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

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.

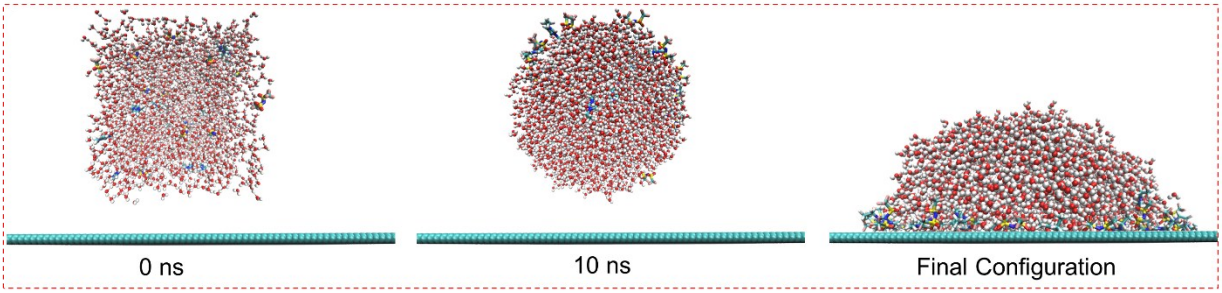

Figure S1. Shape evolution during equilibration of aqueous IL droplet.

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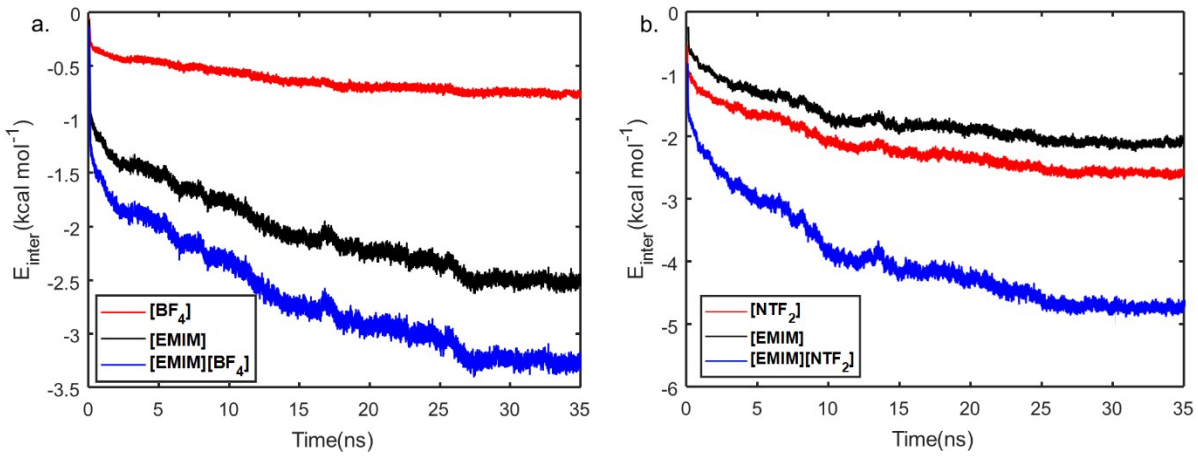

Figure S2. Solid-fluid interaction energy per number of molecules for pure ILs (a.) [EMIM][BF_4] and (b.)[EMIM][NTF_2].

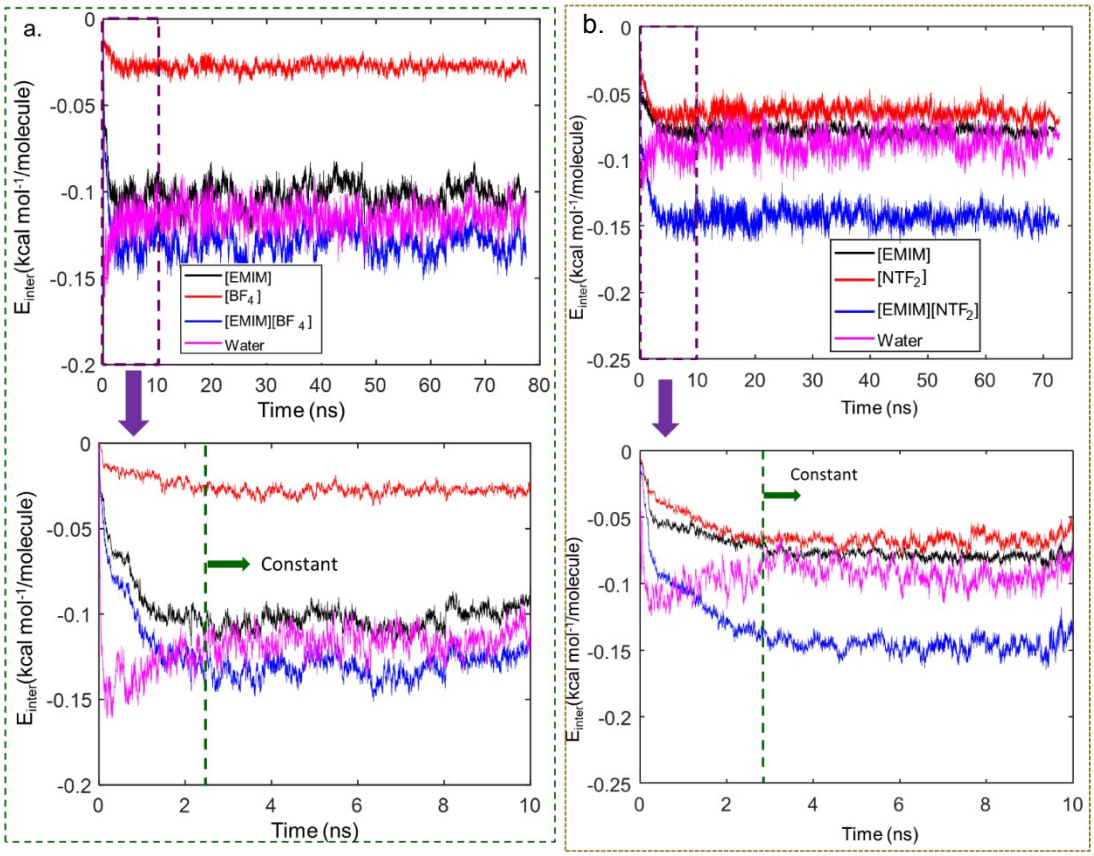

Figure S3. Evolution of various interaction energy for 20wt%ILs (a.) Solid-fluid interaction energy per number of molecule for [EMIM][BF_4], and corresponding zoomed view from the

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 S1. Contact angle of aqueous ILs with different number of water molecules for 40wt%IL

Number of water-molecules	**Contact angle (°)**	
	[EMIM][NTF_2]	**[EMIM][BF_4]**
2000	68 ± 1.1	72 ± 1.3
3000	68 ± 1.6	72 ± 1.6
4000	69 ± 1.2	73 ± 1.2
6000	69 ± 1.5	73 ± 1.4