

Supporting Information

Molecular Insights into the Electrowetting Behavior of Aqueous Ionic Liquid

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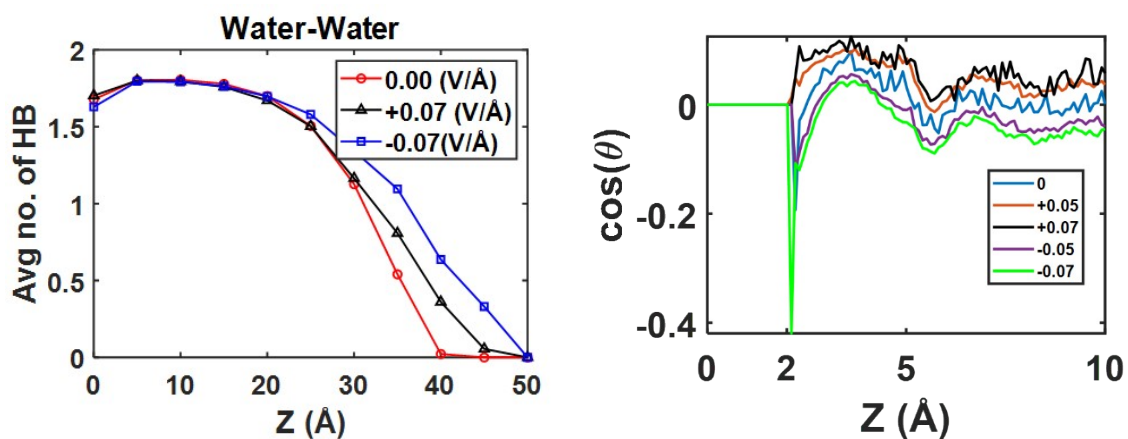


Figure S1: (a) Average hydrogen bond profile along the z-axis. (b) Dipole orientation of water at the solid-fluid interface on the application of the electric field.

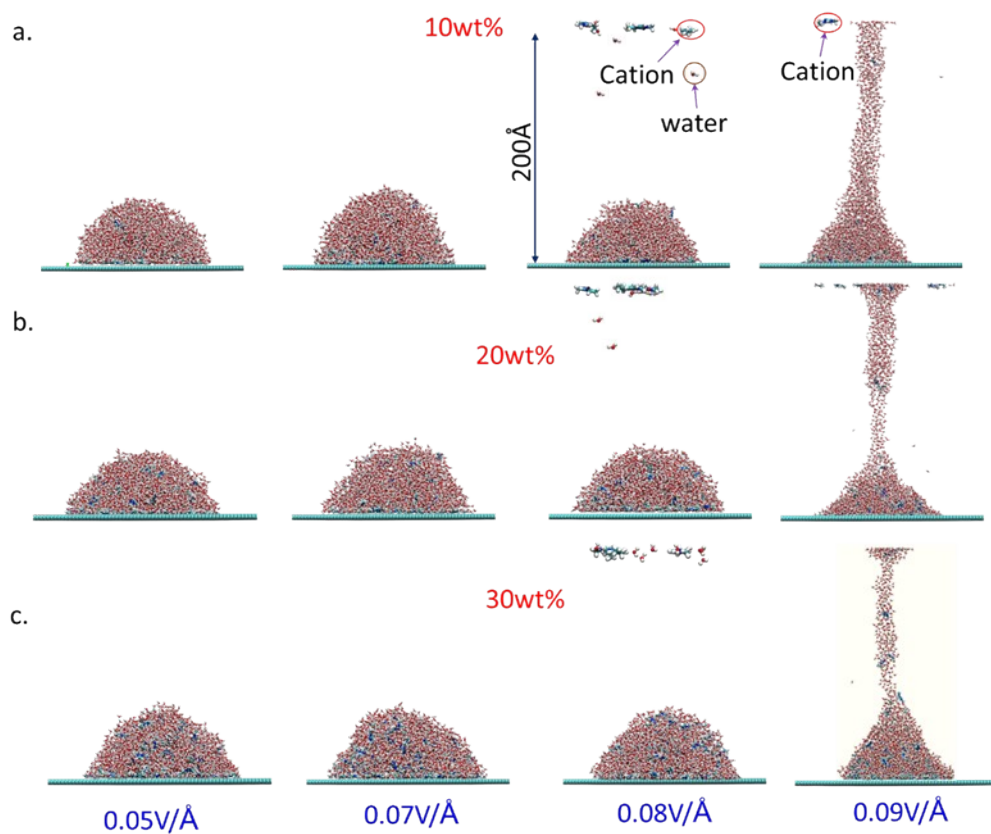


Figure S2: Snapshot of aqueous [EMIM][BF₄] drop at the various electric fields.

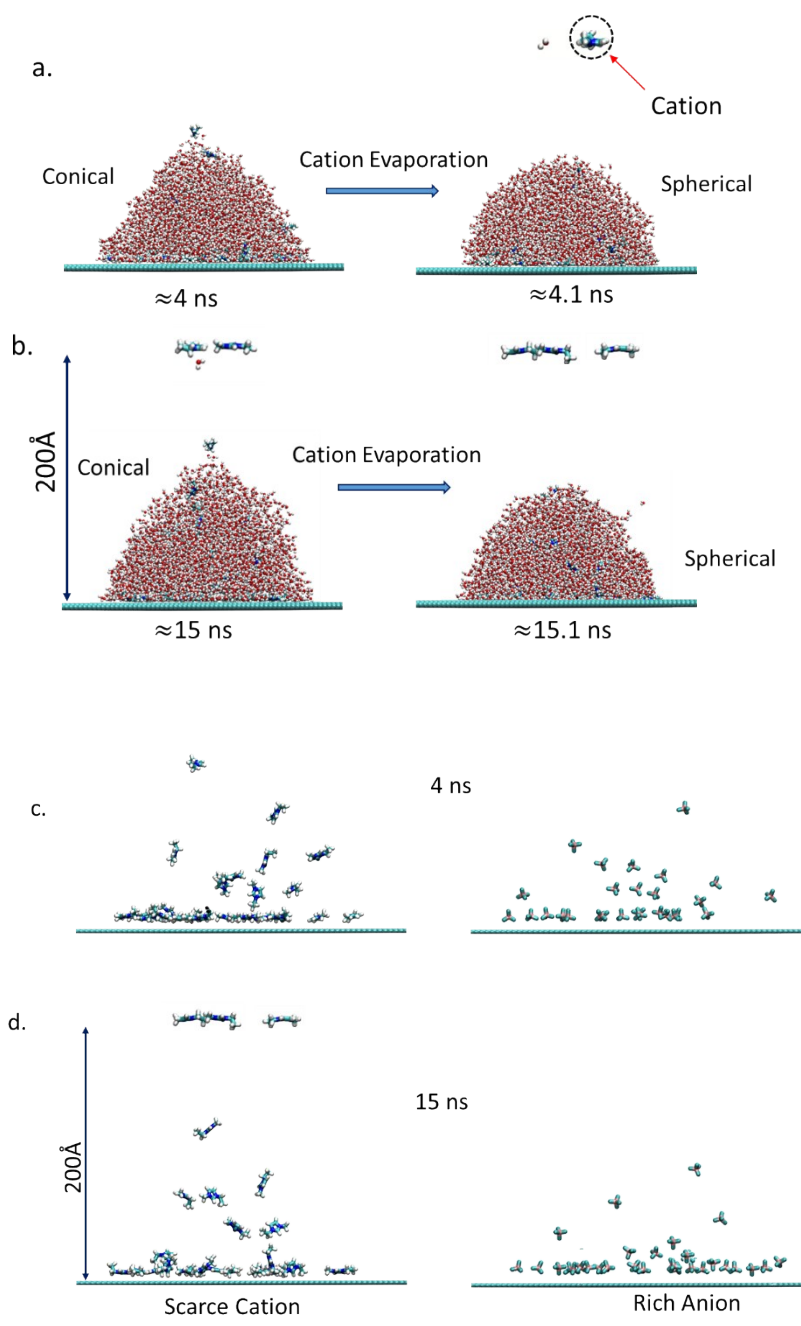


Figure S3: Droplet deformation of 10 wt.-% aqueous [EMIM][BF₄] under application of an external electric field $E = 0.08 \text{ V/\AA}$.

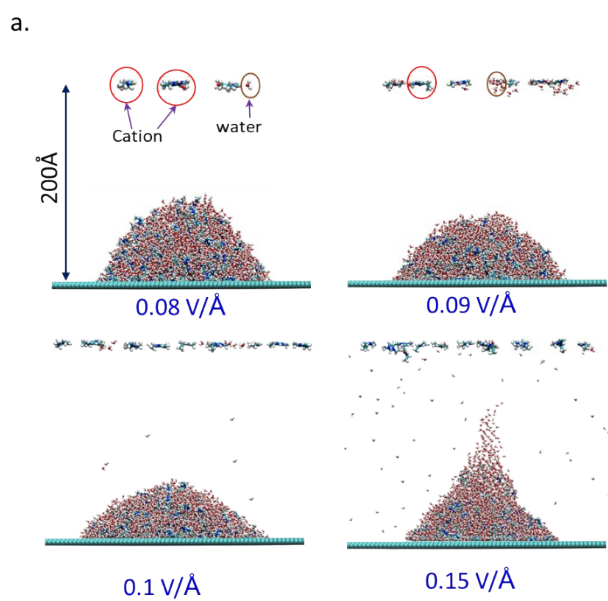


Figure S4: Snapshot of aqueous 50 wt-% [EMIM][BF₄] drop at the various positive electric fields.

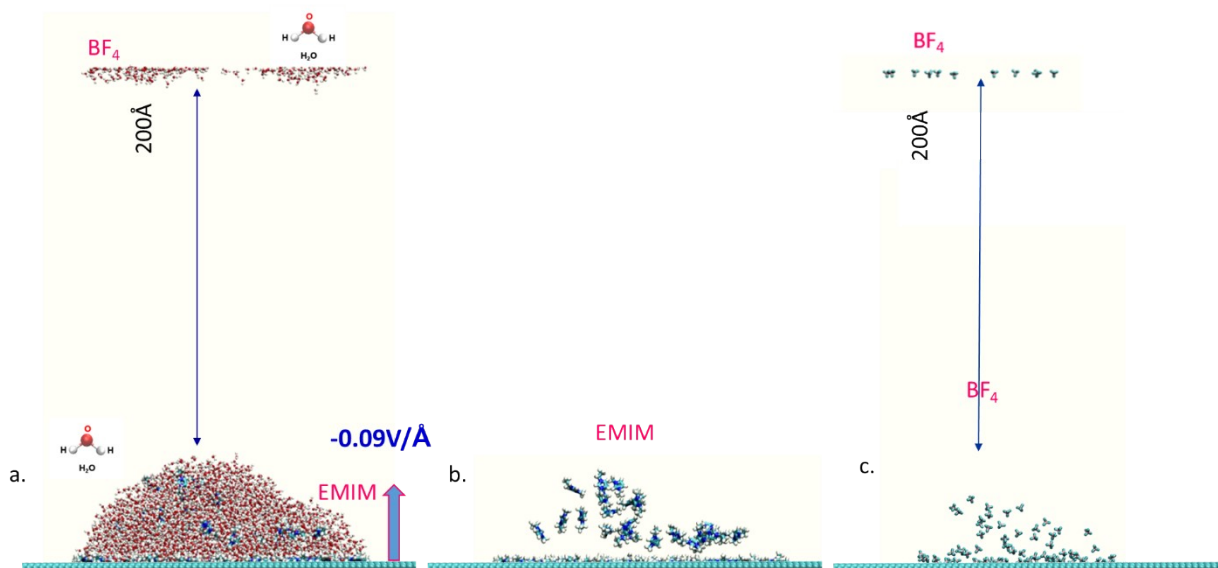


Figure S5: Configurational snapshot of 30 wt-% of [EMIM][BF₄] at -0.09 V/Å a) Aqueous droplet b) Cations c) Anions

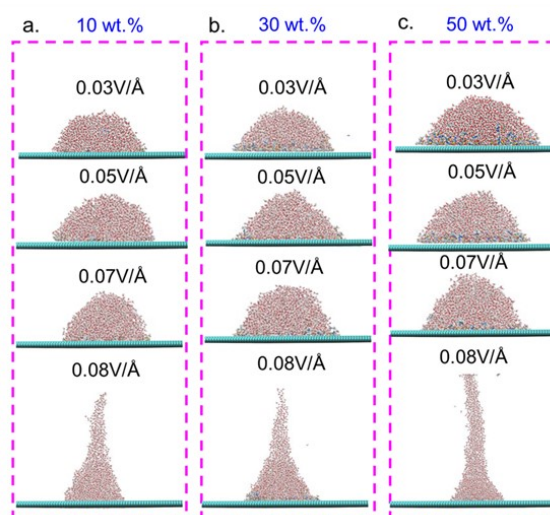


Figure S6: Snapshot of aqueous IL [EMIM][NTF₂] droplet at the various electric fields (can be moved to SI)

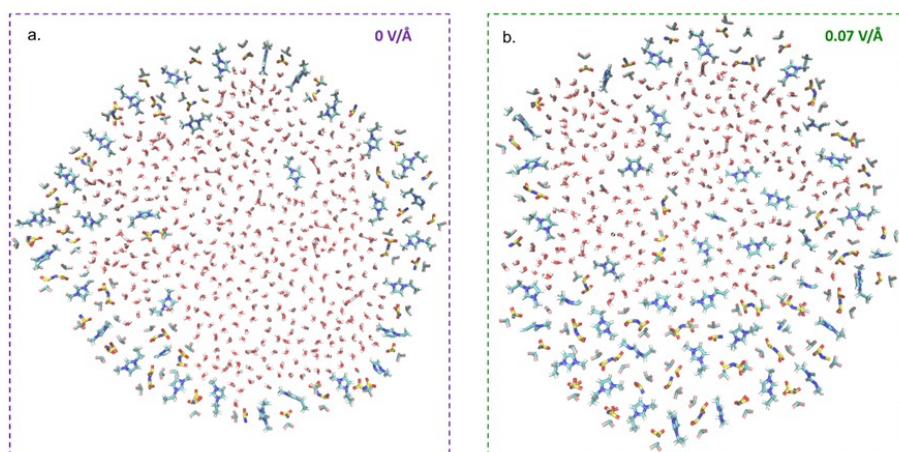


Figure S7. Snapshot of the first layer (near the surface) of aqueous 30 wt.% [EMIM][NTF₂] ILs droplet with a) $E=0$ V/Å and b) 0.07 V/Å, representing the distribution and orientation of molecules near graphene surface at the three-phase contact line.

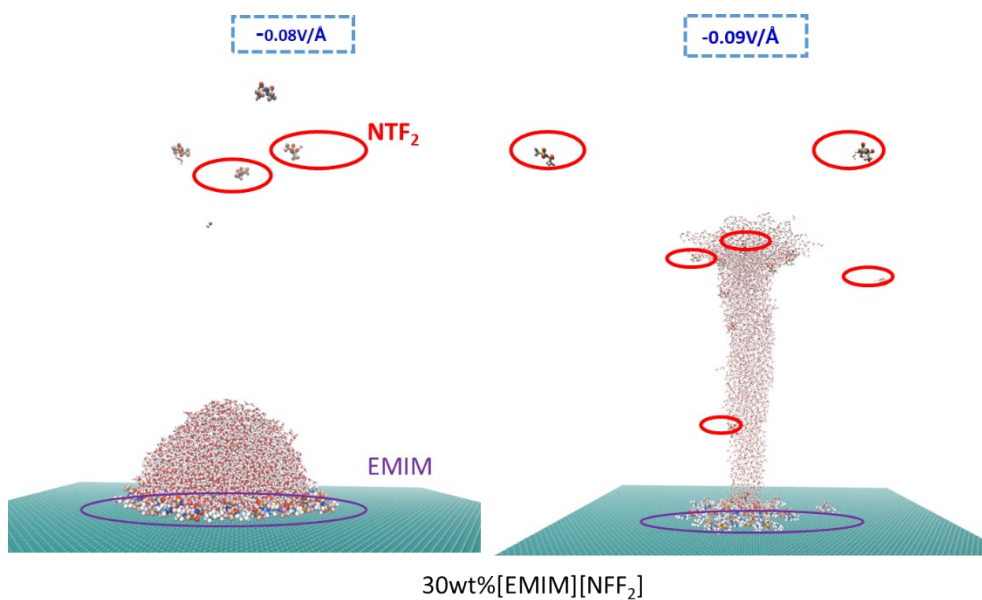


Figure S8: Snapshot of 30 wt.-% [EMIM][NTF₂] at -0.08 V/Å and -0.09 V/Å

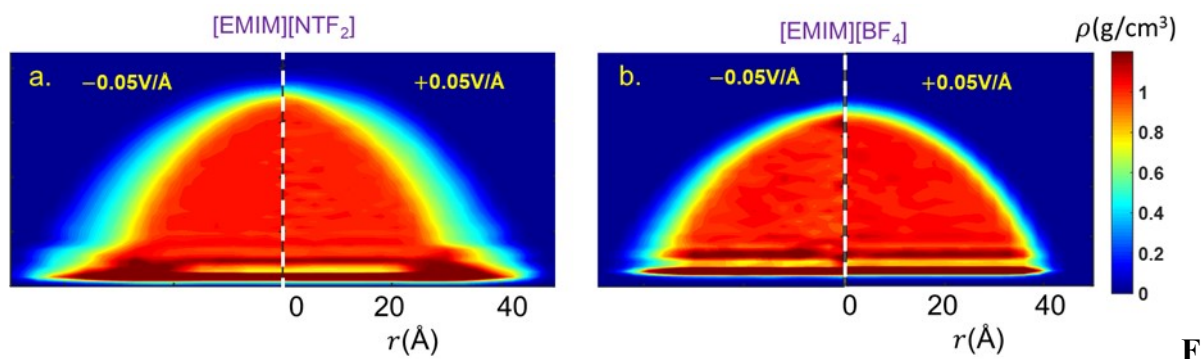


Figure S9. Density profiles of 30wt% a.) [EMIM][NTF₂]. b) [EMIM][BF₄] at ± 0.05 V/Å

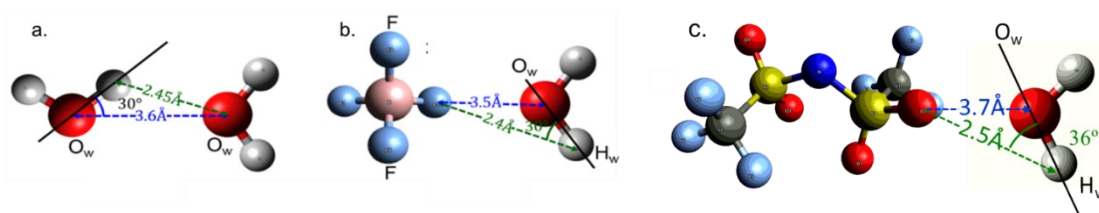


Figure S10: Hydrogen bond (HB) geometric criteria (a) for water-water (b) for BF_4 -water (c) for NTF_2 -water

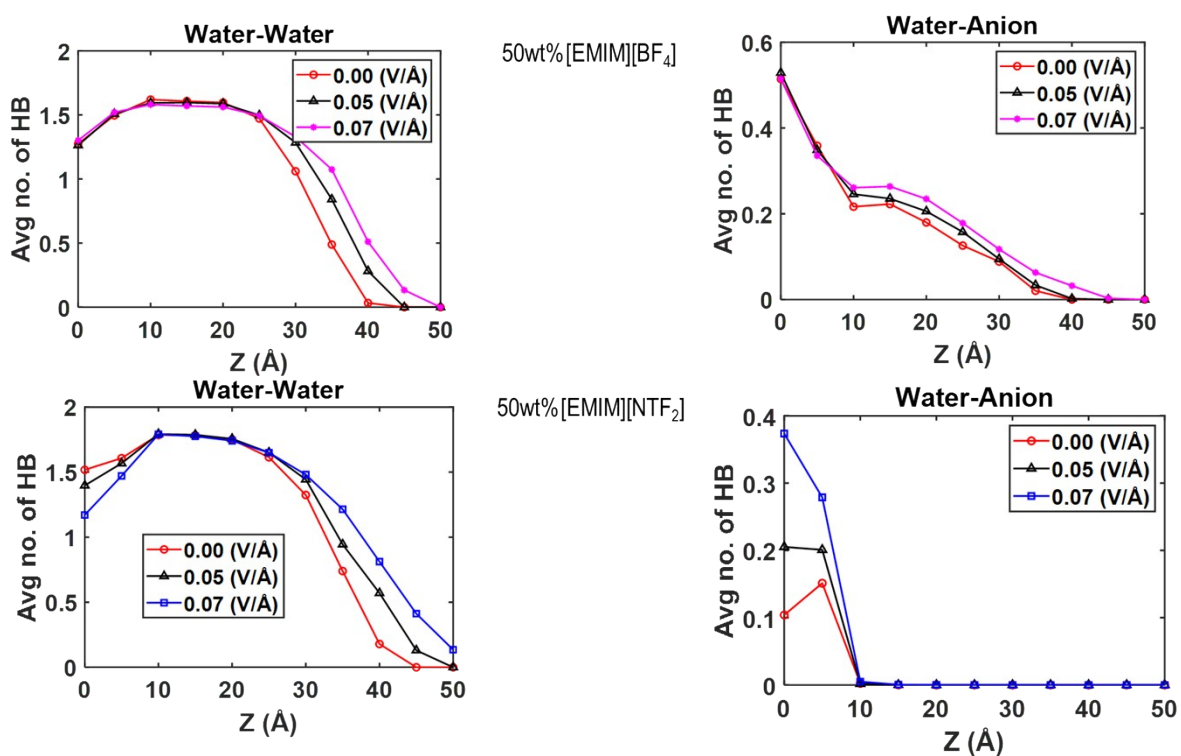


Figure S11: Hydrogen bond profile of 50 wt. % aqueous IL droplet at different electric fields

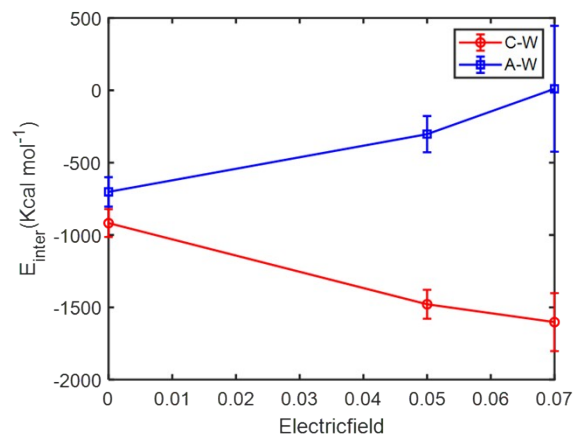
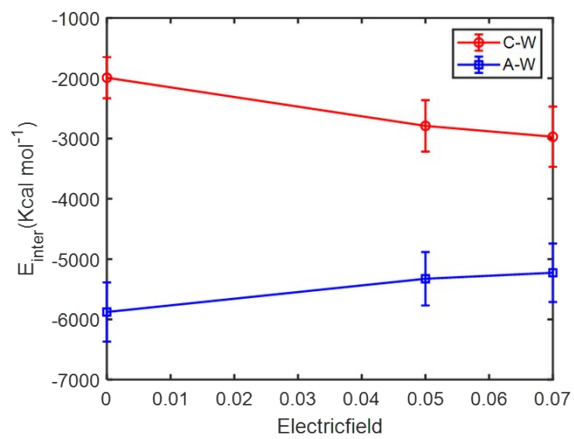


Figure S12: Interaction energy between a) [EMIM] –[Water] & [BF₄]-[Water] b) [EMIM][Water] and [NTF₂]-[Water]