Table I. Intermolecular model parameters used in the MD simulations of $MOENM_2E$ TFSI and BNME TFSI. (See atom numbering in Fig. 1).

Group	ε (10^{-20} J)		σ (Å)		q (e)	
	O	CH_2	O	CH_2	O	CH_2
1 - CH_3	0.036	0.036	4.432	4.432	0.225	-0.110
2 - X	0.063	0.081	3.108	3.991	-0.390	0.210
3 – CH_2	0.081	0.081	3.991	3.991	0.370	0.150
4 – CH_2	0.081	0.081	3.991	3.991	-0.057	-0.150
5 - N^+	0.104	0.104	3.25	3.25	0.310	0.370
6 - CH_2	0.081	0.081	3.991	3.991	0.160	0.160
7 - CH_3	0.036	0.036	4.432	4.432	0.060	0.060
8 - CH_3	0.036	0.036	4.432	4.432	0.160	0.160
9 - CH_3	0.036	0.036	4.432	4.432	0.160	0.160

Table II. Intramolecular model parameters used in the MD simulations of $MOENM_2E$ TFSI and BNME TFSI.

	k_r (10^{-20} J.Å^{-2})		r_{eq} (Å)			k_θ (*k*J.mol^{-1}.rad^{-2})		θ_{eq} (angle)	
	O	CH_2	O	CH_2		O	CH_2	O	CH_2
CH_3-X	222.295	186.172	1.41	1.53	CH_3XCH_2	34.734	40.620	109.5	111.6
X-CH_2	222.295	186.172	1.41	1.53	XCH_2CH_2	34.734	40.620	109.5	111.6
CH_2-CH_2	186.172	186.172	1.53	1.53	CH_2CH_2N	55.574	55.574	111.2	111.2
CH_2-N	254.944	254.944	1.47	1.47	CH_2NCH_2	34.734	34.734	113.0	113.0
N-CH_2	254.944	254.944	1.47	1.47	NCH_2CH_3	55.574	55.574	111.2	111.2
N-CH_3	254.944	254.944	1.47	1.47	CH_3NCH_3	34.734	34.734	113.0	113.0
CH_2-CH_3	186.172	186.172	1.53	1.53					

	$k_{\psi,n}$ (kJ mol^{-1})		N		δ (angle)	
CXCC	-0.1994	0.1046	1	1	0	0
CXCC	-0.3463	-	2	-	180	-
XCCN	2.0357	2.0357	1	1	0	0
XCCN	-0.1456	-0.1456	2	2	0	0
XCCN	0.5595	0.5595	3	3	0	0
CCNC	0.5992	0.5992	1	1	0	0
CCNC	-0.4168	-0.4168	2	2	0	0
CCNC	0.9176	0.9176	3	3	0	0