SUPPORTING INFORMATION

Symmetric Effect on Electrical Double Layer Characteristics and Molecular Assembly Interplay in Imidazolium–based Ionic Liquids Electrolyte in Supercapacitor Models

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Contents

Figure S10. RDF and coordination number (C.N.) of each H atom type in [C1mim]+ paired with (a) OBT, (b) F1, and (c) NBT atom type in [NTf2]– between 0.0 V to 4.0 V at the distance within 10 Å from negatively charged electrode.

Figure S11. RDF and coordination number (C.N.) of each H atom type in [C1mim]+ paired with (a) OBT, (b) F1, and (c) NBT atom type in [NTf2]– between 0.0 V to 4.0 V at the distance within 10 Å from positively charged electrode.

Figure S12. RDF analysis of each atom type in [C2mim][NTf2] within bulk region. Colored solid lines are g(r) for each voltage from 0.0 V to 4.0 V (purple, blue, green, yellow and red, respectively). Colored dash lines are C.N. for each voltage.

S4 Electrostatic Potential Profile of [C1mim][NTf2] and [C2mim][NTf2] at each Voltage

Figure S13. Electrostatic potential profiles of (a) [C1mim][NTf2] and (b) [C2mim][NTf2] between 0.0 V to 4.0 V.

S1 RMSD Plots, Whole Charge Density Profiles, and Whole Mass/number Density Profiles of [C_1mim][NTf_2] and [C_2mim][NTf_2]

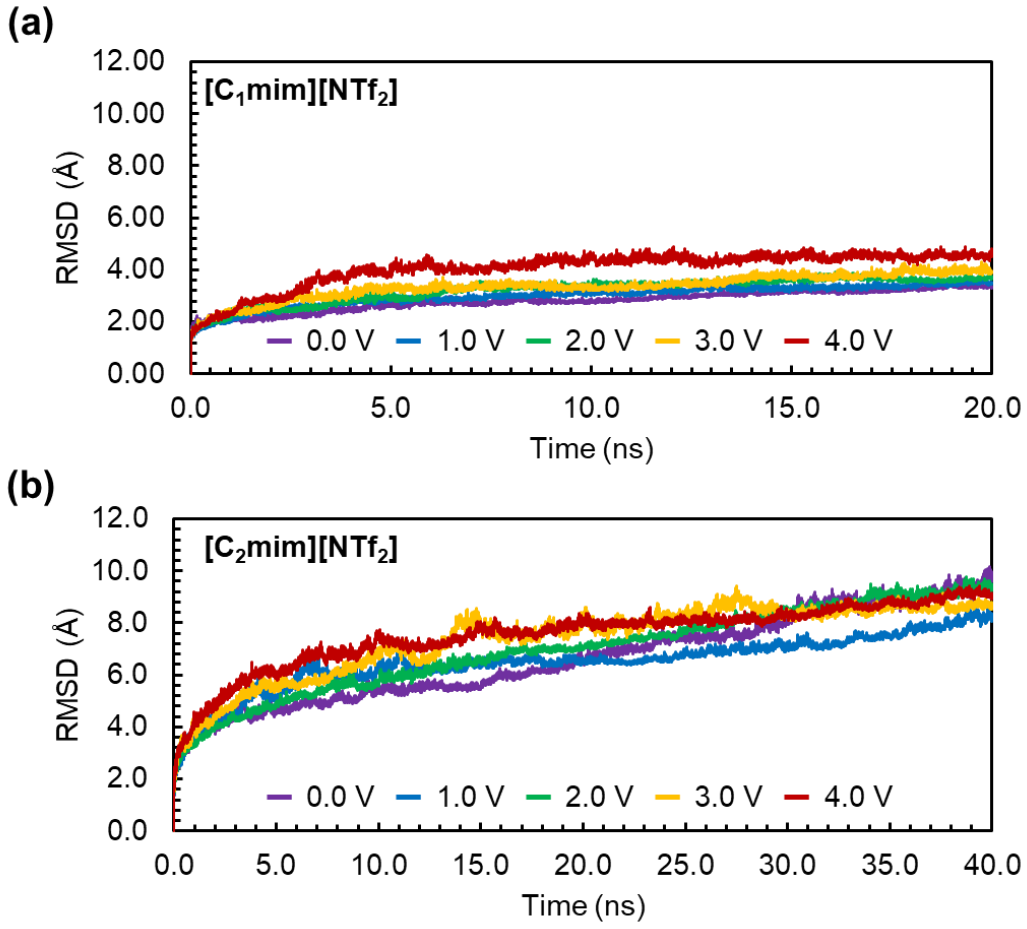


Figure S1. RMSD plots of (a) [C_1mim][NTf_2] and (b) [C_2mim][NTf_2] and in each $\Delta\Psi$.

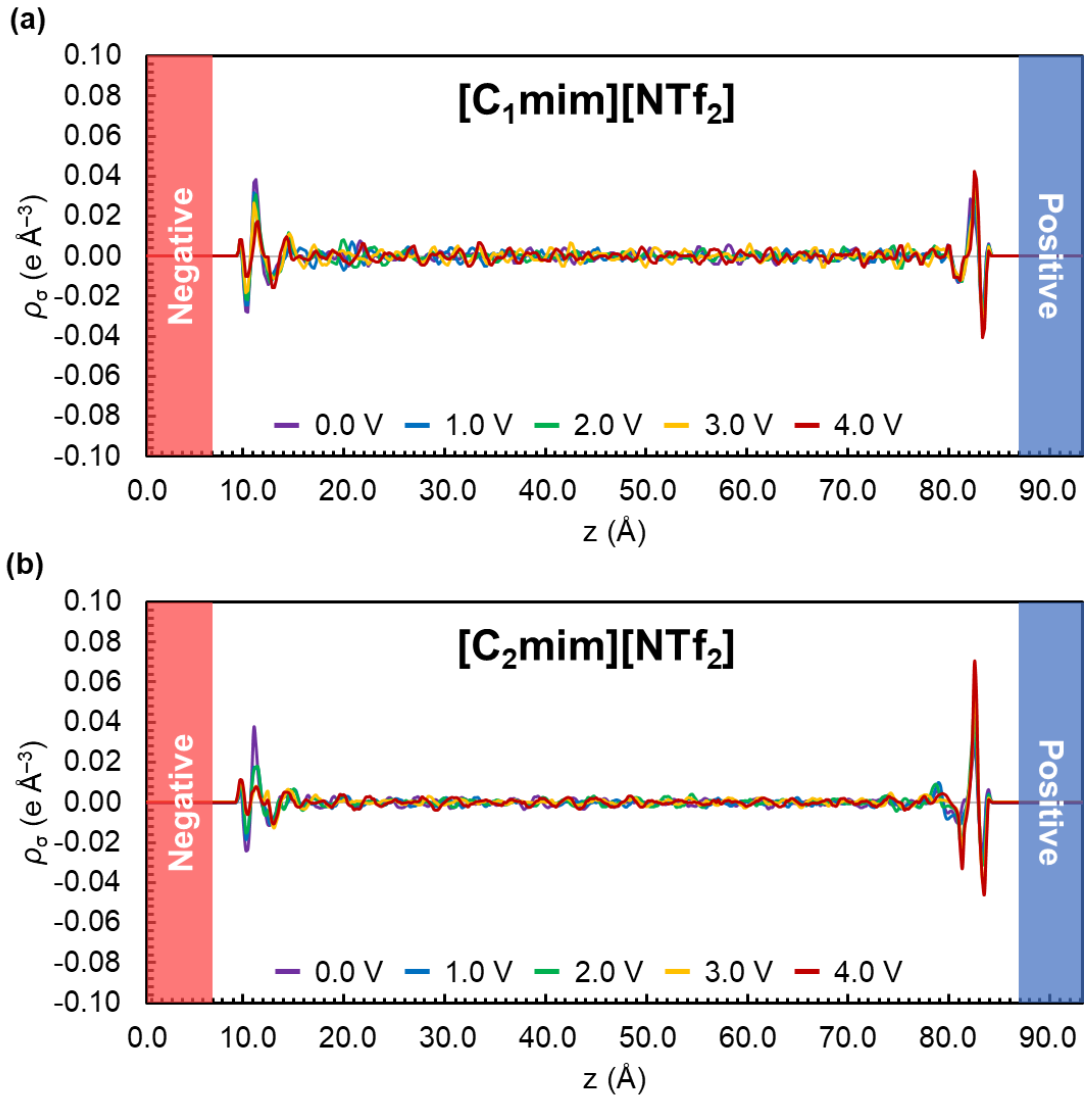


Figure S2. Charge density (ρ_σ) distribution plot of (a) [C_1mim][NTf_2] and (b) [C_2mim][NTf_2] at each $\Delta\Psi$.

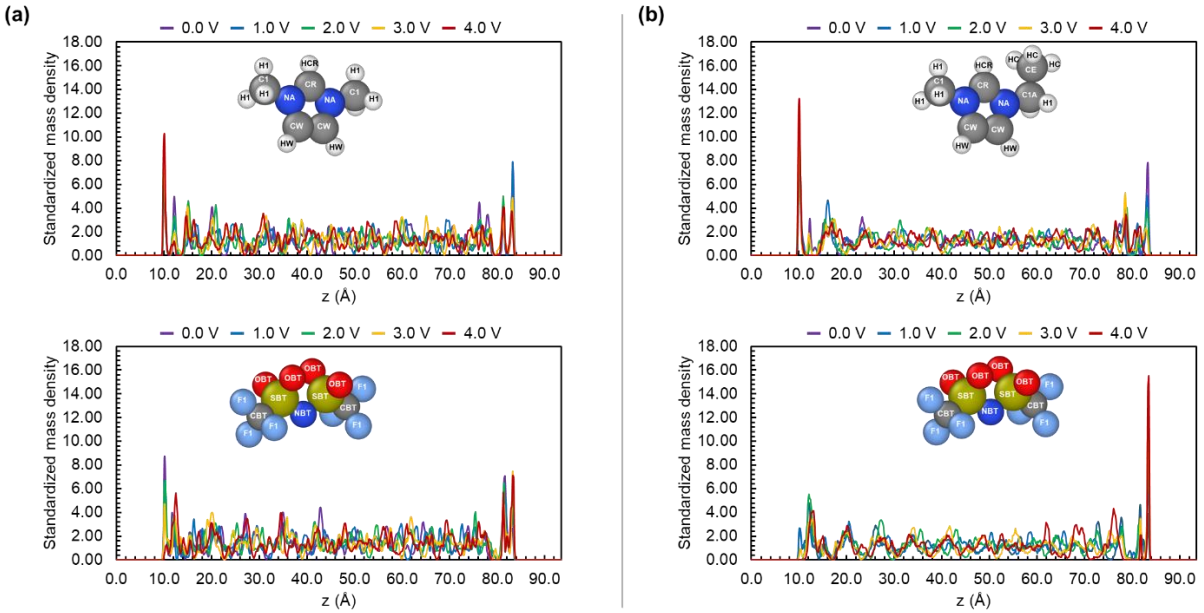


Figure S3. Standardized mass density distribution of (a) $[C_1mim]^+$ $[NTf_2]^-$ and (b) $[C_2mim]^+$ $[NTf_2]^-$ between 0.0 V to 4.0 V.

S2 Concentration Difference and Total Number of Molecular Ions in EDL Region of $[C_1mim][NTf_2]$ and $[C_2mim][NTf_2]$

The concentration difference between molecular ions in EDL region and bulk region was calculated by finding an average number of ions in each region divided by the volume of the region (9569 $Å^3$ for EDL region and 57416 $Å^3$ for bulk region). Then the difference of ion concentration in EDL to bulk was presented as mol L^{-1}. In addition, to determine the ion diffusion between EDL and bulk, the average number of ions within EDL region was calculated and presented as EDL total number where we compared the total number of ions in EDL region at the first 0.5 ns of the production run to the last 0.5 ns.

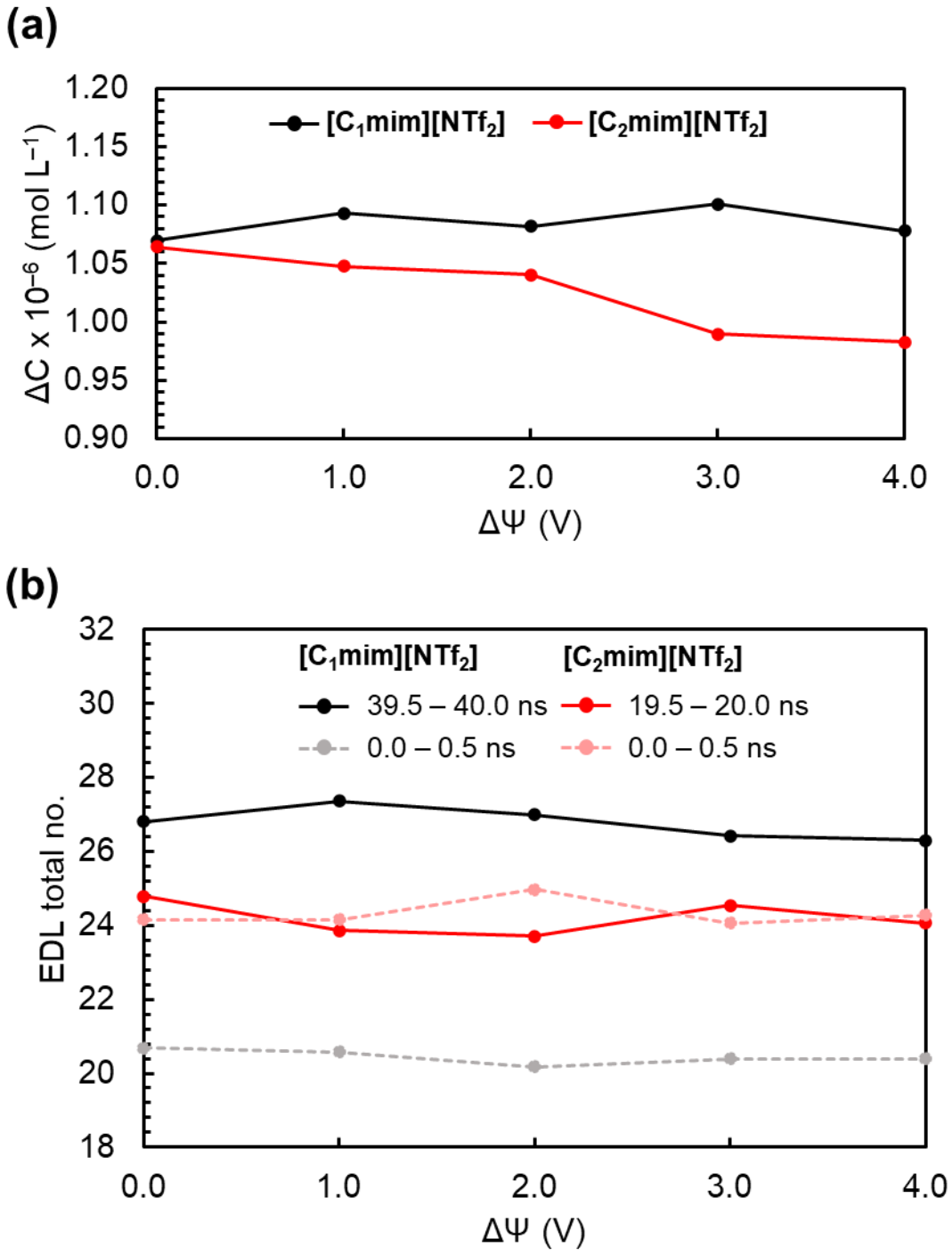


Figure S4. (a) Concentration differences (ΔC) between EDL region and bulk region of $[C_1mim][NTf_2]$ and $[C_2mim][NTf_2]$ at each voltage and (b) total number of molecular ions in EDL region of $[C_1mim][NTf_2]$ and $[C_2mim][NTf_2]$ at the first 0.5 ns of the simulation and the last 0.5 ns of the simulation at each voltage.

S3 Orientation Analysis of $[C_1mim][NTf_2]$ and $[C_2mim][NTf_2]$ in the Whole Cell, and Orientation of $[C_2mim][NTf_2]$ 10 Å from the Electrode Surface

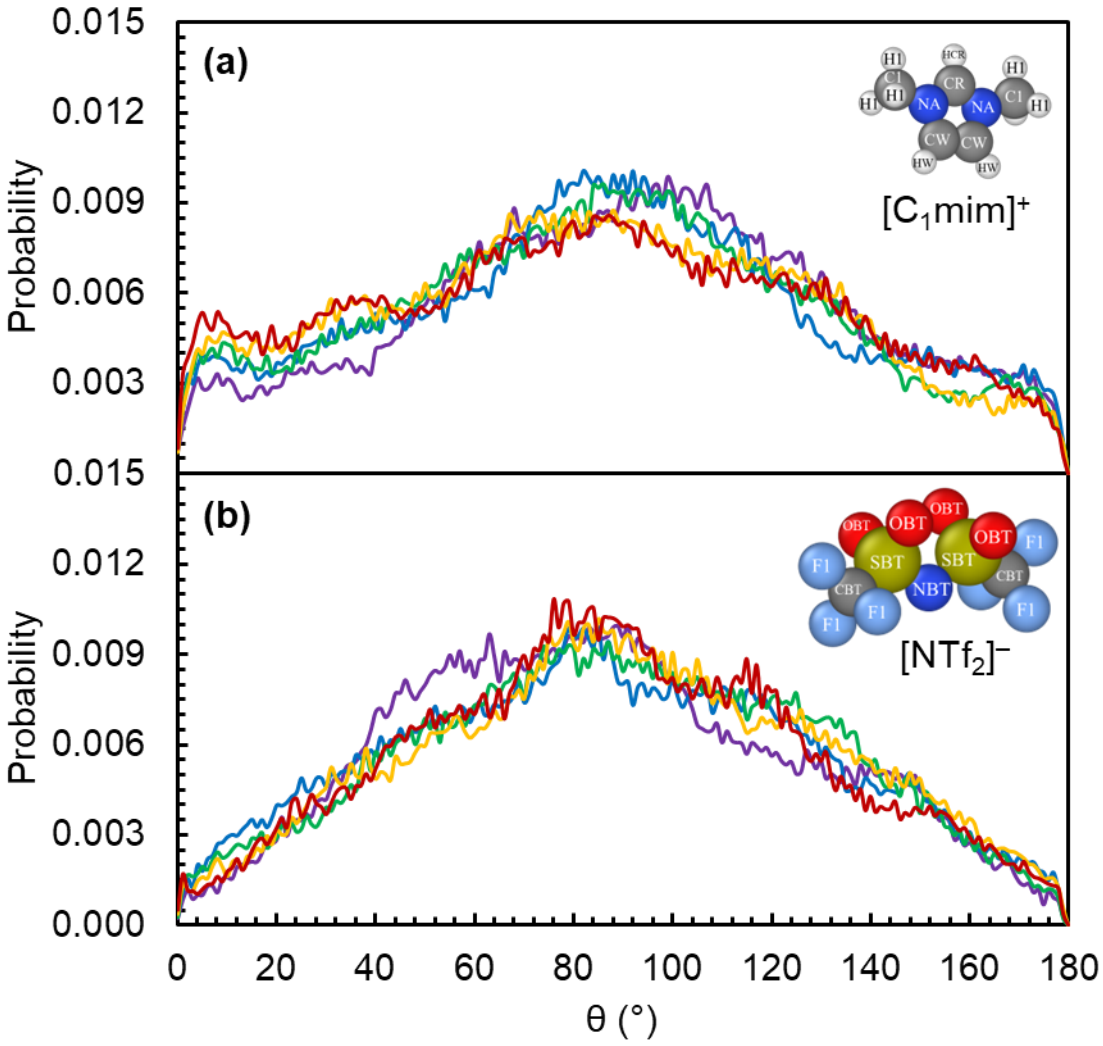


Figure S5. Probability plots across the whole cell of (a) $[C_1mim]^+$ and (b) $[NTf_2]^-$ between 0.0 V to 4.0 V.

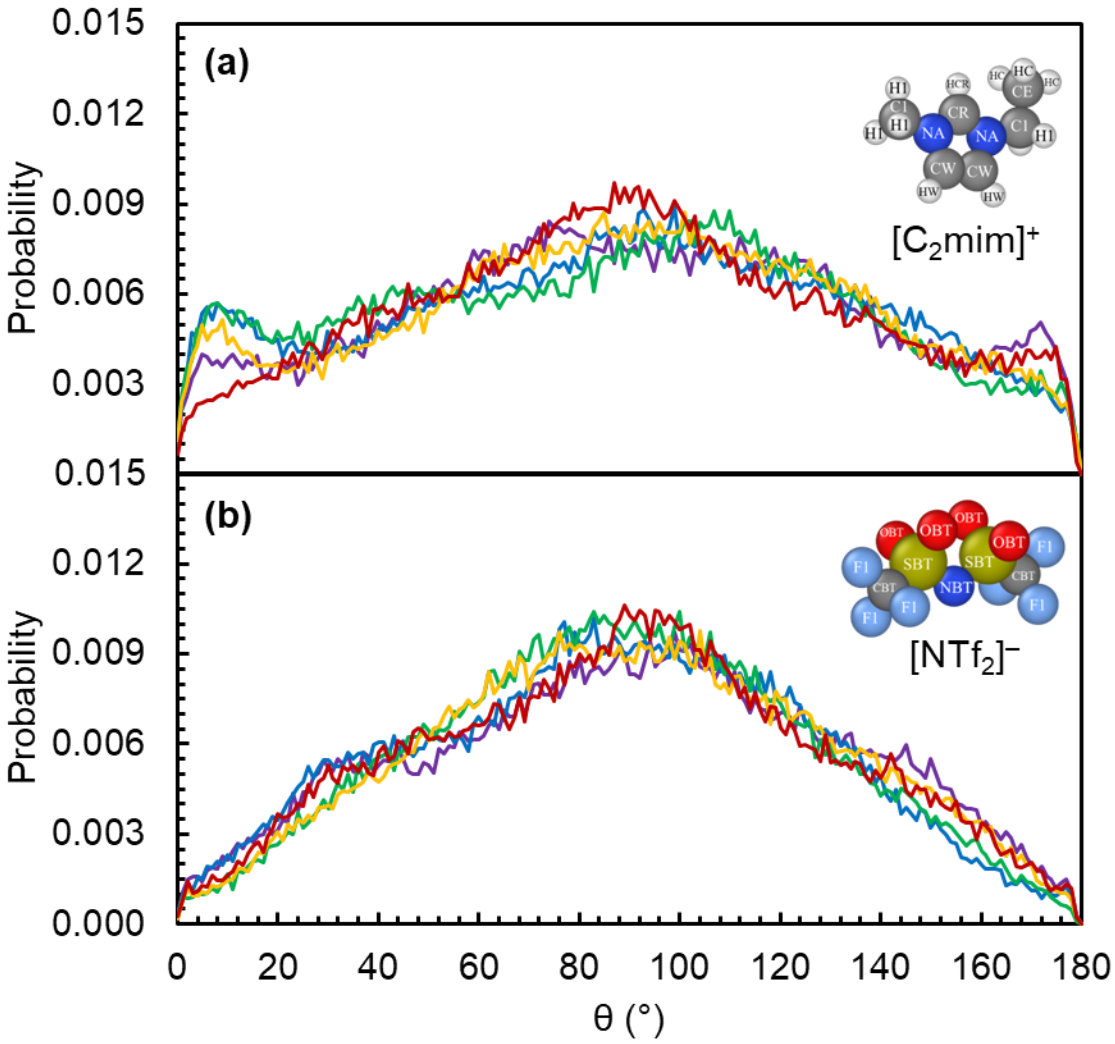


Figure S6. Probability plots across the whole cell of (a) $[C_2mim]^+$ and (b) $[NTf_2]^-$ between 0.0 V to 4.0 V.

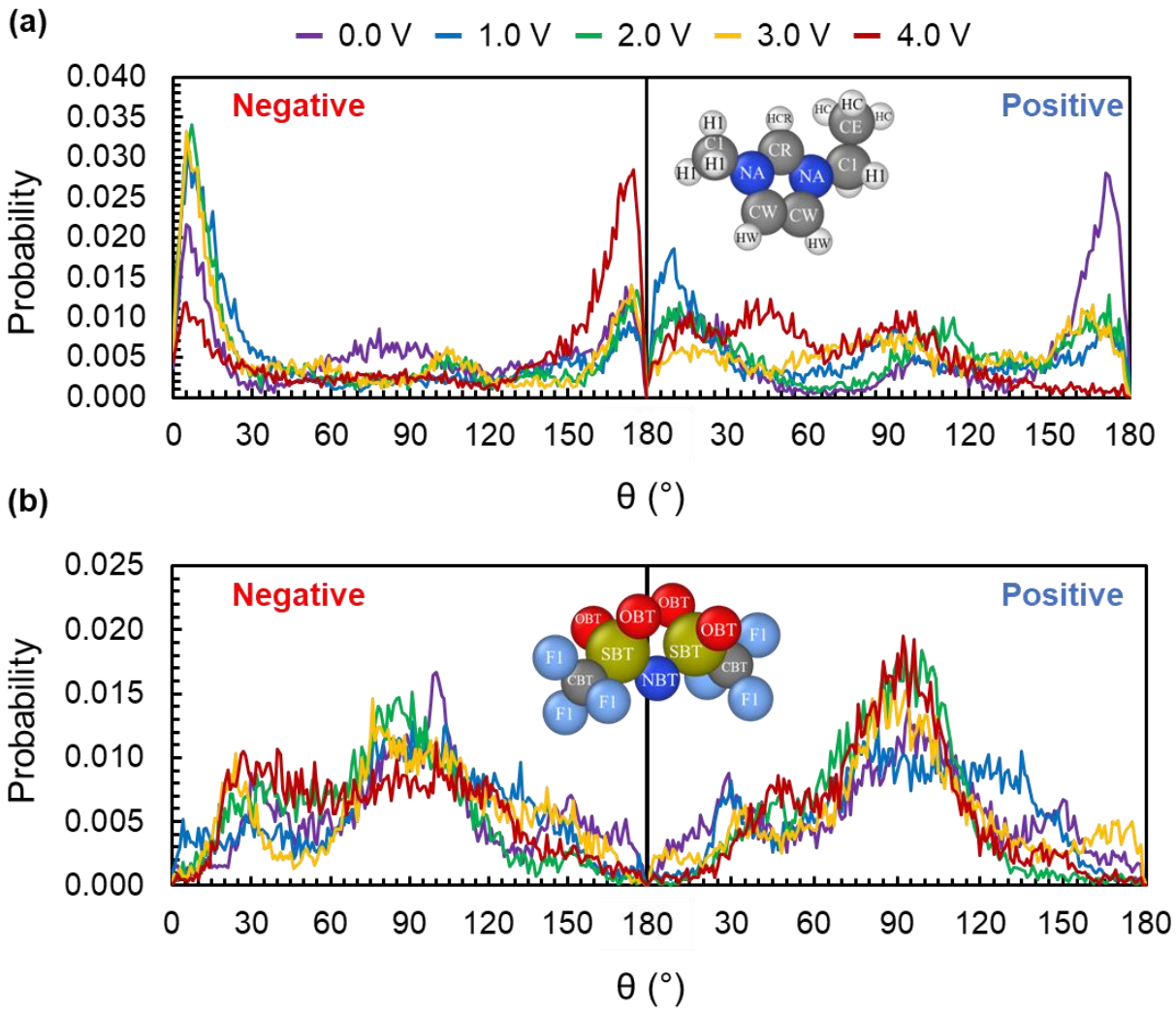


Figure S7. Orientation analysis of (a) $[C_2mim]^+$ and (b) $[NTf_2]^-$ within a distance of 10 Å from each electrode surface.

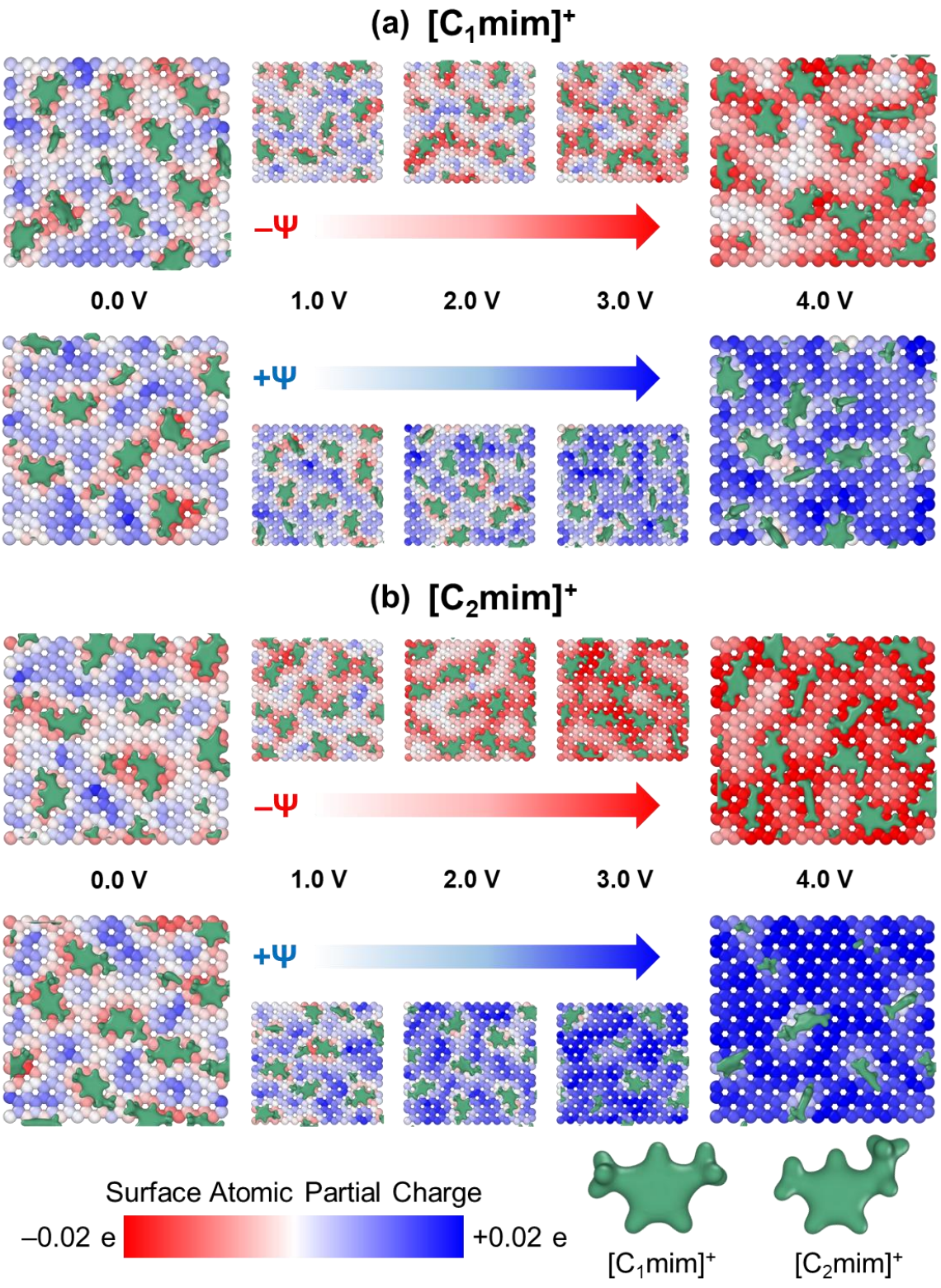


Figure S8. Snapshots of (a) $[C_1mim]^+$ and (b) $[C_2mim]^+$ on electrode surface visualized by gaussian density method (iso value = 1.0) at each voltage. Each snapshot was captured at the last frame of the simulation.

S4 Radial Distribution Function of [C_1mim][NTf_2] and [C_2mim][NTf_2] in the Bulk Region and [C_1mim][NTf_2] in the EDL Region

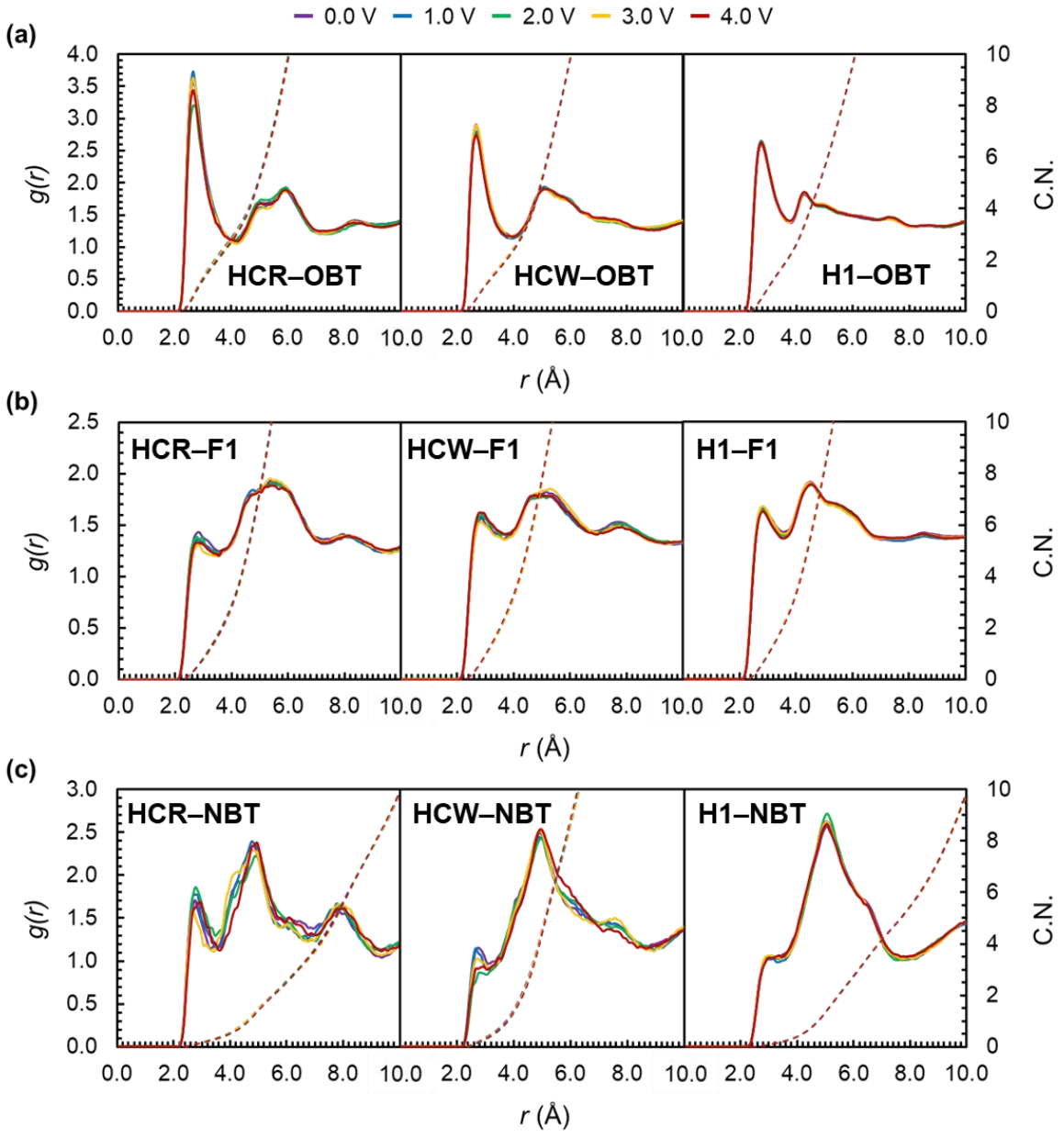


Figure S9. RDF analysis of each atom type in [C_1mim][NTf_2] within bulk region. Colored solid lines are gyration function (*g(r)*) for each voltage from 0.0 V to 4.0 V (purple, blue, green, yellow and red, respectively). Colored dash lines are C.N. for each voltage.

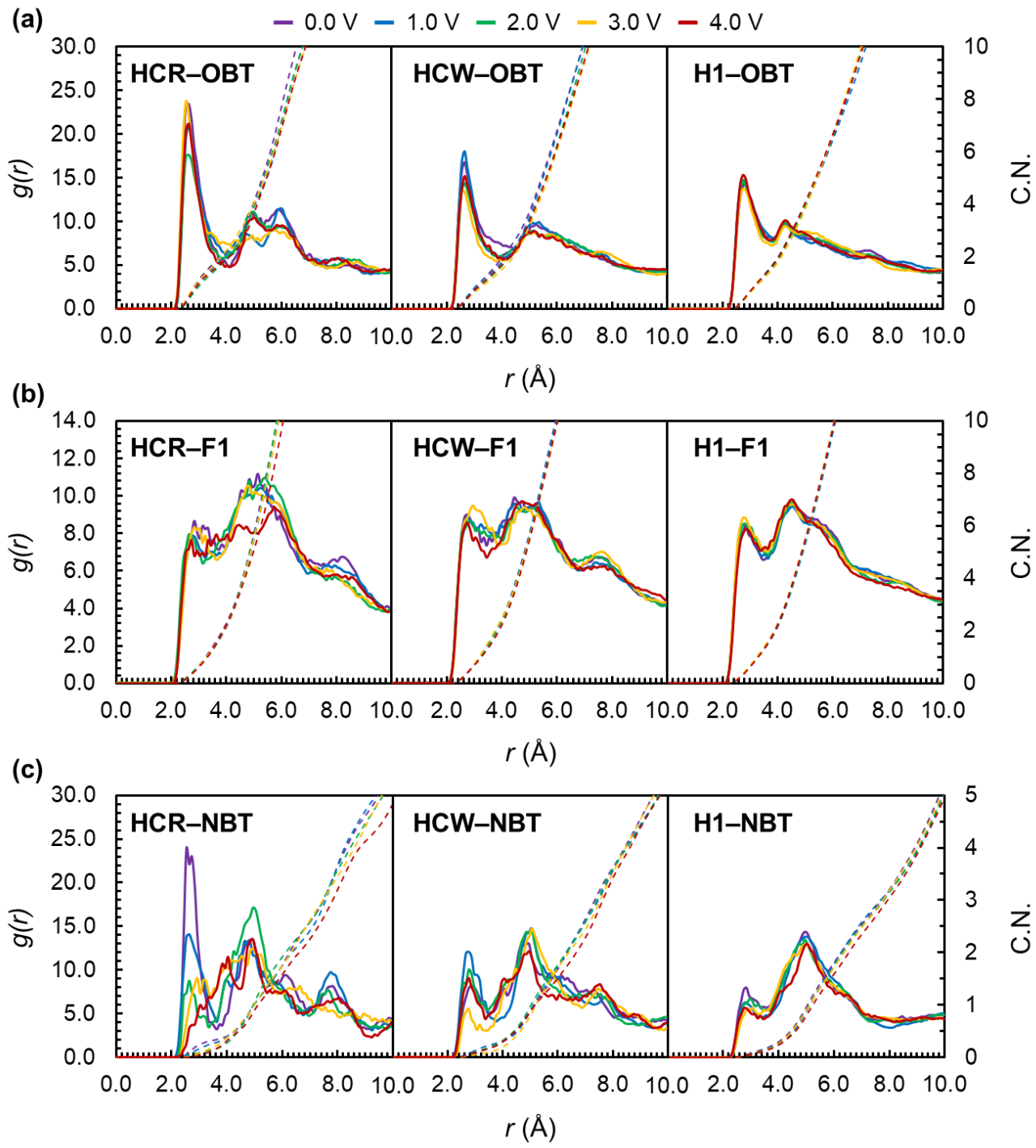
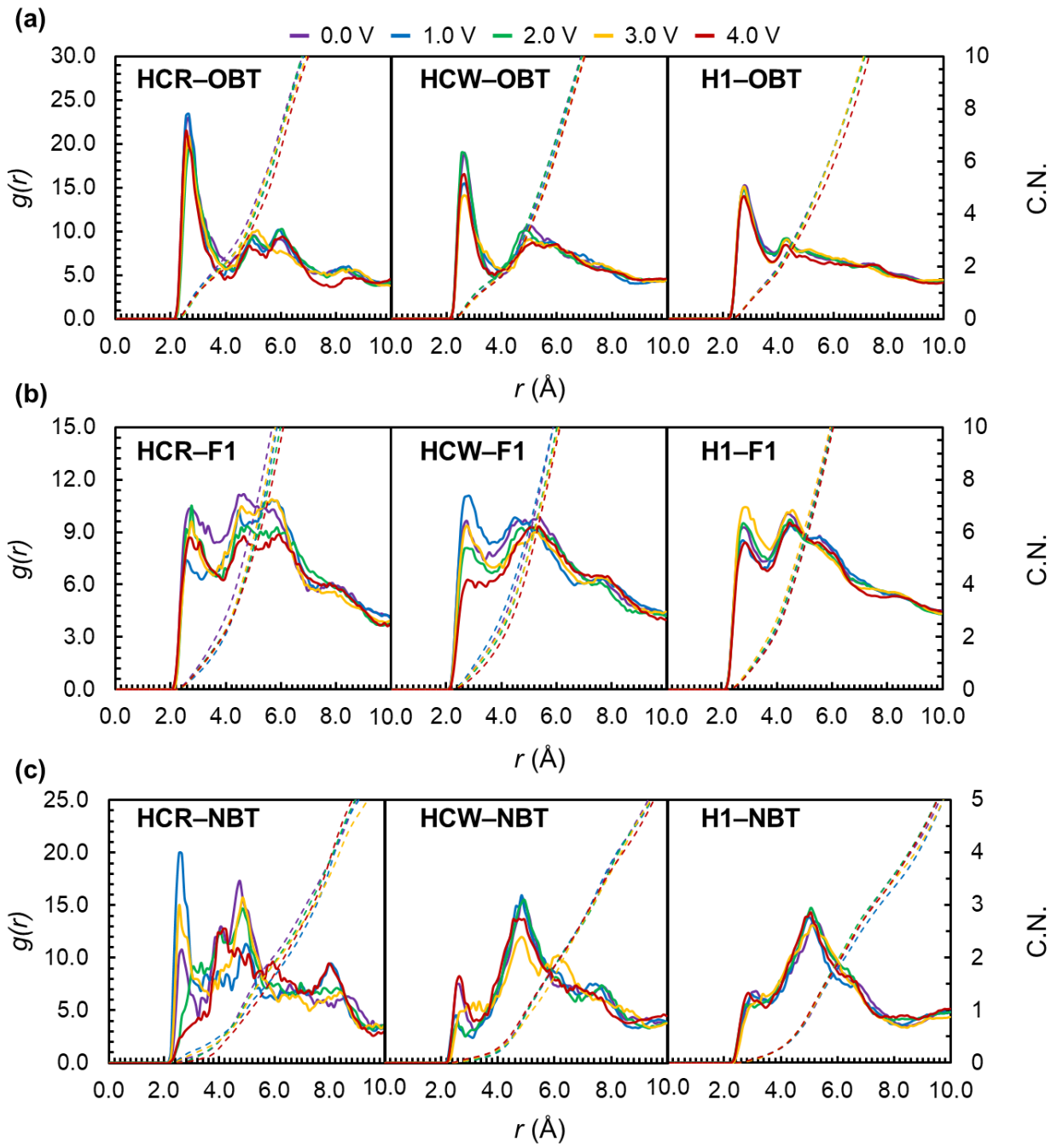


Figure S10. RDF and coordination number (C.N.) of each H atom type in $[C_1mim]^+$ paired with (a) OBT, (b) F1, and (c) NBT atom type in $[NTf_2]^-$ between 0.0 V to 4.0 V at the distance within 10 Å from negatively charged electrode.



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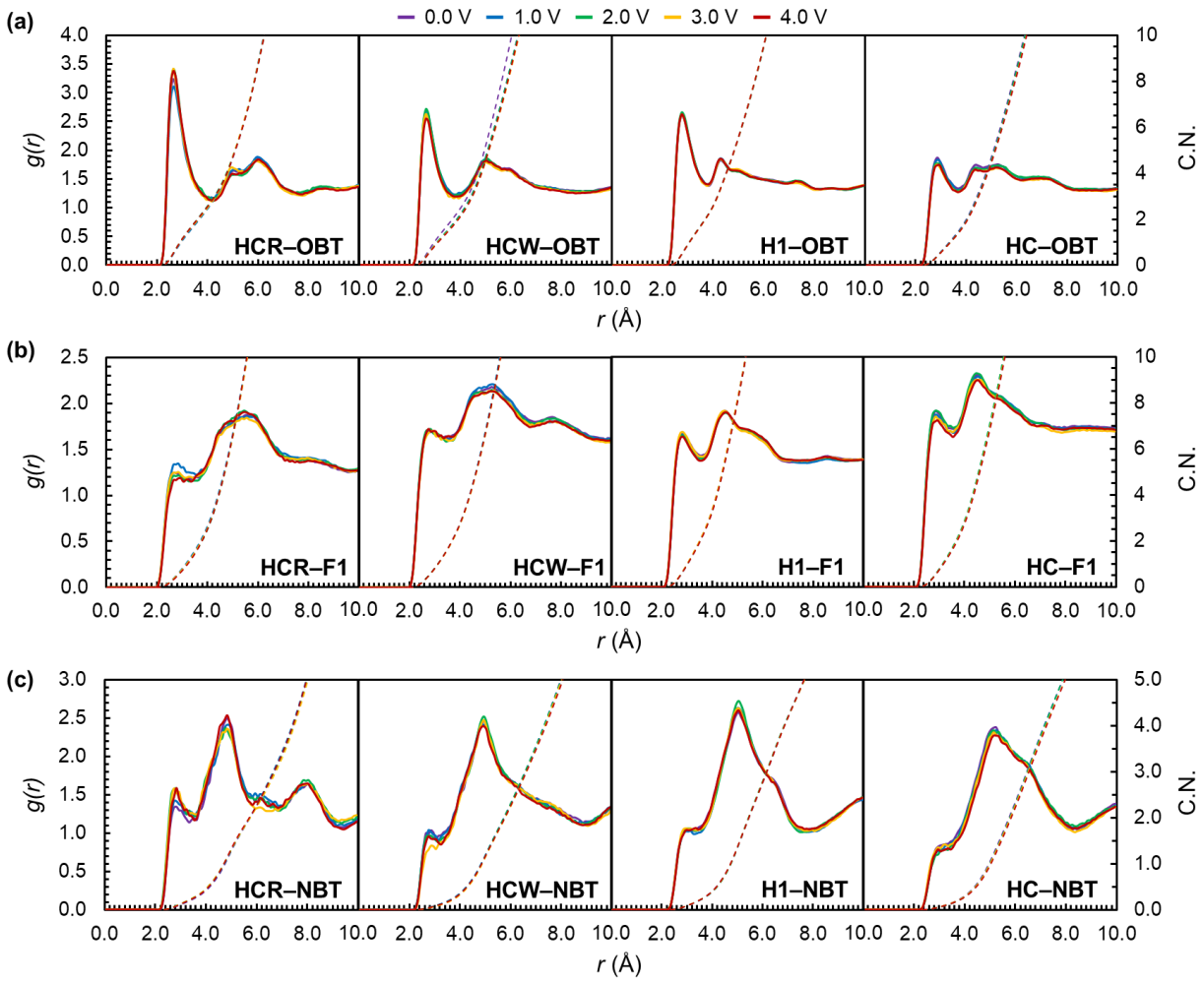

Figure S12. RDF analysis of each atom type in [C_2mim][NTf_2] within bulk region. Colored solid lines are g(r) for each voltage from 0.0 V to 4.0 V (purple, blue, green, yellow and red, respectively). Colored dash lines are C.N. for each voltage.

S4 Electrostatic Potential Profile of [C_1mim][NTf_2] and [C_2mim][NTf_2] at each Voltage

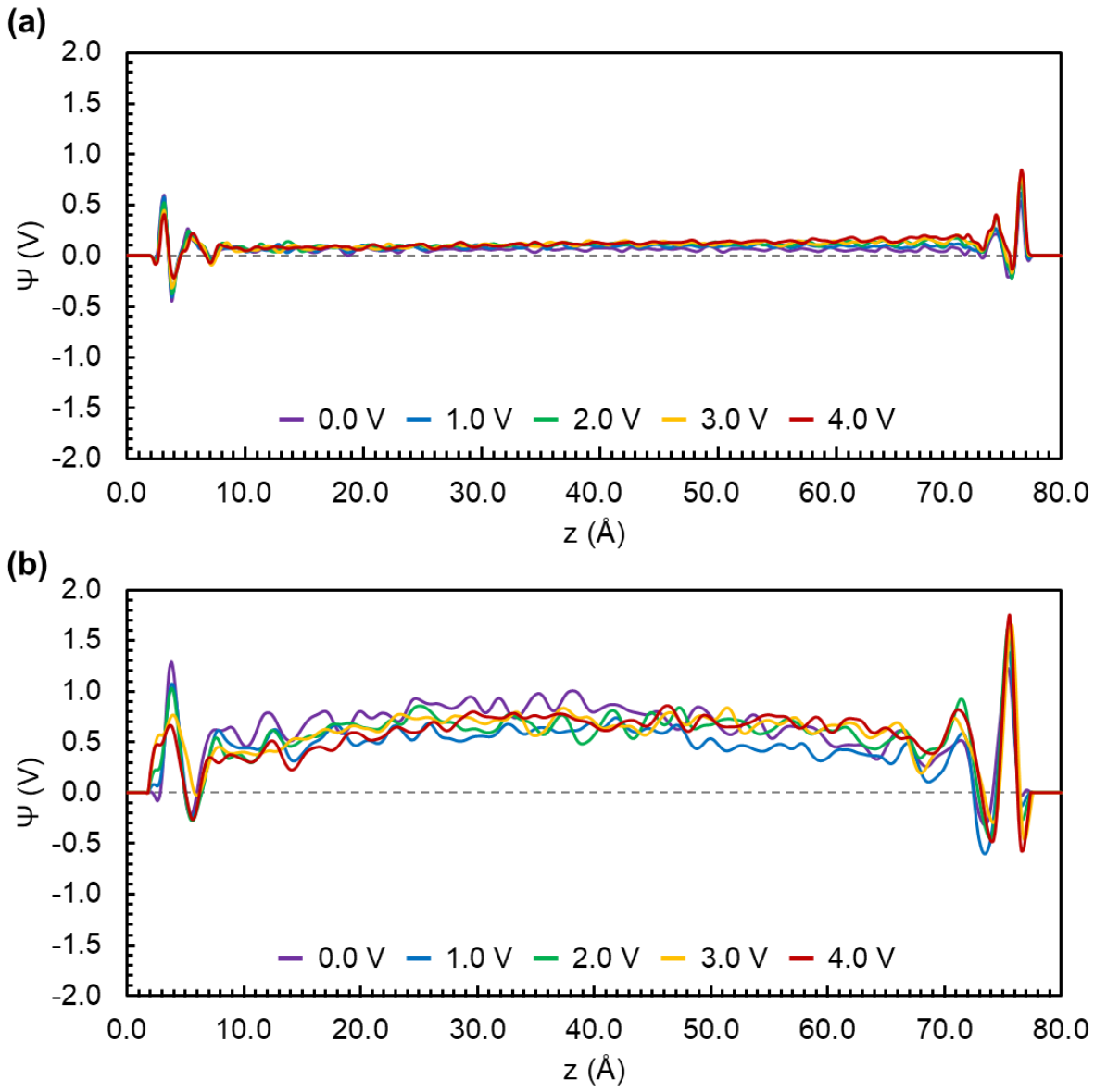

Figure S13. Electrostatic potential profiles of (a) [C_1mim][NTf_2] and (b) [C_2mim][NTf_2] between 0.0 V to 4.0 V.