Supplementary Information

The Wetting Behavior of Aqueous Imidazolium Based Ionic Liquids: A Molecular Dynamics Study

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Section S1: Interaction Energy

The equilibration of droplet was traced by observing the interaction energy (solid-fluid interaction energy per molecule) to be constant (after graphite sheet being close to the droplet, i.e. after 10 ns see Figure S1). It can be observed from Figure S2, and Figure S3 that time required to reach the equilibration is significantly high (about 30-40 ns) for pure ILs compared to that of aqueous IL (about 3-8 ns, see bottom Figure S3) Furthermore, cations were found to have a larger contribution compare to that of the anions or water in solid-fluid interaction for both the ILs.

Figure S1. Shape evolution during equilibration of aqueous IL droplet.

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Figure S2. Solid-fluid interaction energy per number of molecules for pure ILs (a.) [EMIM][BF₄] and (b.)[EMIM][NTF₂].

Figure S3. Evolution of various interaction energy for 20wt%ILs (a.) Solid-fluid interaction energy per number of molecule for [EMIM][BF₄], and corresponding zoomed view from the
selected portion is shown bottom. All energy found nearly constant after the time $> 2.5$ ns. (b.)

Solid-fluid interaction energy per number of molecule for [EMIM][NTF$_2$].

**Section S2: System size effect**

To investigate the system size effect, we vary the number of water molecules from 2000 to 6000), for 40wt% (ion pair vary accordingly), and analyze the wetting behavior of the droplet by observing the contact angle. Table S1 shows the contact angle dependency on the droplet size. For all the system size contact angle of [EMIM][BF$_4$] droplet always higher than [EMIM][NTF$_2$] droplet. No significant change is found in contact angle with system size.

<table>
<thead>
<tr>
<th>Number of water-molecules</th>
<th>Contact angle ($^\circ$)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[EMIM][NTF$_2$]</td>
<td>[EMIM][BF$_4$]</td>
</tr>
<tr>
<td>2000</td>
<td>68 ± 1.1</td>
<td>72 ± 1.3</td>
</tr>
<tr>
<td>3000</td>
<td>68 ± 1.6</td>
<td>72 ± 1.6</td>
</tr>
<tr>
<td>4000</td>
<td>69 ± 1.2</td>
<td>73 ± 1.2</td>
</tr>
<tr>
<td>6000</td>
<td>69 ± 1.5</td>
<td>73 ± 1.4</td>
</tr>
</tbody>
</table>

**Table S1.**

Contact angle dependency on the droplet size.