Supporting Information

Simulation of Wetting and Interfacial Behavior of Quaternary Ammonium and Phosphonium Ionic Liquid Nanodroplets Over Face-Centered Cubic Metal Surfaces

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\( Z / \AA \)

\( \rho / \text{atoms.Å}^3 \)

(a) NI  O  F  N  CT
(b) NI  O  F  N  CT
(c) NI  O  F  N  CT
(d) NI  O  F  N  CT
Figure S1. Atomic number density as a function of distance $z$ from the metallic substrates for (a) $[\text{N}_{2225}][\text{NTf}_2]/\text{Cu}(100)$, (b) $[\text{N}_{2225}][\text{NTf}_2]/\text{Cu}(111)$, (c) $[\text{N}_{2225}][\text{NTf}_2]/\text{Pt}(100)$, (d) $[\text{N}_{2225}][\text{NTf}_2]/\text{Pt}(111)$, (e) $[\text{P}_{2225}][\text{NTf}_2]/\text{Pt}(100)$ and (f) $[\text{P}_{2225}][\text{NTf}_2]/\text{Pt}(111)$. 
Figure S2. Total charge densities of $[\text{N}_{2225}][\text{NTf}_2]$ and $[\text{P}_{2225}][\text{NTf}_2]$ ILs nano-droplets as a function of $z$-axis of simulation box. Metal surfaces are at $z = 0$.

Figure S3. Top view of adsorbed $[\text{N}_{2225}]\text{NTf}_2$ IL nano-droplet on Cu(100) surface for the large system.
Figure S4. Top view of the first adsorbed layer of [N_{2225}]NTf$_2$ IL nano-droplet on Cu(111) surface for the large system. The circles highlight the possible anion-cation coordination.

Figure S5. Top view of adsorbed [N_{2225}]NTf$_2$ IL nano-droplet on Pt(100) surface for the large system.
Figure S6. Top view of adsorbed [N_{2225}]NTf$_2$ IL nano-droplet on Pt(111) surface for the large system. Circle used to highlight the possible anion-cation coordination.

Figure S7. Top view of adsorbed [P_{2225}]NTf$_2$ IL nano-droplet on Pt(100) surface for the large system.
Figure S8. Top view of adsorbed $[P_{2225}]NTf_2$ IL nano-droplet on Pt(111) surface for the large system. Circle used to highlight the possible anion-cation coordination.

Table S1. Neighbor count histogram of $[NTf_2]$ anion around $[N_{2225}]$ and $[P_{2225}]$ cations on Cu(111) and Pt(111) surfaces. Only the major ones are shown.

<table>
<thead>
<tr>
<th>IL/Substrate system</th>
<th>Neighbor count</th>
<th>percent of the time</th>
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<tbody>
<tr>
<td>$[N_{2225}][NTf_2]/Cu(111)$</td>
<td>2, 3, 4</td>
<td>20.29, 63.25, 13.33</td>
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<tr>
<td>$[N_{2225}][NTf_2]/Pt(111)$</td>
<td>2, 3, 4</td>
<td>19.37, 43.12, 21.27</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>---------------------</td>
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<td>-----</td>
</tr>
<tr>
<td>[P_{2225}][NTf_2]/Pt(111)</td>
<td>21.57</td>
<td>41.08</td>
</tr>
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