

Supplementary Information

Electro-wetting behavior of Imidazolium based Hydrophilic Ionic Liquid on Rough surface: A molecular dynamics study

*Devargya Chakraborty, Sandip Khan **

Department of Chemical & Biochemical Engineering

Indian Institute of Technology Patna

Patna, India- 801106

1. Ionic Liquid (IL) model

Table S1. Equilibrium density of Ionic liquids used in our work at 300 K and 1 bar pressure

Ionic liquid	Literature		Present work (g/cm^3)
	Experimental-work (g/cm^3)	Simulation-work (g/cm^3)	
[EMIM] [BF ₄]	1.2798 [1]	~ 1.28 [2]	~1.28

2. Effect of Positive Electric field

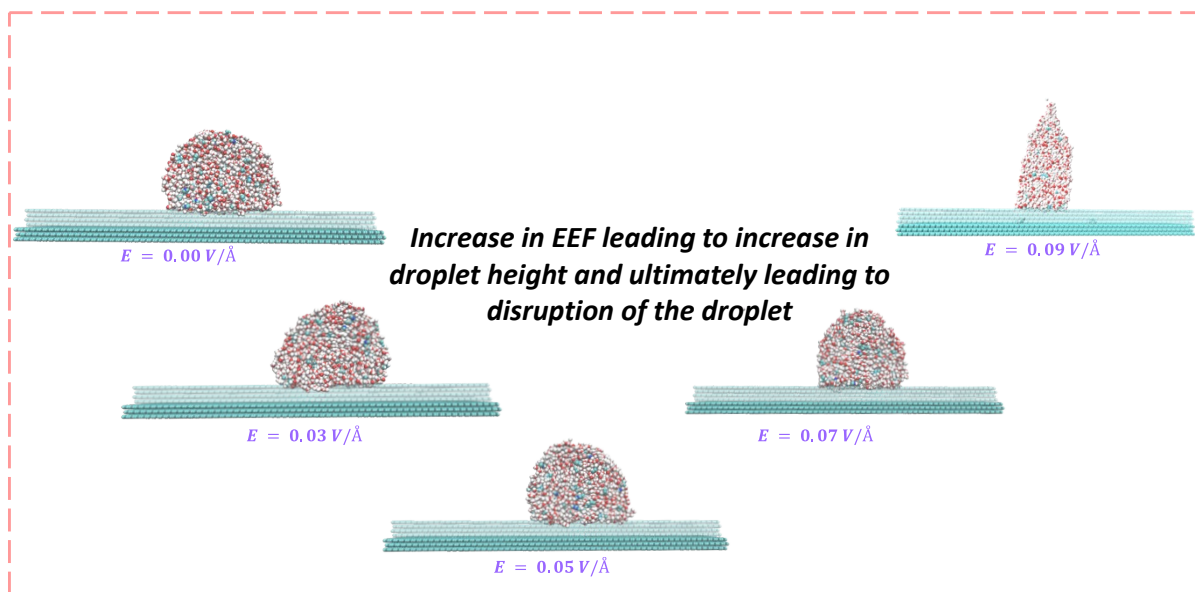


Figure S1. Change in droplet shape with the increase in positive EEF on 30 wt.% [EMIM] [BF₄] system

3. Hydrogen Bond Criteria

Table S2. Geometric criteria for the Existence of HB in water-water and IL-water systems

- **Condition for the existence of water-water HB**

$$r_{O_w O_w} \leq 3.5 \text{ \AA}$$

$$r_{H_w O_w} \leq 2.4 \text{ \AA}$$

$$\varphi \leq 30^\circ$$

- **Condition for the existence of water-anion HB**

$$r_{FO} \leq 3.6 \text{ \AA}$$

$$r_{FH} \leq 2.45 \text{ \AA}$$

$$\varphi \leq 30^\circ$$

References

- [1] W.-G. Xu, L. Li, X.-X. Ma, J. Wei, W.-B. Duan, W. Guan, J.-Z. Yang, Density, Surface Tension, and Refractive Index of Ionic Liquids Homologue of 1-Alkyl-3-methylimidazolium Tetrafluoroborate [C_nmim][BF₄] (n = 2,3,4,5,6), *Journal of Chemical & Engineering Data*, 57 (2012) 2177-2184.
- [2] O.Y. Fajardo, S. Di Lecce, F. Bresme, Molecular dynamics simulation of imidazolium C_nMIM-BF₄ ionic liquids using a coarse grained force-field, *Physical Chemistry Chemical Physics*, 22 (2020) 1682-1692.