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

Supporting Information:

Evaluation of Static Differential Capacitance at the [C_4mim^+][$TFSA^-$]/Electrode Interface Using Molecular Dynamics Simulation Combined with Electrochemical Surface Plasmon Resonance Measurements

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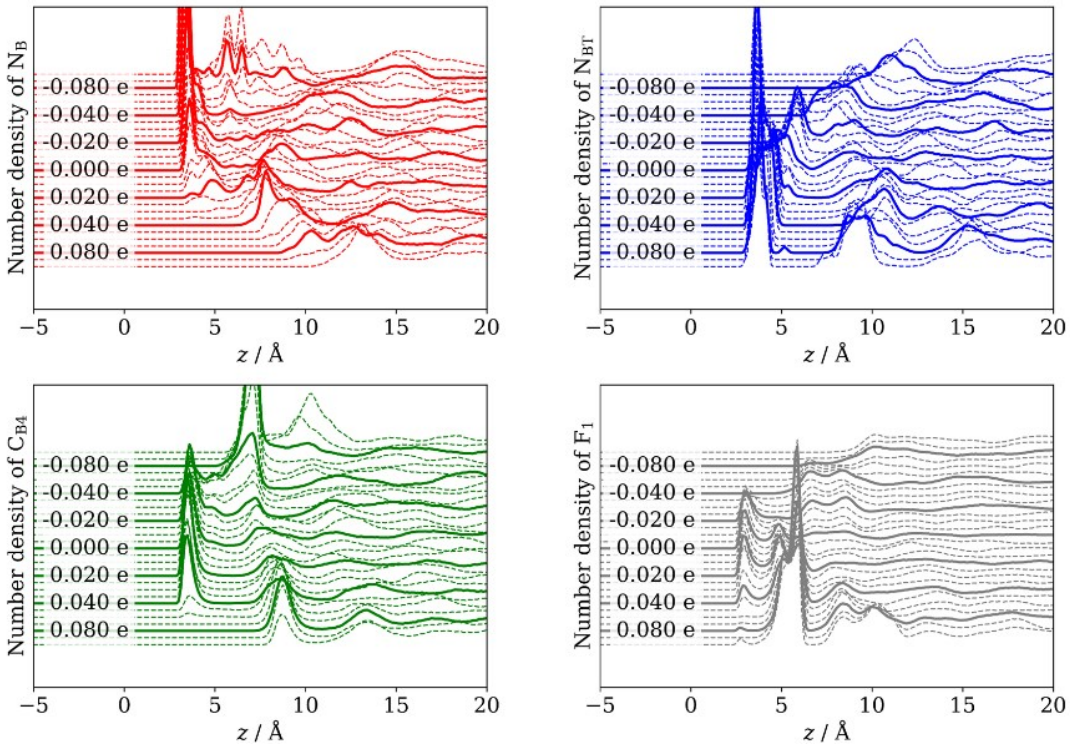

Figure S1. Atomic number density distributions profiles of N_B, C_{B4}, N_{BT} and F_1 atoms (see Fig. 1 for the atom name definition) produced from the MD trajectories as examples.

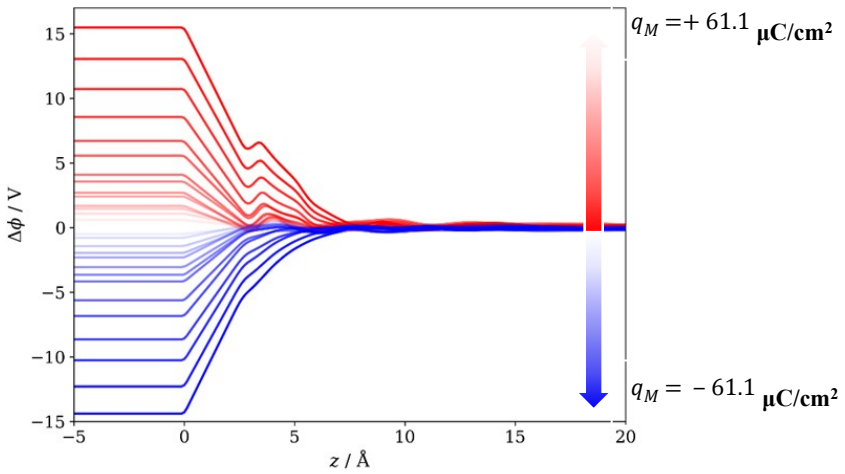

Figure S2. Potential distribution calculated by the one-dimensional Poisson equation.

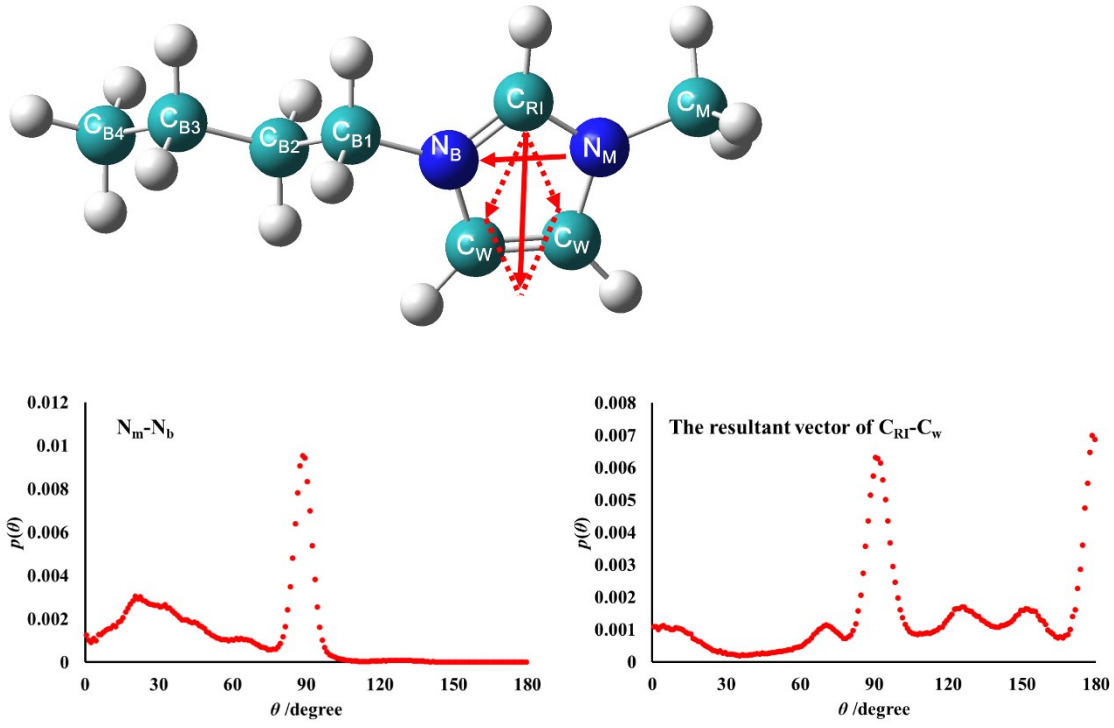

Figure S3. Orientation of imidazolium ring in the first and semi layers at q_M = −61.1 μC/cm². The probability density functions for the vector between the two N atoms (left) and the resultant vector of the two C_{RI}-C_w (right) are investigated. The two vectors both exhibit high peaks besides those at 90°, which means that some of the imidazolium rings are "standing up" if we include the semi-layer into the first ionic layer.

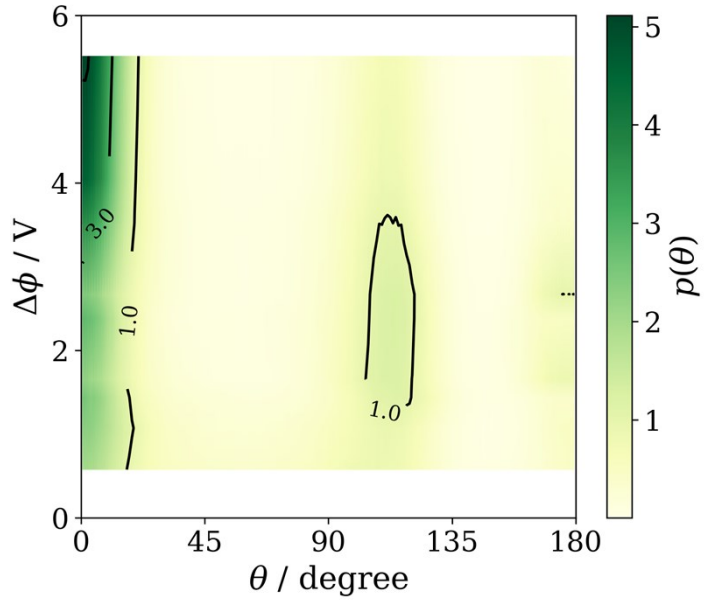

Figure S4. Dihedral angle of C_{BT}-S_{BT}-S_{BT}-C_{BT} in the anion near the positively charged electrode. Three peaks can be seen in all the potentials around 0°, 120° and 180°. The peak around 0° is corresponding to the cis conformation, while those around 120° and 180° are to the trans conformation. At 2 V, the ratio of cis to trans conformation is about 2. As the potential goes positive, all the anions are tend to be in cis conformation.

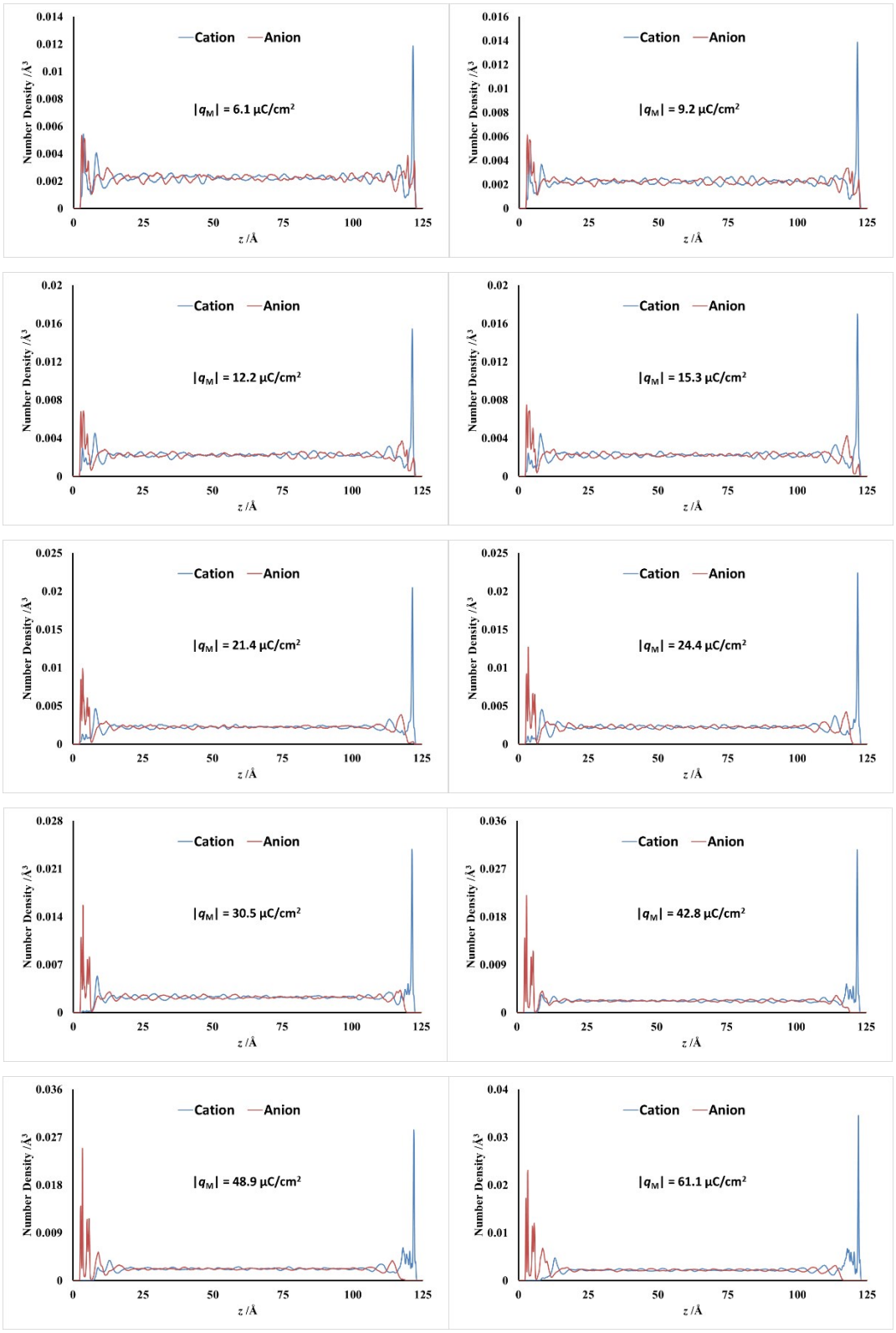

Figure S5. Ionic number density distributions in all the other charging conditions other than $|q_M|$ = 0, 18.3, 36.6, and 55.0 μC/cm^2, which are shown in Fig. 7.