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

Supplementary Information: Electric double layer structure and differential capacitance at the electrode interface of tributylmethylammonium bis(trifluoromethanesulfonyl)amide studied using molecular dynamics simulation.

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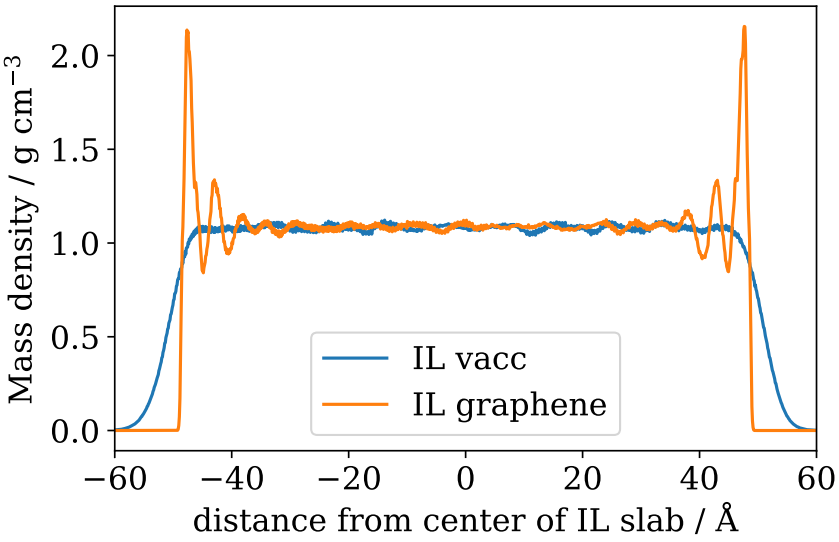

Figure S1: Mass density distribution of $[N^{+}_{1444}][TFSA^{-}]$ slab at the vacuum interface and the graphene interface.

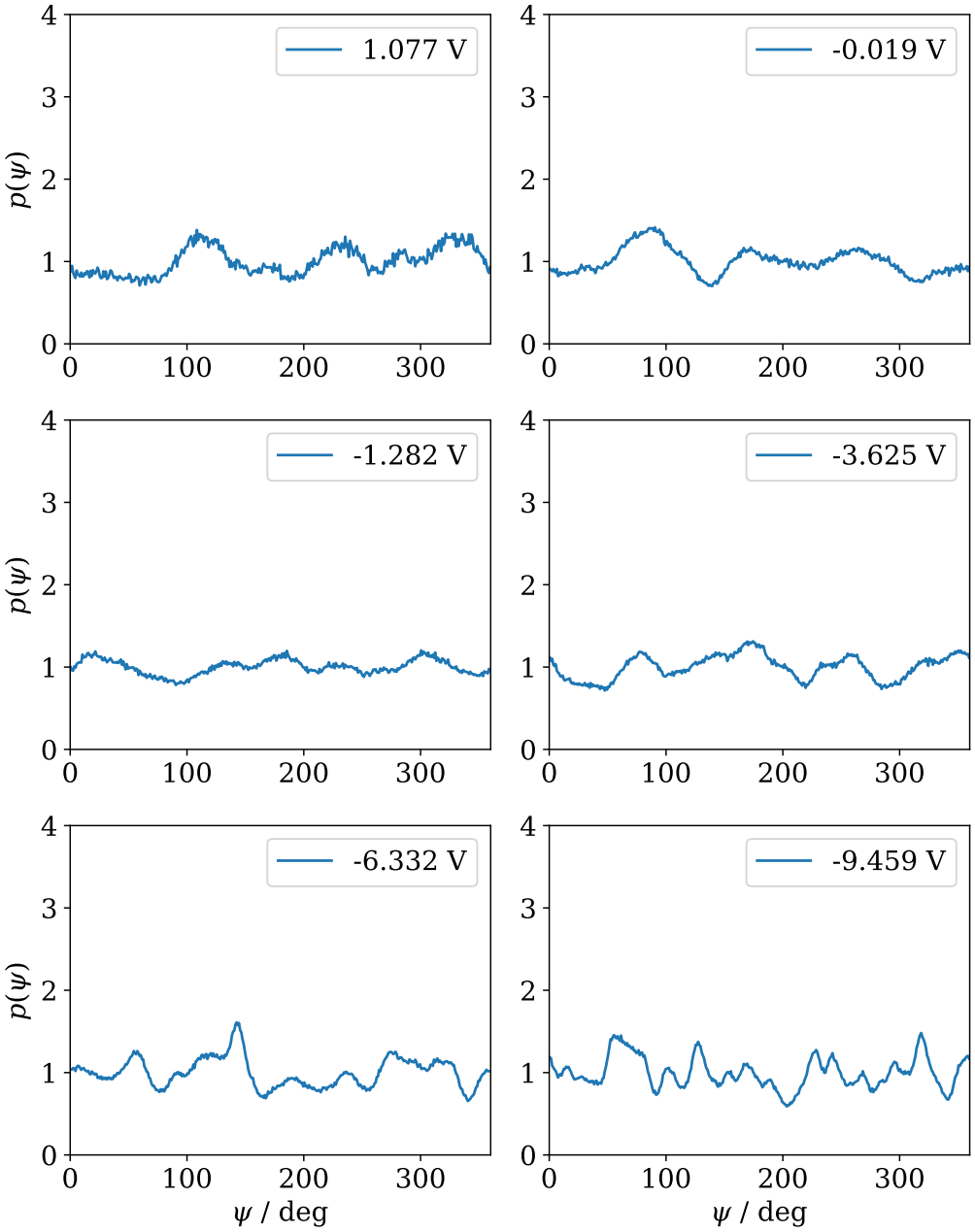

Figure S2: Orientational distribution on azimuthal angle $p(\psi) = \int_0^\pi p(\theta, \psi) \mathrm{d}\theta$.

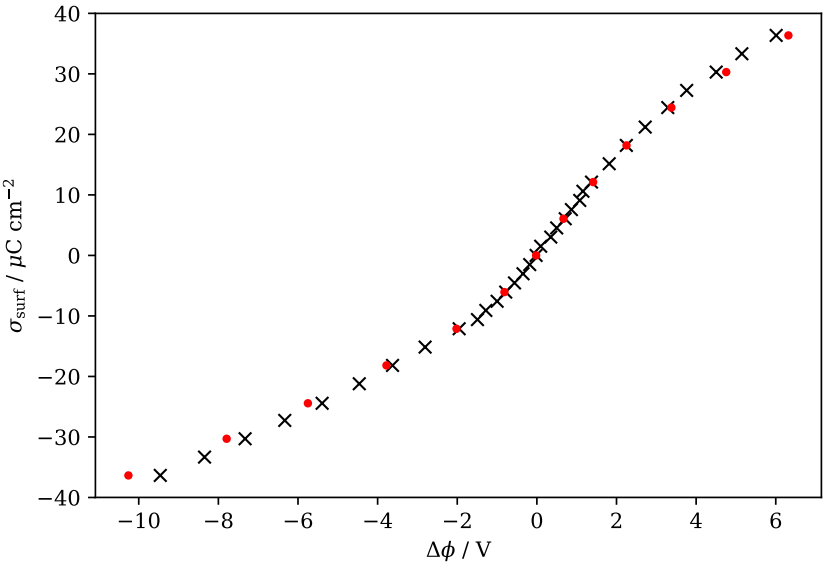

Figure S3: Relationship between the given surface charge density of electrode σ_{elec} and the calculated interfacial potential difference $\Delta\phi$. Black plots; results using SPME. Red plots; results using SPME with slab correction.[1]

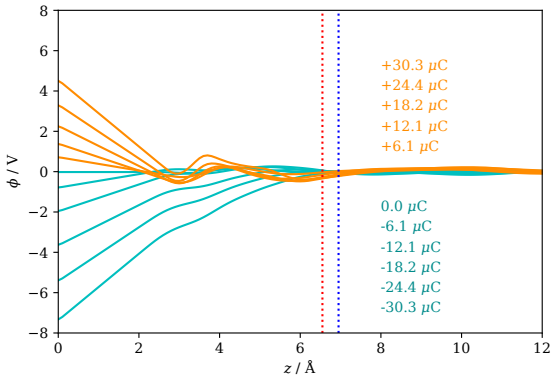

Figure S4: Potential profiles as a function of the distance from electrode (z). The potential at IL_{bulk} was set to be zero. The dotted lines are the border between the first and second layers (z_{div}) of N_{Qa} (red) and N_{BT} (blue).

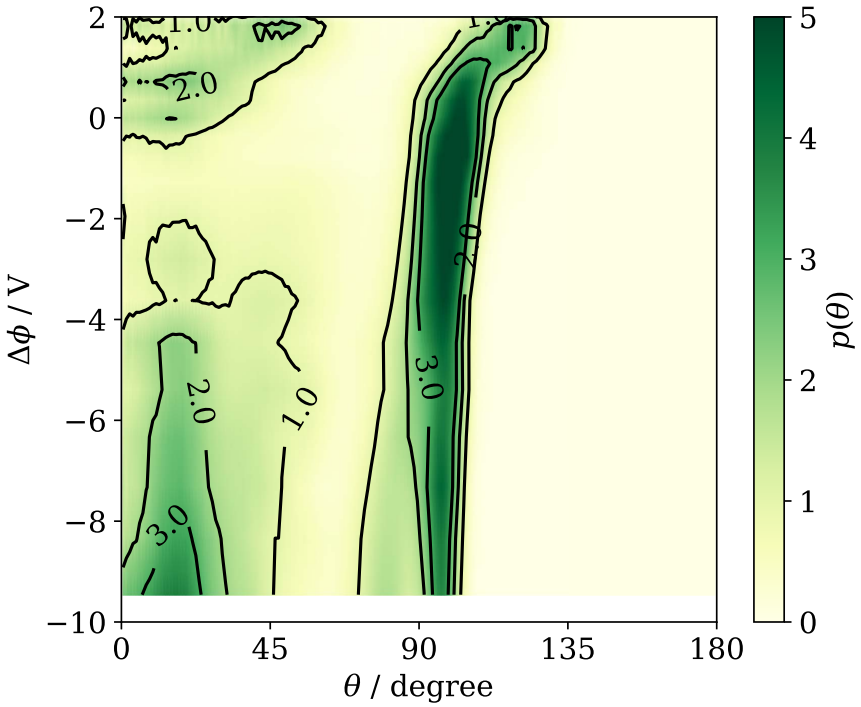

Figure S5: Contour map of $p_{NQa\text{-}CB4}(\theta)$ on the $\Delta\phi$-θ plane.

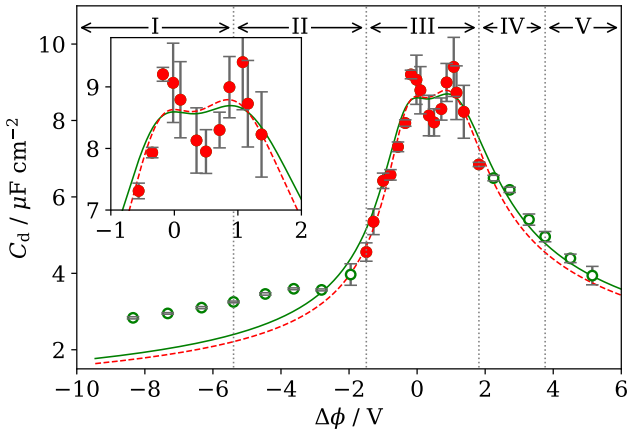

Figure S6: $\Delta\phi$-C_d plot. The plot and red dashed line are the same as in Fig.11. The green solid line is the fitting curve to all the plots. There is no qualitative difference between the red dashed line and the green solid line.

References

[1] I.-C. Yeh and M. L. Berkowitz, *J. Chem. Phys.*, 1999, **111**, 3155–3162.