Supporting Information

Interface Enhanced CO_2 Capture through Synthetic Effects of Nanomaterial Supported Ionic Liquid Thin Film

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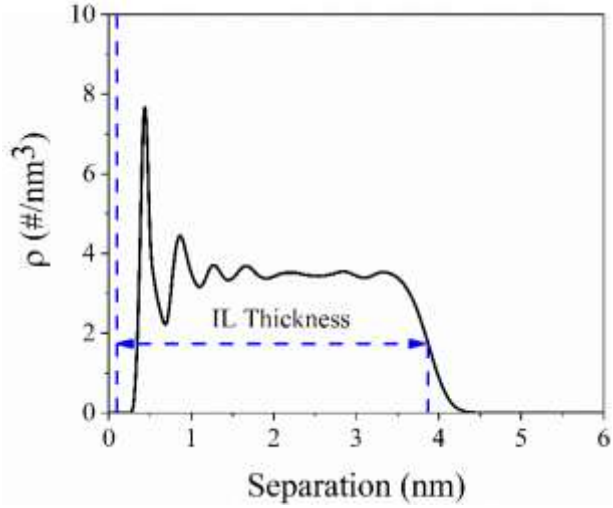

Figure S1 Defination of the IL film thickness. The thickess is defined as the distance from the nanosheet to the liquid-gas interface, where the IL density is half of the bulk value.

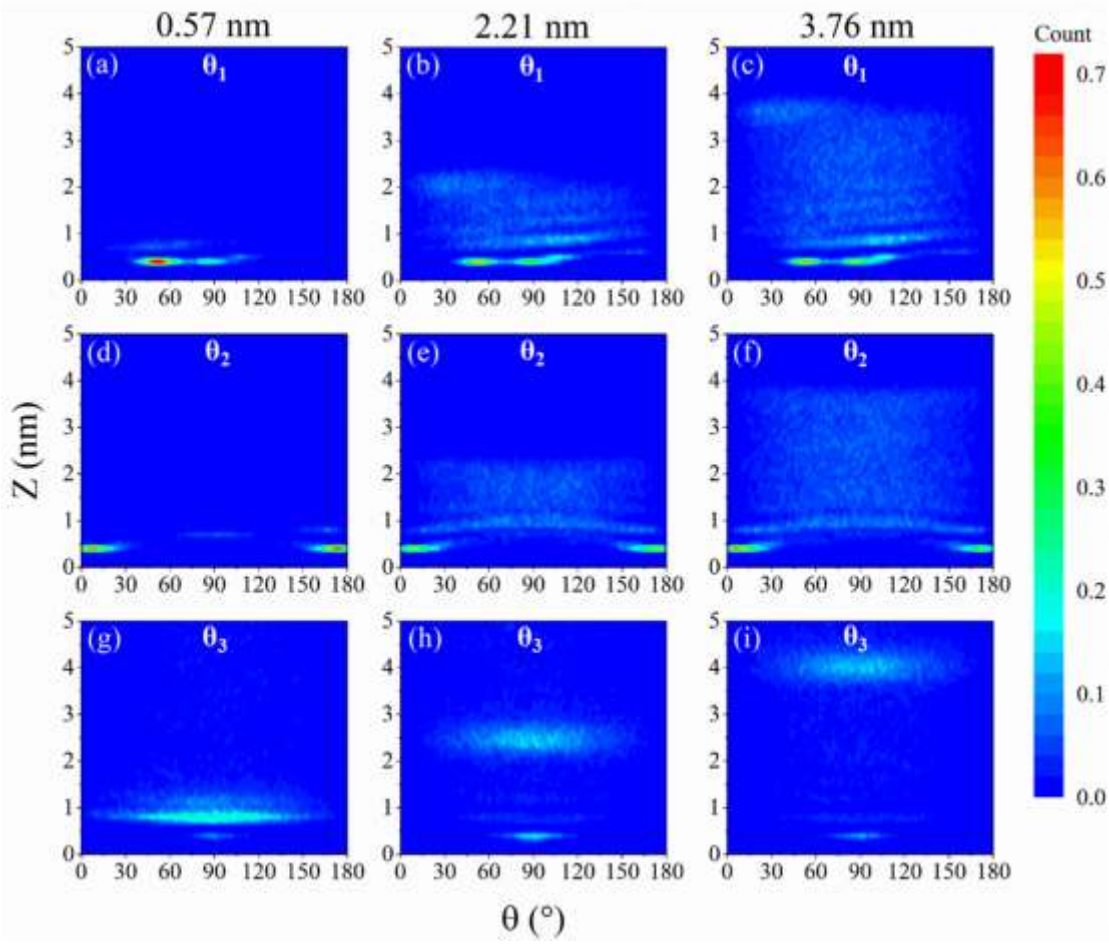

Figure S2 Distribution of the tilt angles of the ethyl side chain of cations (a-c), imidazolium ring of cations (d-g) and CO_2 (g-i) in three IL films attached to C_3N with IL thickness of 0.57 nm, 2.21 nm and 3.76 nm, respectively.

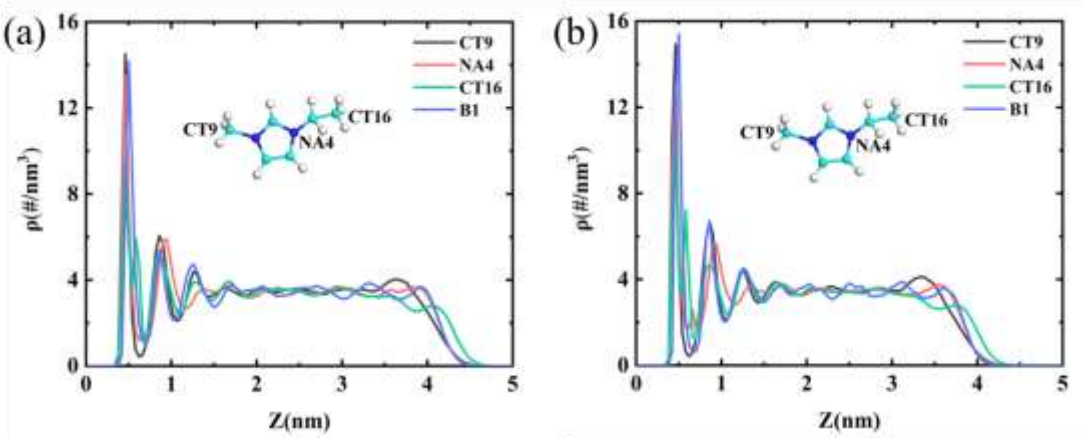

Figure S3 Number density profiles of atomic groups of cations and anions in the (a) GRA systems and (b) C_3N systems. The profiles are generated based on the last 30 ns trajectories of the system containing 140 ion pairs. The methyl group, imidazolium ring and ethyl group of the cation are represented by CT9, NA4 and CT16 atoms, respectively, as illustrated by the embedded molecular structure. The anion is represented by the boron atom.

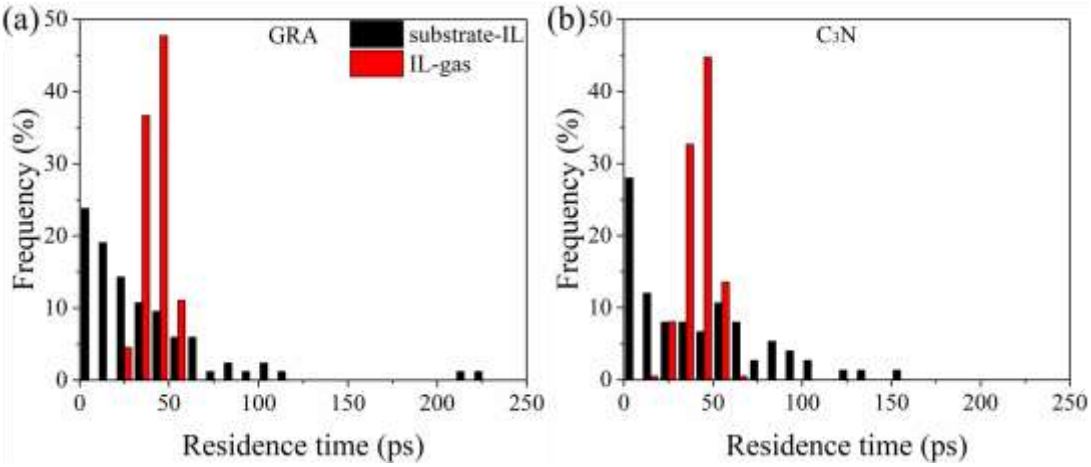

Figure S4 Distribution of the residence time of CO_2 molecules in the two interfacial regions of the GRA system (a) and C_3N system (b). The residence time is calculated based on the simulation systems with IL thickness of 4.09 nm (GRA) and 3.76 nm (C_3N). The substrate-IL interfaces are defined as the region with z-coordinates from 0.34 nm to 1.02 nm in both the GRA system and the C_3N system. The IL-gas interfaces are defined as the region with z-coordinates from 3.66 nm to 5.58 nm in the GRA system and z-coordinates from 3.06 nm to 4.98 nm in the C_3N system.

Table S1 Percentage of the captured and uncaptured CO_2 in the GRA systems.

Thickness (nm)	Captured CO_2 (%)			Uncaptured CO_2 (%)
	Solid-liquid interface	Bulk liquid	Liquid-gas interface	
0.57	N.A	N. A.	N.A	71.1
1.57	4.0	N. A.	29.3	66.7
2.41	5.4	4.7	28.3	61.6
3.26	4.0	9.5	28.2	58.3
4.09	4.1	15.5	27.4	53.0

Table S2 Percentage of the captured and uncaptured CO_2 in the C_3N systems.

Thickness (nm)	Captured CO_2 (%)			Uncaptured CO_2 (%)
	Solid-liquid interface	Bulk liquid	Liquid-gas interface	
0.57	N.A	N. A.	N.A	71.1
1.43	4.5	N. A.	28.4	67.1
2.21	5.0	4.0	27.9	63.1
3.00	4.4	8.8	27.7	59.1
3.76	3.7	13.1	28.4	54.8