Supporting information for

Atomistic insights into confinement and electric potential effects on the Electric Double Layer of CO_2/IL at slits

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Table S1 Detailed LJ interaction parameters for each atom in the CO_2/IL.

Molecule	Atom	ε_0 (kcal/mol)	σ_0 (Å)	Charge(e)
CO_2	C	0.056	2.757	0.7
	O	0.16	3.033	-0.35
$Bmim^+$	C in Imidazole ring	0.066	3.5	+0.131
	N in Imidazole ring	0.17	3.25	-0.347
	H in Imidazole ring	0.03	2.5	+0.186
	C in Methyl	0.066	3.5	-0.043
	H in Methyl	0.03	2.5	0.09
	C in Butyl chain	0.066	3.5	-0.043
	H in Butyl chain	0.03	2.5	0.09
Tf_2N^-	O	0.17	2.96	-0.53
	S	0.25	3.55	1.02
	N	0.17	3.25	-0.53
	C	0.066	3.5	0.35
	F	0.06	2.9	-0.16

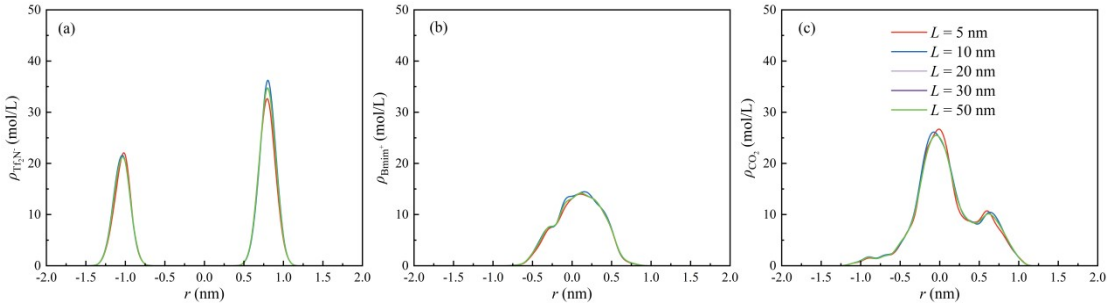

FIG: S1 The density distribution of (a) Tf_2N^- , (b) $Bmim^+$, and (c) CO_2 along the r when φ = -1.4 V under different lengths of CNT at d = 0.8 nm.

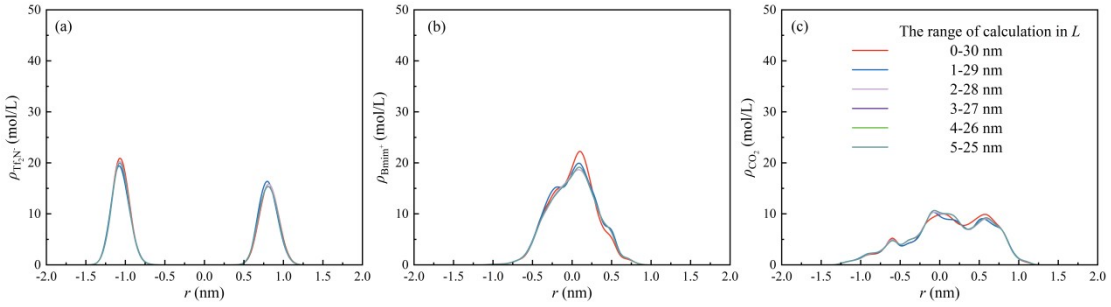

FIG: S2 The density distribution of (a) Tf_2N^- , (b) $Bmim^+$, and (c) CO_2 along the r when φ = 1.4 V under different regions of slit at d = 0.8 nm.

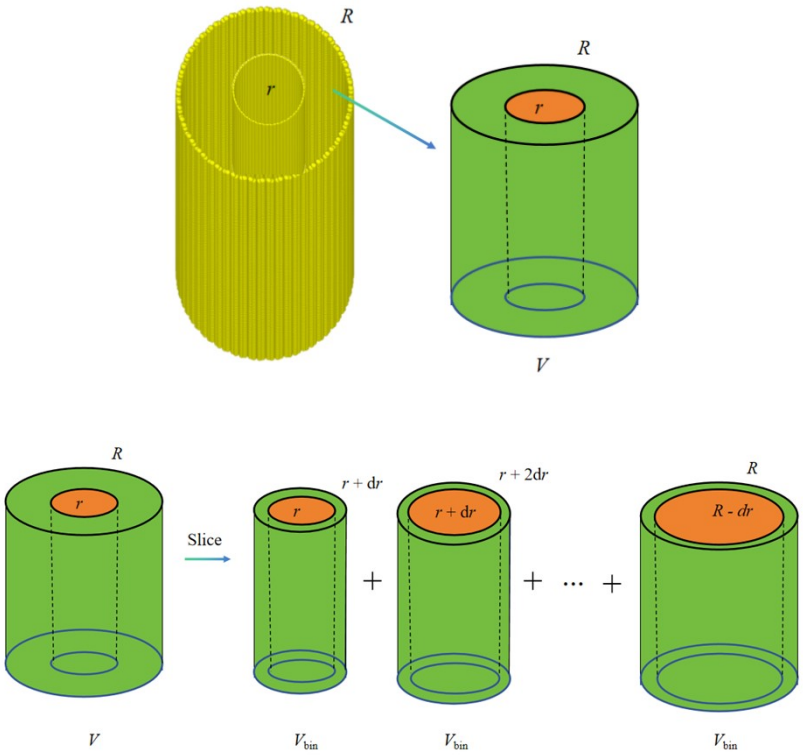

FIG: S3 Illustrations of the method of slice each layer inside the slit.