Electronic Supplementary Material (ESI) for Faraday Discussions

2D or not 2D: Structural and charge ordering at the solid-liquid interface of the 1-(2-hydroxyethyl)-3-methylimidazolium tetrafluoroborate ionic liquid

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Table 1: Force Field parameters. The "tab" potential type refers to tabulated potential functions, whose values are given as separate files, one for each type of glass (TABLE.alu, TABLE.bk7, TABLE.sio2).

Al_2O_3						
atoms	potential type	q (au)	A (kJ mol^{-1})	ρ (Å)	C (Å)	
Al – Al	buck	3.0	0.00	1.00	0.00	
Al – HW	buck		0.00	1.00	0.00	
HW – HW	buck	1.0	0.00	1.00	0.00	
O – O	tab	-2.0				
O – Al	tab					
O – HW	tab					
O – OW	tab					
OW – OW	tab	-2.0				
OW – Al	tab					
OW – HW	tab					
angles	potential type	k (kJmol^{-1} rad$^{-(a+4)}$)	t (deg)	a	r (Å)	cutoff (Å)
O – Al – O	bvs2	0.4824	109.47	1.2	2.6	3.45
Al – O – HW	bvs2	0.2412	109.47	1.2	1.0	3.45
Al – OW – HW	bvs2	0.2412	109.47	1.2	1.0	3.45

BK7						
atoms	potential type	q (au)	A (kJ mol^{-1})	ρ (Å)	C (Å)	
K – K	buck	1.0	0.00	1.00	0.00	
K – Na	buck		0.00	1.00	0.00	
K – Si	buck		0.00	1.00	0.00	
K – B	buck		0.00	1.00	0.00	
K – HW	buck		0.00	1.00	0.00	
Na – Na	buck	1.0	0.00	1.00	0.00	
Na – Si	buck		0.00	1.00	0.00	
Na – B	buck		0.00	1.00	0.00	
Na – HW	buck		0.00	1.00	0.00	
Si – Si	buck	4.0	0.00	1.00	0.00	
Si – B	buck		0.00	1.00	0.00	
Si – HW	buck		0.00	1.00	0.00	
B – B	buck	3.0	0.00	1.00	0.00	
B – HW	buck		0.00	1.00	0.00	
HW – HW	buck	1.0	0.00	1.00	0.00	
O – K	buck		823.66	0.37	0.00	
O – Na	buck		523.62	0.36	0.00	
OW – K	buck		823.66	0.37	0.00	
OW – Na	buck		523.62	0.36	0.00	
O – O	tab	-2.0				
O – Si	tab					
O – B	tab					
O – HW	tab					
O – OW	tab					
OW – OW	tab	-2.0				
OW – Si	tab					
OW – B	tab					
OW – HW	tab					
angles	potential type	k (kJmol^{-1} rad$^{-(a+4)}$)	t (deg)	a	r (Å)	cutoff (Å)
O – Si – O	bvs2	0.4824	109.47	1.2	2.6	3.45
Si – O – Si	bvs2	0.2412	144.00	4.0	2.6	3.45
Si – O – HW	bvs2	0.2412	109.47	1.2	1.0	3.45
Si – OW – HW	bvs2	0.2412	109.47	1.2	1.0	3.45
B – O – HW	bvs2	0.2412	109.47	1.2	1.0	3.45
B – OW – HW	bvs2	0.2412	109.47	1.2	1.0	3.45

SiO_2						
atoms	potential type	q (au)	A (kJ mol^{-1})	ρ (Å)	C (Å)	
Si – Si	buck	4.0	0.00	1.00	0.00	
Si – HW	buck		0.00	1.00	0.00	
HW – HW	buck	1.0	0.00	1.00	0.00	
O – O	tab	-2.0				
O – Si	tab					
O – HW	tab					
O – OW	tab					
OW – OW	tab	-2.0				
OW – Si	tab					
OW – HW	tab					
angles	potential type	k (kJmol^{-1} rad$^{-(a+4)}$)	t (deg)	a	r (Å)	cutoff (Å)
O – Si – O	bvs2	0.4824	109.47	1.2	2.6	3.45
Si – O – Si	bvs2	0.2412	144.00	4.0	2.6	3.45
Si – O – HW	bvs2	0.2412	109.47	1.2	1.0	3.45
Si – OW – HW	bvs2	0.2412	109.47	1.2	1.0	3.45

1-(2-Hydroxyethyl)-3-methylimidazolium, $[C_2OHmim]^+$				
atoms	potential type	q (au)	ε (kJ mol^{-1})	σ (Å)
C_R	vdw	-0.11	0.29288	3.55
C_W	vdw	-0.13	0.29288	3.55
N_A	vdw	0.15	0.71128	3.25
H_{CR}	vdw	0.21	0.12552	2.42
H_{CW}	vdw	0.21	0.12552	2.42
C_1	vdw	-0.17	0.27614	3.50
C_{2O}	vdw	0.275	0.27614	3.50
H_1	vdw	0.13	0.12552	2.50
H_C	vdw	0.06	0.12552	2.50
O_H	vdw	-0.683	0.71176	3.12
H_O	vdw	0.418	0.00000	0.00
bonds	r_0 (Å)	k_r (kJ mol^{-1} Å^{-2})		
$C_R – H_{CR}$	1.08	(constrained)		
$C_W – H_{CW}$	1.08	(constrained)		
$C_1 – H_1$	1.09	(constrained)		
$C_{2O} – H_C$	1.09	(constrained)		
$O_H – H_O$	0.95	(constrained)		
$C_R – N_A$	1.315	3991.54		
$C_W – N_A$	1.378	3573.14		
$C_W – C_W$	1.341	4351.36		
$C_1 – N_A$	1.466	2820.02		
$C_1 – C_{2O}$	1.529	2242.62		
$C_{2O} – O_H$	1.410	2679.55		
angles	θ_0 (deg)	K_θ (kJ mol^{-1} rad^{-2})		
C_R-N_A-C_W	108.0	585.76		
C_1-N_A-C_R	126.4	585.76		
C_1-N_A-C_W	125.6	585.76		
N_A-C_R-N_A	109.8	585.76		
H_{CR}-C_R-N_A	125.1	292.88		
C_W-C_W-N_A	107.1	585.76		
C_W-C_W-H_{CW}	130.9	292.88		
H_{CW}-C_W-N_A	122.0	292.88		
H_1-C_1-N_A	110.7	313.80		
H_1-C_1-H_1	107.8	276.14		
C_{2O}-C_1-N_A	112.7	418.40		
C_{2O}-C_1-H_1	110.7	313.80		
C_1-C_{2O}-H_C	110.7	313.80		
H_C-C_{2O}-H_C	107.8	276.14		
C_1-C_{2O}-O_H	109.5	418.68		
H_C-C_{2O}-O_H	109.5	293.08		
C_{2O}-O_H-H_O	108.5	460.55		
dihedralangles	potential type	V1(kJmol-1)	V2(kJmol-1)	V3(kJmol-1)
C_W-N_A-C_R-N_A	cos3	0.0000	19.460	0.0000
C_W-N_A-C_R-H_{CR}	cos3	0.0000	19.460	0.0000
C_1-N_A-C_R-N_A	cos3	0.0000	19.460	0.0000
C_1-N_A-C_R-H_{CR}	cos3	0.0000	19.460	0.0000
C_R-N_A-C_W-C_W	cos3	0.0000	12.550	0.0000
C_R-N_A-C_W-H_{CW}	cos3	0.0000	12.550	0.0000
C_1-N_A-C_W-C_W	cos3	0.0000	12.550	0.0000
C_1-N_A-C_W-H_{CW}	cos3	0.0000	12.550	0.0000
N_A-C_W-C_W-N_A	cos3	0.0000	44.980	0.0000
H_{CW}-C_W-C_W-N_A	cos3	0.0000	44.980	0.0000
H_{CW}-C_W-C_W-H_{CW}	cos3	0.0000	44.980	0.0000
C_W-H_{CW}-N_A-C_W	cos3	0.0000	9.2000	0.0000
C_W-H_{CW}-C_W-N_A	cos3	0.0000	9.2000	0.0000
C_R-H_{CR}-N_A-N_A	cos3	0.0000	9.2000	0.0000
N_A-C_1-C_R-C_W	cos3	0.0000	8.3700	0.0000
N_A-C_1-C_W-C_R	cos3	0.0000	8.3700	0.0000
C_W-C_R-C_1-N_A	cos3	0.0000	8.3700	0.0000
C_W-N_A-C_1-H_1	cos3	0.0000	0.0000	0.5190
C_R-N_A-C_1-H_1	cos3	0.0000	0.0000	0.0000
C_{2O}-C_1-N_A-C_W	cos3	-7.1535	6.1064	0.7939

C_{2O}-C_1-N_A-C_R	cos3	-5.2691	0.0000	0.0000
H_C-C_{2O}-C_1-N_A	cos3	0.0000	0.0000	0.3670
H_1-C_1-C_{2O}-H_C	cos3	0.0000	0.0000	1.3305
H_1-C_1-C_{2O}-O_H	cos3	0.0000	0.0000	1.9594
C_1-C_{2O}-O_H-H_O	cos3	-1.4905	-0.7285	2.0599
H_C-C_{2O}-O_H-H_O	cos3	0.0000	0.0000	1.8841
N_A-C_1-C_{2O}-O_H	cos3	-3.5787	-1.6564	4.9154