Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Molecular Dynamics Study of Fluorosulfonyl Ionic Liquids as Electrolyte for Electrical Double Layer Capacitors

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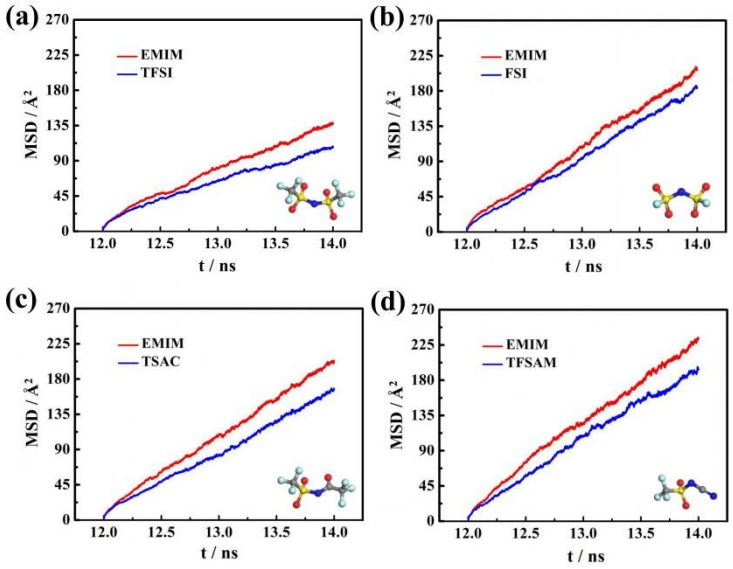

Figure S1. Mean Square Displacement (MSD) curves of the four fluorinated sulfonyl ILs using OPLS-VSIL force field.

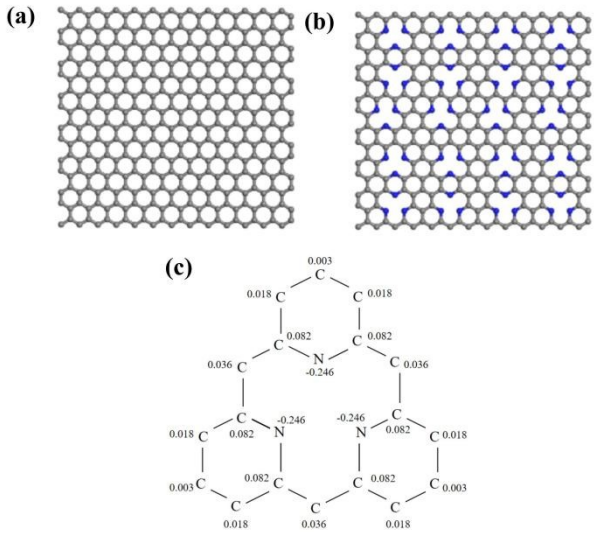

Figure S2. (a) Pristine graphene electrode; (b) defect graphene electrode; (c) Local charge distribution of defective graphene electrode

Table S1. Self diffusion parameters of four fluorinated sulfonyl ionic liquids

	$D^{+}(10^{-10}m^2/s)$	$D^{-}(10^{-10}m^2/s)$
EMIMTFSI	0.332	0.211
EMIMFSI	0.552	0.394
EMIMTSAC	0.34	0.219
EMIMTFSAM	0.511	0.299

Table S2. Values of Beta Factors

		OPLS	OPLS-VSIL
EMIMTFSI	EMIM	0.6	0.8
	TFSI	0.7	0.7
EMIMFSI	EMIM	0.6	0.9
	FSI	0.7	0.9
EMIMFSAC	EMIM	0.8	1
	TSAC	0.6	1
EMIMTFSAM	EMIM	0.8	0.9
	TFSAM	0.6	0.8

Table S3. Comparison of self diffusion coefficients simulated by OPLS and OPLS-VSIL force field

	OPLS		OPLS-VSIL	
	$D^+(10^{-10}m^2/s)$	$D^-(10^{-10}m^2/s)$	$D^+(10^{-10}m^2/s)$	$D^-(10^{-10}m^2/s)$
EMIMTFSI	0.332	0.211	1.041	0.785
EMIMFSI	0.552	0.394	1.642	1.481
EMIMTSAC	0.34	0.219	1.6	1.3
EMIMTFSAM	0.511	0.299	1.728	1.542

Table S4. Comparison of Conductivity simulated by OPLS and OPLS-VSIL force field

	OPLS	OPLS-VSIL
EMIMTFSI	6.69 S • cm^{-1}	21.45 S • cm^{-1}
EMIMFSI	14 S • cm^{-1}	46.14 S • cm^{-1}
EMIMTSAC	7.12 S • cm^{-1}	36.46 S • cm^{-1}
EMIMTFSAM	12.23 S • cm^{-1}	45.92 S • cm^{-1}