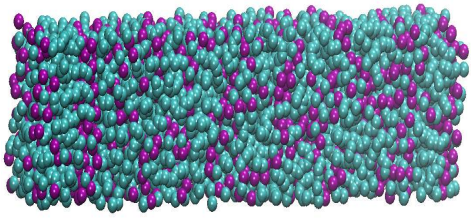
$[C_9(mim)_2][BF_4]_2$ (AA)



$[C_9(mim)_2][BF_4]_2$ (CG (1))



$[C_{12}(mim)_2][BF_4]_2$ (AA)



$[C_{12}(mim)_2][BF_4]_2$ (CG (1))

Fig. S5

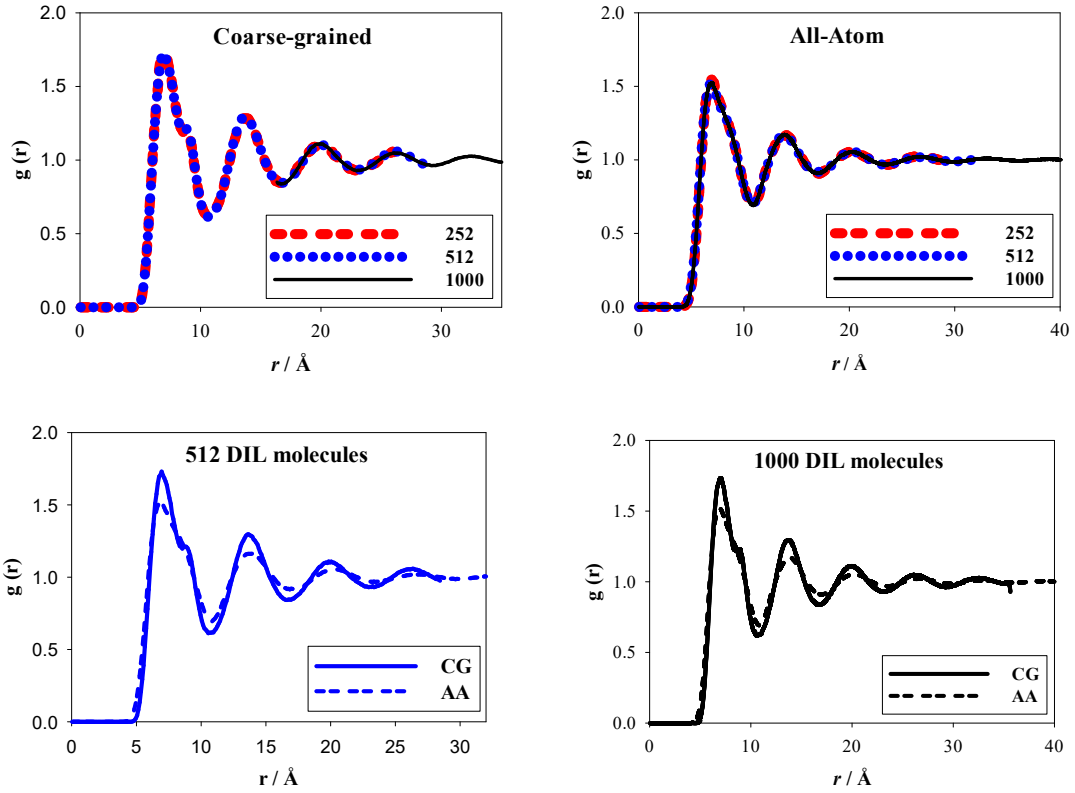

Coarse-grained
All-Atom
512 DIL molecules
1000 DIL molecules
g (r)
r / Å
252
512
1000
CG
AA

Fig. S6

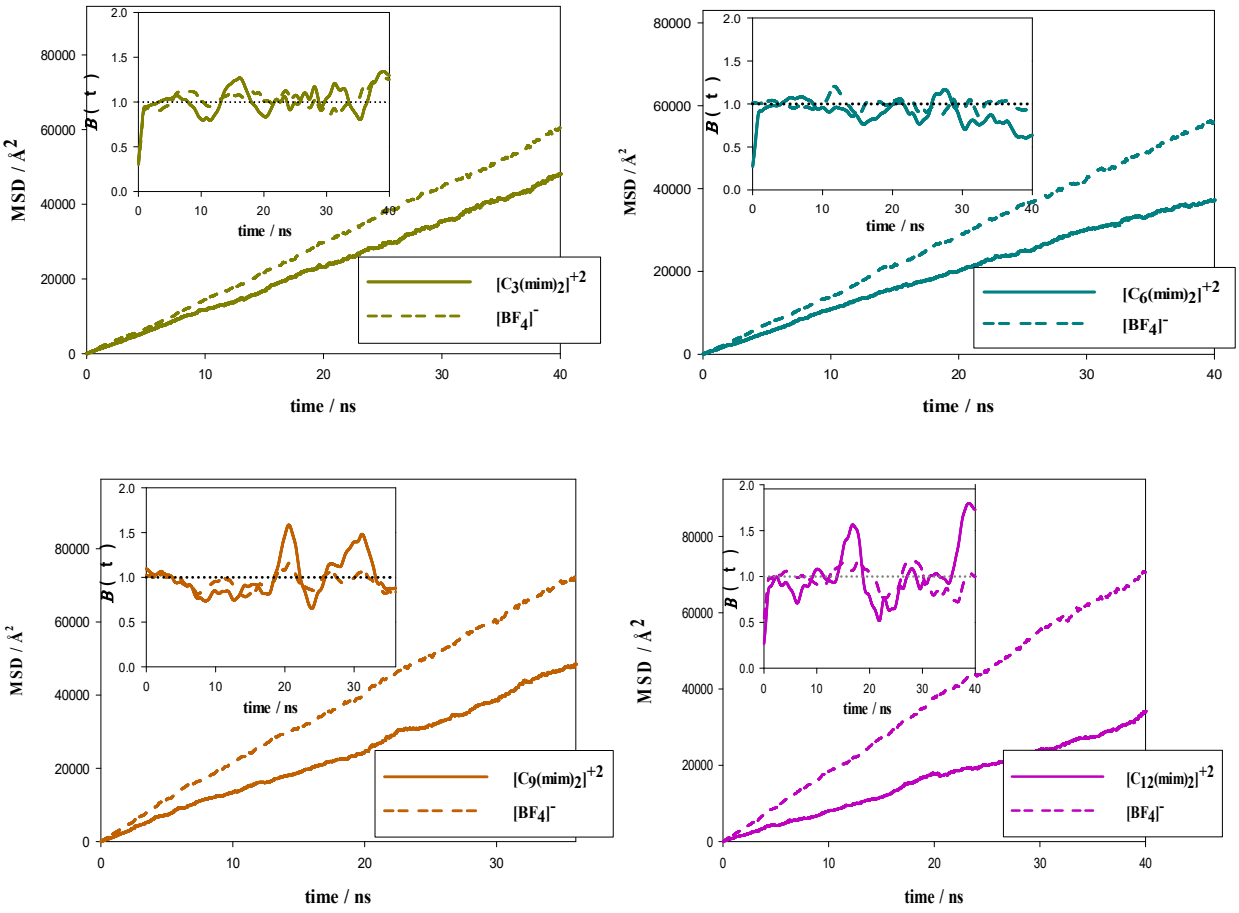

MSD / Å²
time / ns
B (t)
[C3(mim)2]+2
[BF4]-
[C6(mim)2]+2
[BF4]-
[C9(mim)2]+2
[BF4]-
[C12(mim)2]+2
[BF4]-

Fig. S7

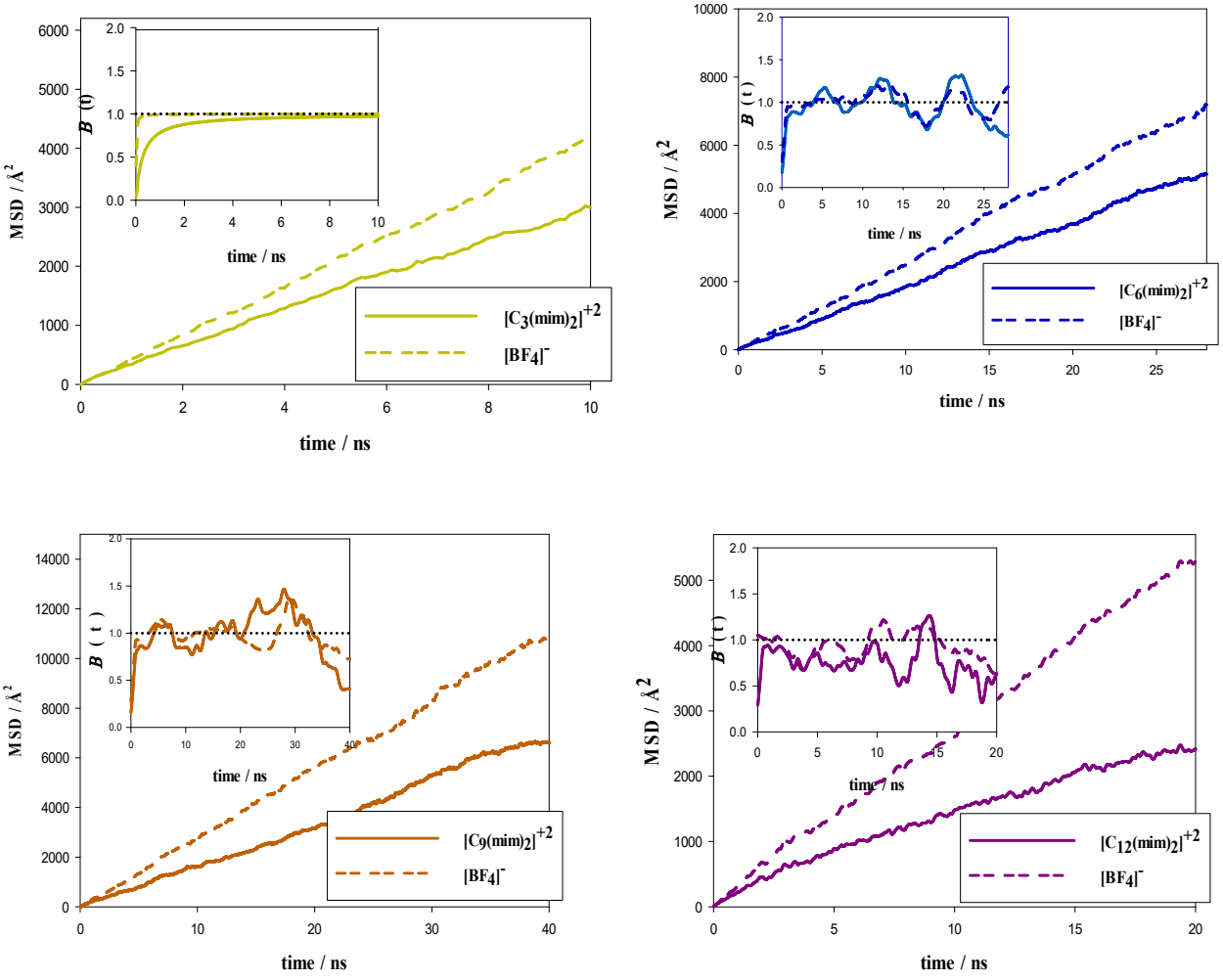

MSD / Å2
time / ns
B (t)
[C3(mim)2]+2
[BF4]-
[C6(mim)2]+2
[BF4]-
[C9(mim)2]+2
[BF4]-
[C12(mim)2]+2
[BF4]-

Fig. S8

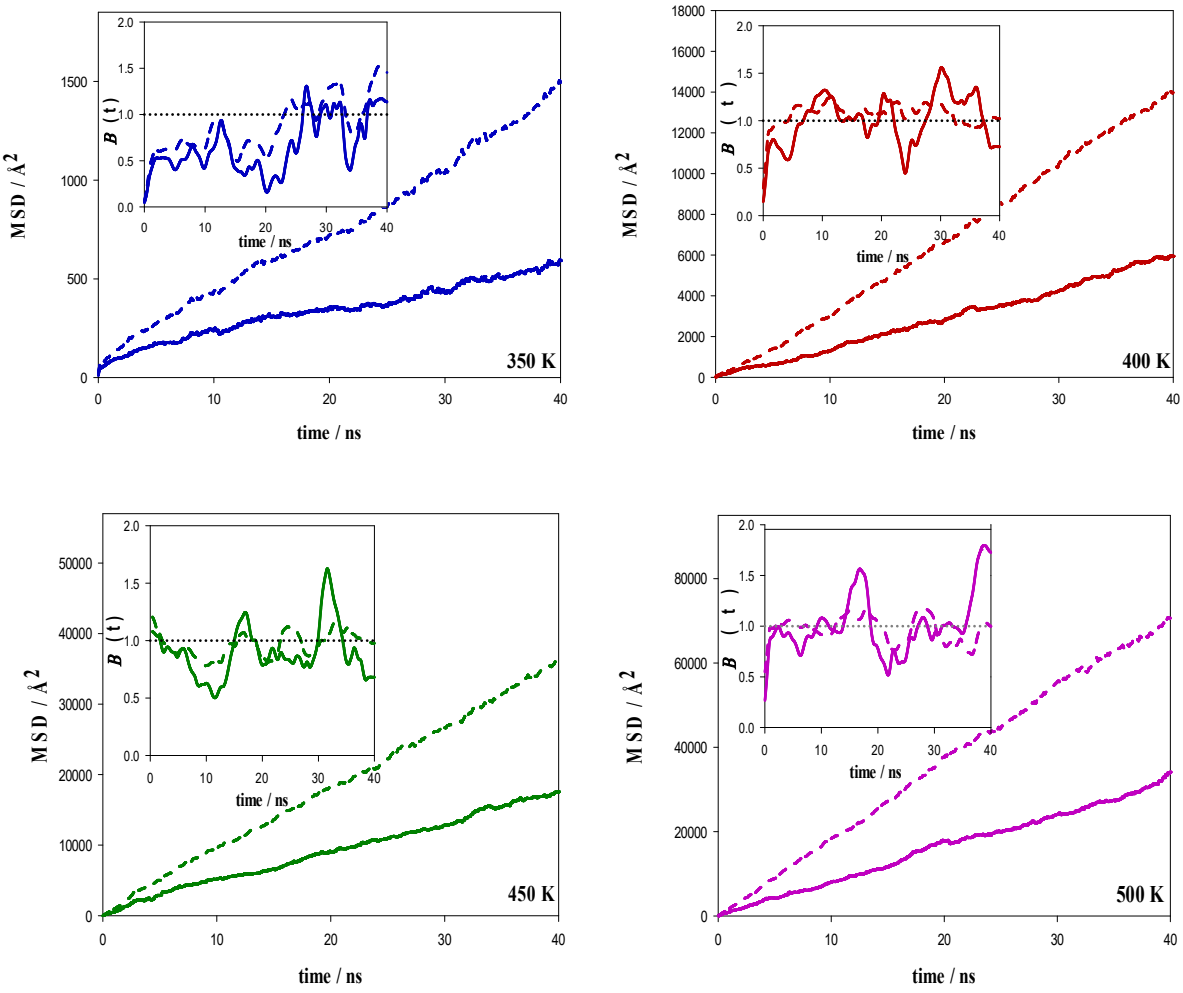


Fig. S9