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Air-Liquid Interface of Imidazolium-Based [Tf_2N^-] Ionic Liquids: Insight from Molecular Dynamics Simulations

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SUPPLEMENTARY INFORMATION

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Additional Results

Figure S1: The surface roughness of $[C_6mim^+][Tf_2N^-]$ at a temperature of 300 K. (a, b) Bivariate distribution of the probability (red=high probability, blue=low probability) that two surface points are located at the lateral distance l and at the normal distance d from each other for (a) the interfacial and (b) sub-interfacial layers. (c) Average normal distance of two surface points $\langle d \rangle$ as a function of their lateral distance l.

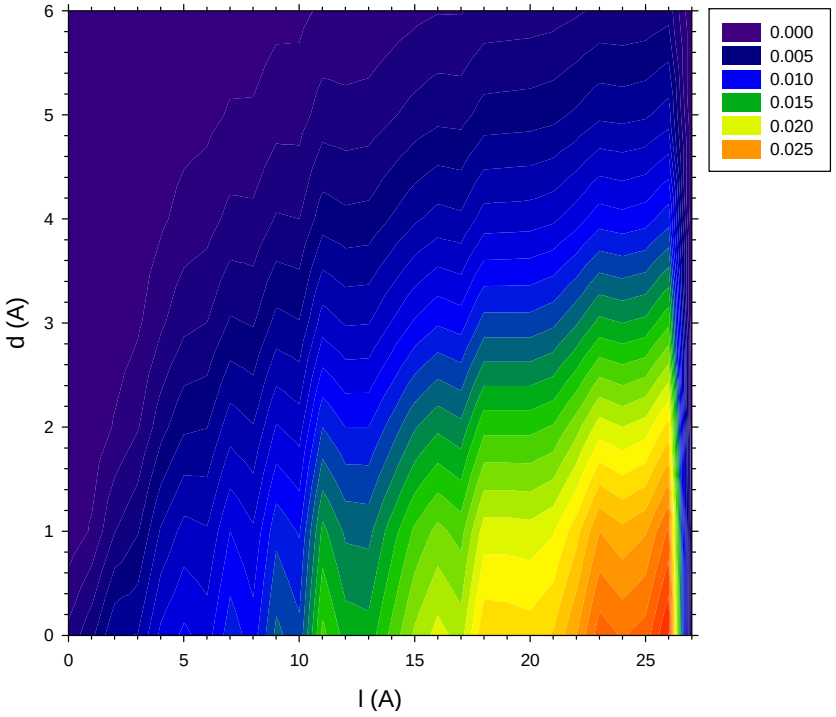
Figure S2: The surface roughness of $[C_8mim^+][Tf_2N^-]$ at a temperature of 300 K. (a, b) Bivariate distribution of the probability (red=high probability, blue=low probability) that two surface points are located at the lateral distance l and at the normal distance d from each other for (a) the interfacial and (b) sub-interfacial layers. (c) Average normal distance of two surface points $\langle d \rangle$ as a function of their lateral distance l.

Figure S3: Orientation of the cation and anion in the interfacial layer for $[C_6mim^+][Tf_2N^-]$ at a temperature of 300 K (red=high probability, blue=low probability). (a) Probability distribution $(\cos\theta, \cos\Phi)$ for the cation ring; θ and Φ are the tilt angles of the vectors CH and NN, respectively, with respect to the interface normal z. (b) Two-dimensional plot $(\cos\theta, z)$ for the cation tail; θ is the tilt angle of the vector CN with respect to z. (c) Probability distribution $(\cos\theta, \cos\Phi)$ for the anion; θ and Φ are the tilt angles of the vectors SC and SS, respectively, with respect to z.

Figure S4: Orientation of the cation and anion in the interfacial layer for $[C_8mim^+][Tf_2N^-]$ at a temperature of 300 K (red=high probability, blue=low probability). (a) Probability distribution $(\cos\theta, \cos\Phi)$ for the cation ring; θ and Φ are the tilt angles of the vectors CH and NN, respectively, with respect to the interface normal z. (b) Two-dimensional plot $(\cos\theta, z)$ for the cation tail; θ is the tilt angle of the vector CN with respect to z. (c) Probability distribution $(\cos\theta, \cos\Phi)$ for the anion; θ and Φ are the tilt angles of the vectors SC and SS, respectively, with respect to z.

Fig. S1 (Lisal et al.)

(a)



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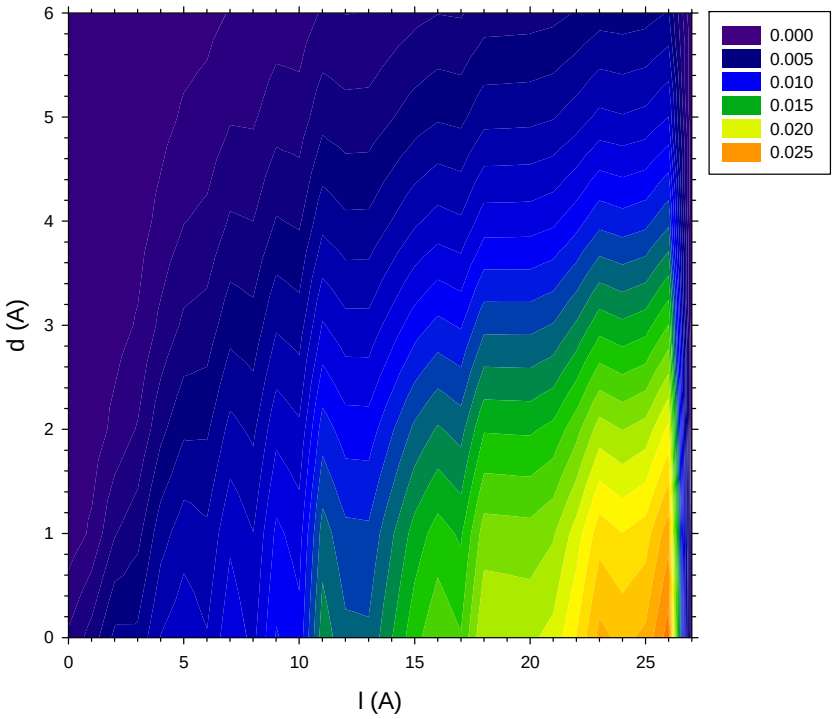

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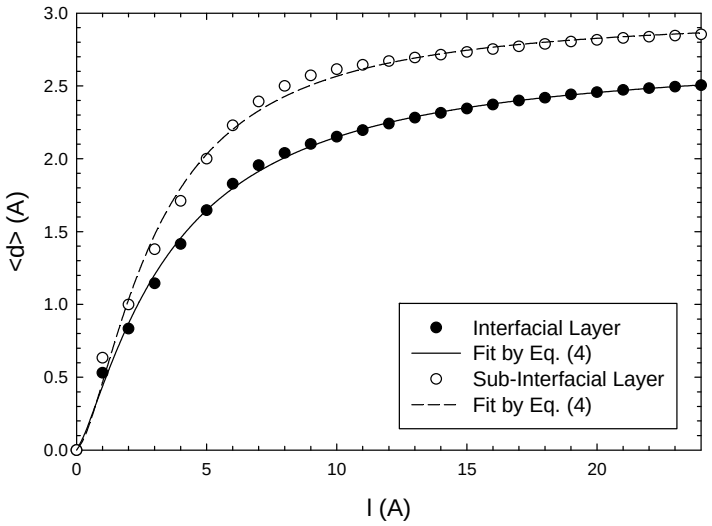
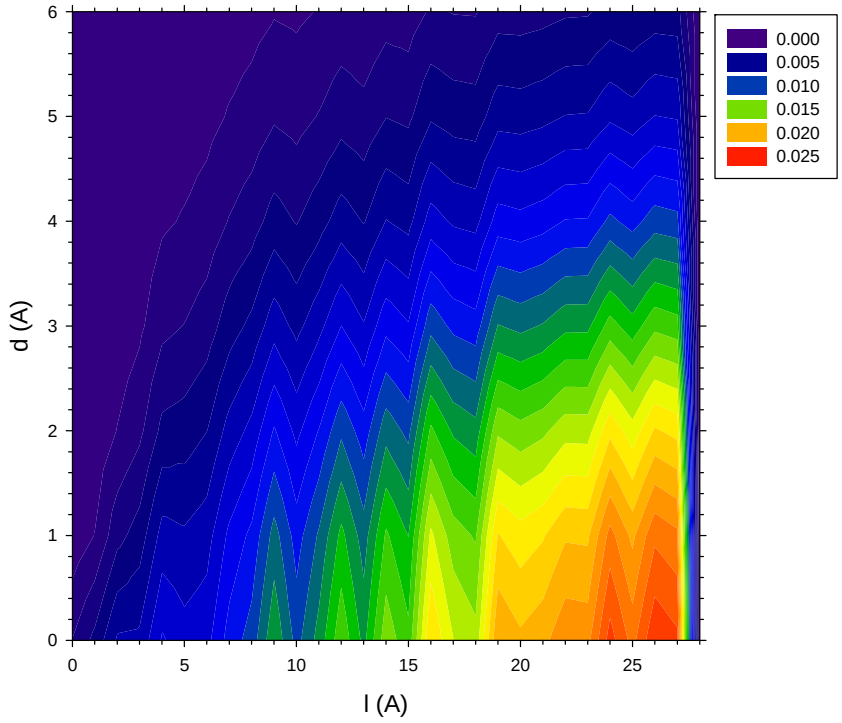


Fig. S2 (Lisal et al.)

(a)



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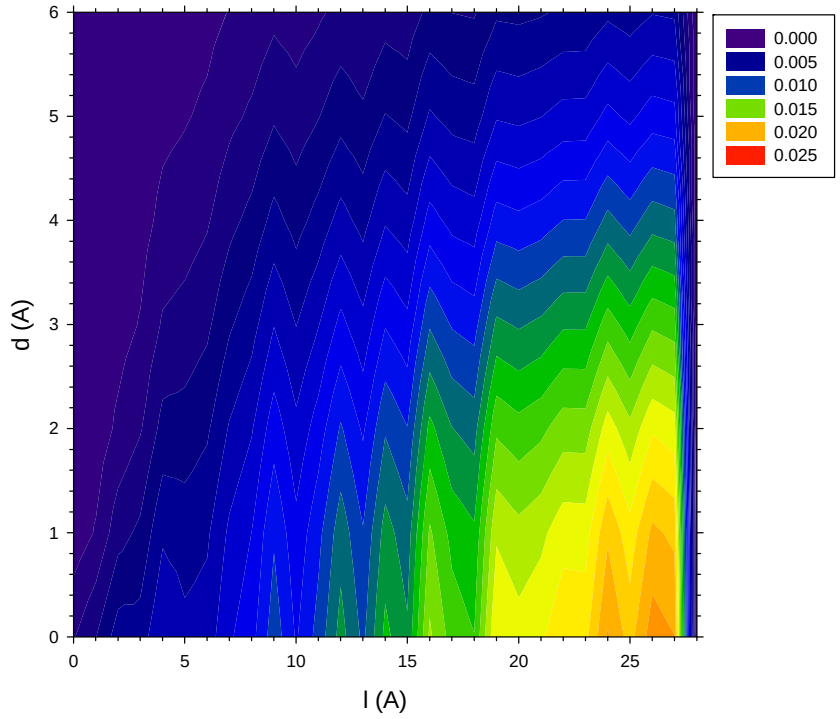

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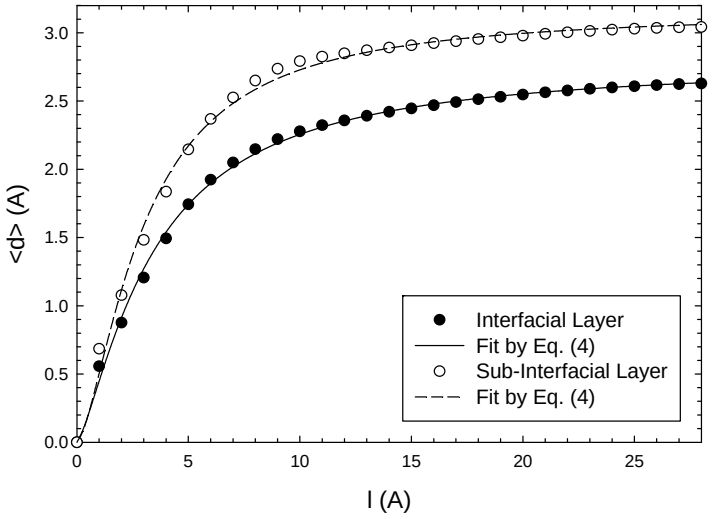
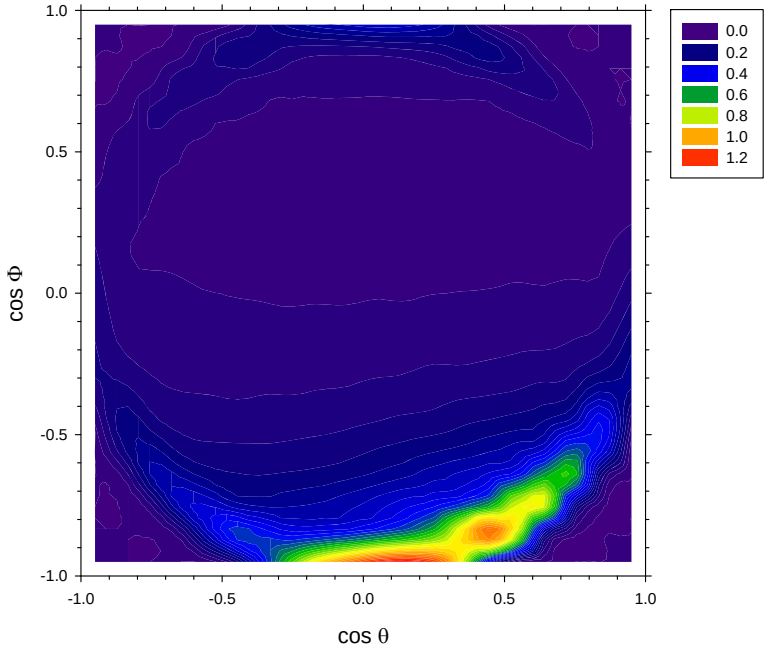


Fig. S3 (Lisal et al.)

(a)



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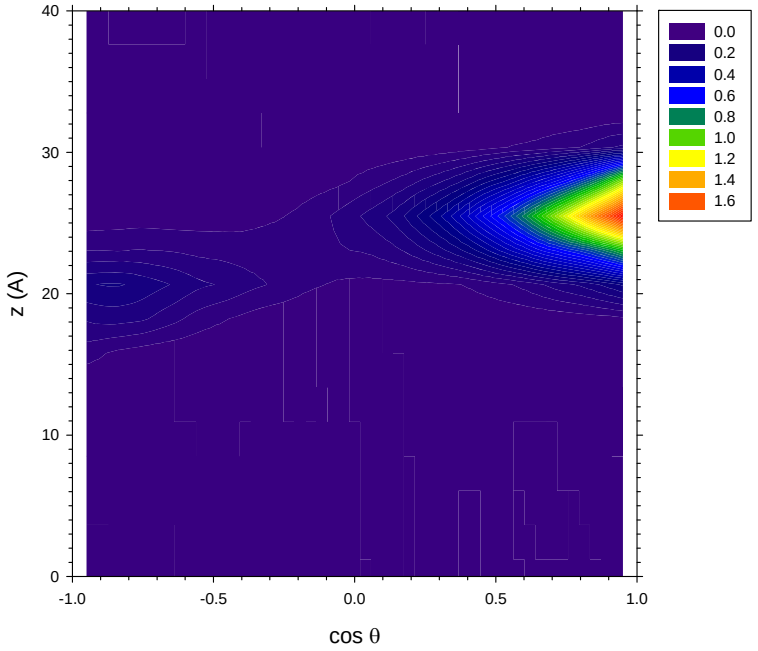

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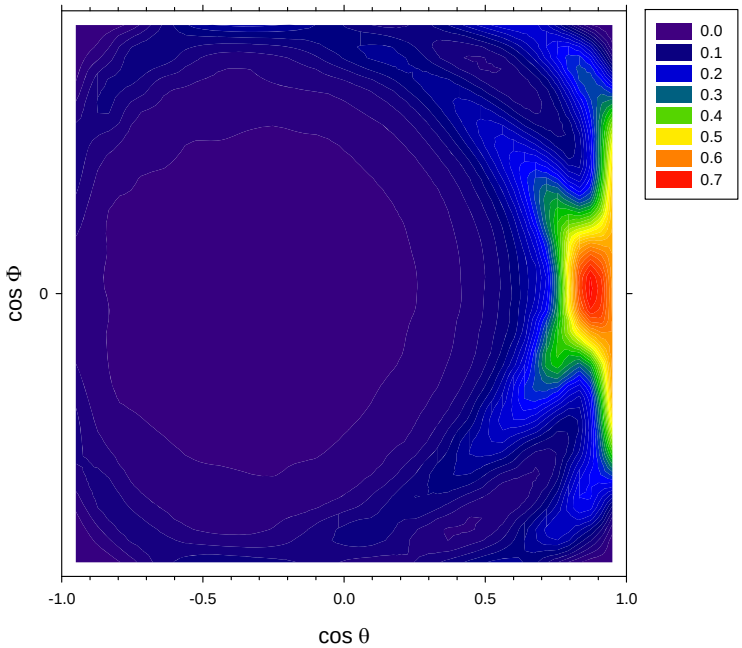
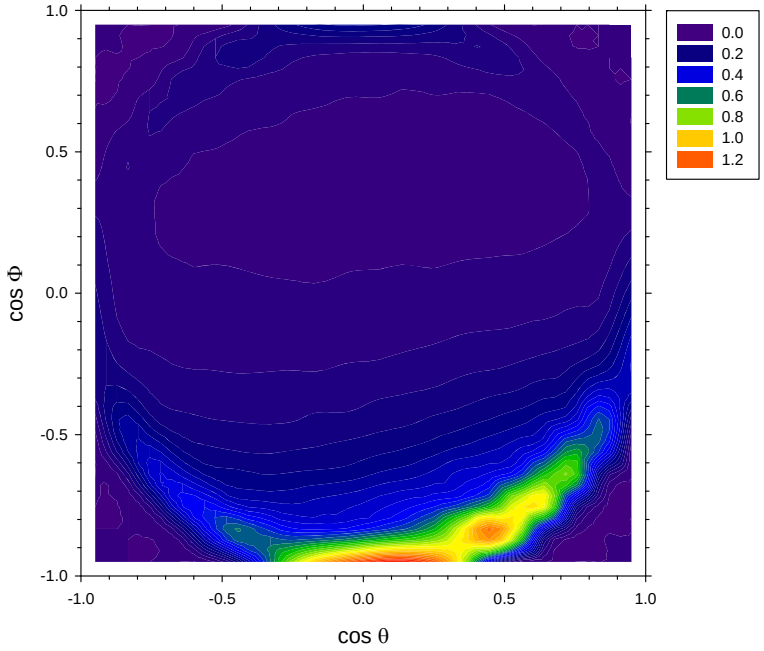


Fig. S4 (Lisal et al.)

(a)



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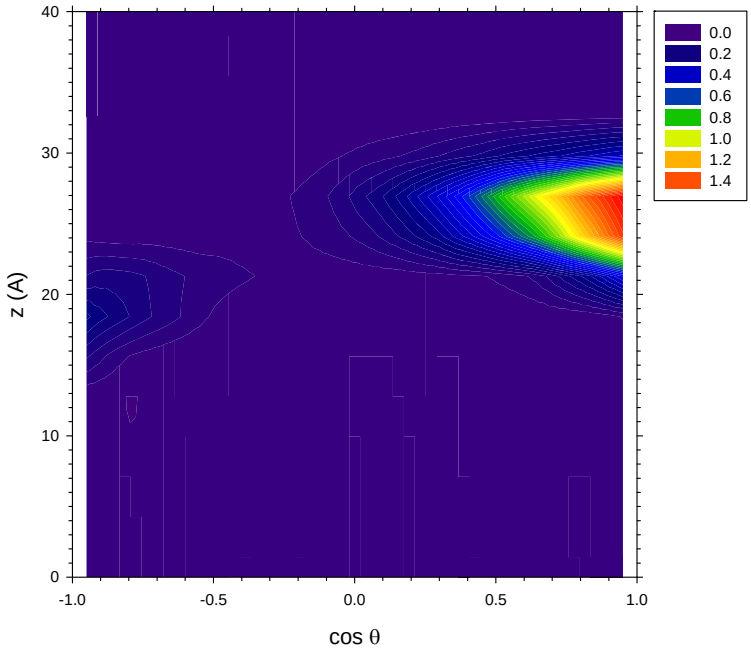
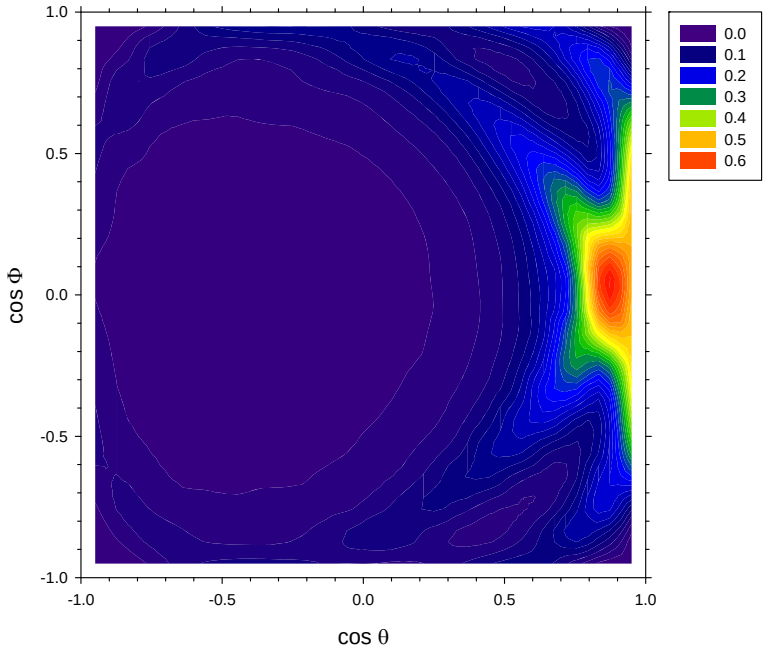
(c)