Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular Dynamics Simulation of Pyrrolidinium and Imidazolium Ionic Liquids at Graphene Interfaces

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SUPPLEMENTARY INFORMATION

Figure S1

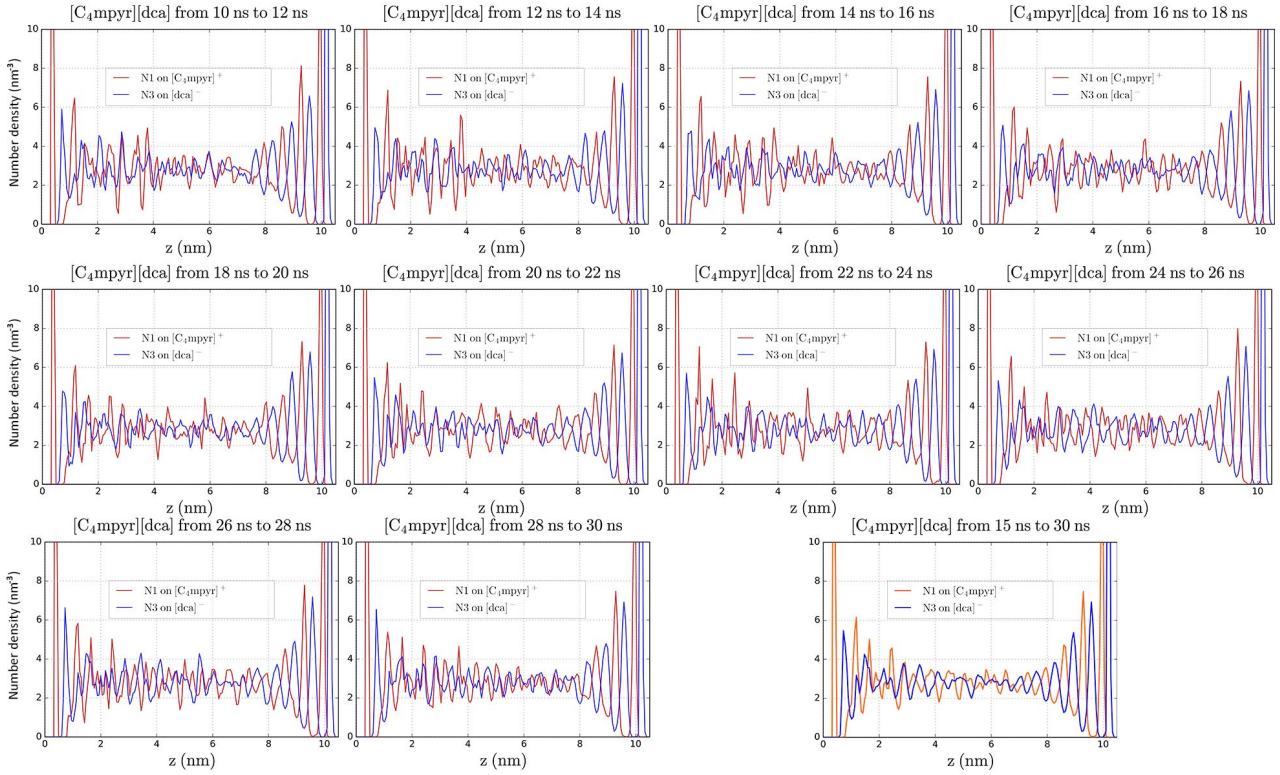

Figure S1 – Time-window analysis of [C_4mpyr][dca] from 10 ns to 30 ns in windows of 2 ns. The number of cationic layers near the negative electrode stabilizes after about 16-18 ns. The last chart shows the 15-30 ns time-window of partial density of the cation and anion. All densities were traced on the nitrogen atoms N1 (cation) and N3 (anion).

FIGURE S2

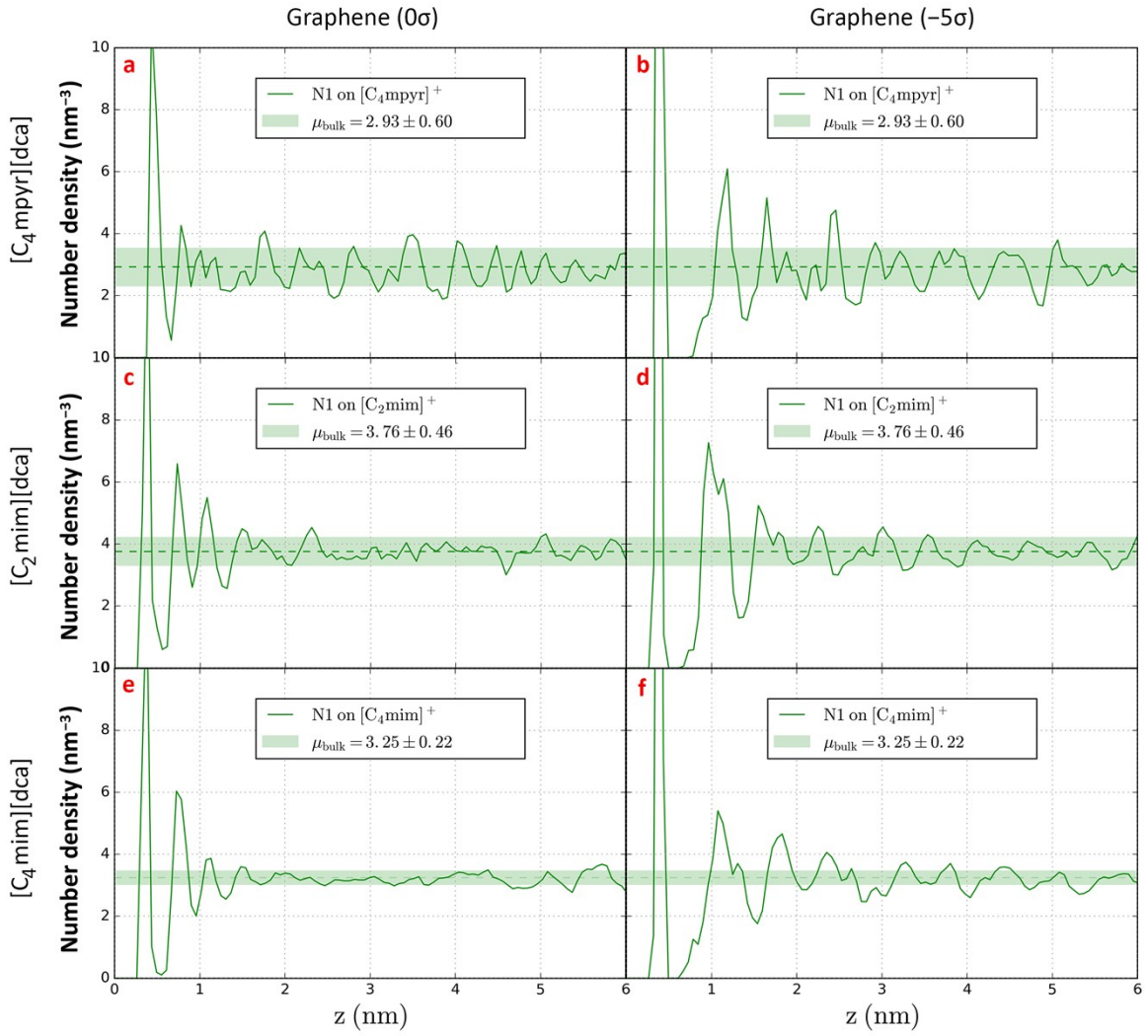

Figure S2 – Zoomed-in cation-only partial densities (N1-atom) of all 3 ILs at both uncharged and negatively charged graphene. The thick green region indicates the mean with standard deviation of partial densities as obtained from the simulations of the corresponding ILs in the absence of electrodes.

Figure S3

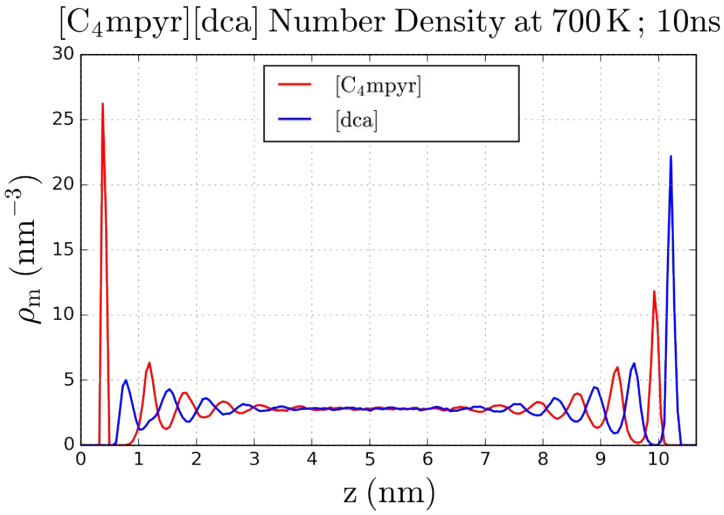

Figure S3 – [C_4mpyr][dca] number density (nitrogen atoms) for a 10 ns NVT simulation at 700 K and 5 σ surface charge density of graphene.

Figure S4

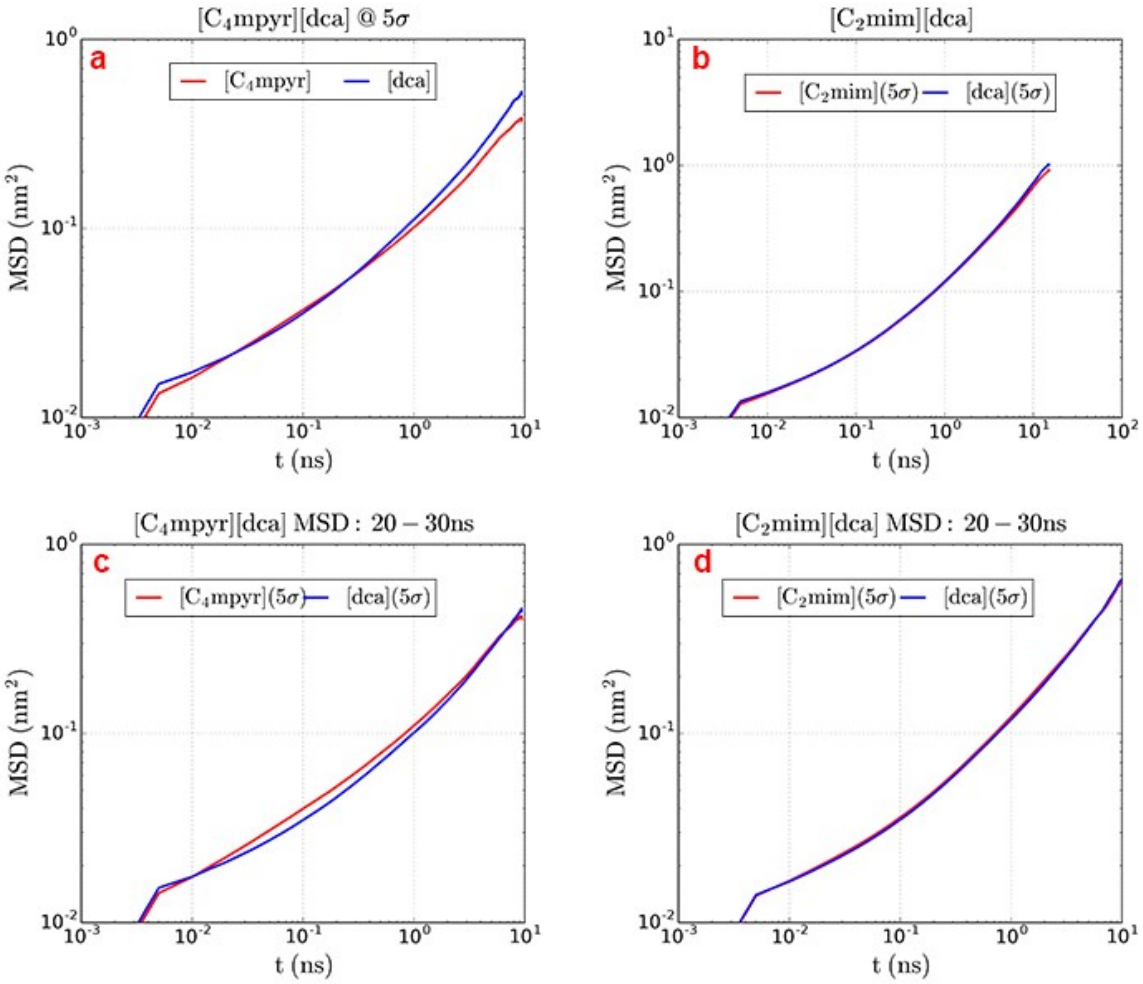

Figure S4 – MSD plots for cations and anions in [C_4mpyr][dca] and [C_2mim][dca] at 5σ for the time domain 20-30ns. (a-b): all IL ions included in the analysis; (c-d): ions in the inner/adsorbed layers excluded from the analysis.