Wetting Transition of Ethanol–Water Droplet on Smooth and Textured Surfaces

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Supporting Information

Table S1: Summarized all the bonding and non–bonding parameters for the ethanol–ethanol and water–water interactions[a].

Table S2: System size of the droplets, microscopic and macroscopic contact angle, and the line tension as a function of ethanol concentration on smooth surface.

Figure S3 Average number of hydrogen bonds per ethanol (a–c) and water (d–e) molecules in ethanol-water droplet on a smooth surface for 10, 20, and 30 wt% of ethanol respectively.

Figure S4: Density profile (A), and average number of HB distribution (B) of ethanol (a–c) and water (d–f) of 10 wt% ethanol solution, $\alpha = 0.25$ with h = 2, 4, 6.

Figure S5: Density profile (a and b) and HB distribution (c and d) of ethanol and water molecules for 75 wt% ethanol solution at h = 6 and $\alpha = 0.25$

Figure S6: Density profile (a and b) and HB distribution (c and d) of ethanol and water molecules for 50 wt% ethanol solution at pillar height, h = 2 and $\alpha = 0.51$.

Table S1: Summarized all the bonding and non–bonding parameters for the ethanol–ethanol and water–water interactions[a].

Molecule	Site	ε (kcal mol^{-1})	σ (Å)	q (e)
Water[1]	O	1.5525	3.166	-0.8476
	H	0.0000	0.000	0.4238
Ethanol[2-4]	O	0.1700	3.120	-0.6830
	C1	0.0660	3.500	0.1450
	C2	0.0660	3.500	0.1800
	H1	0.0300	2.500	0.0600
	H2	0.0300	2.500	0.0600
	HO	0.0000	0.000	0.4180
Graphite[5]	C	0.2364	3.214	0.0000
Molecule	Bond stretching	k_r (kcal mol^{-1} Å^{-2})		r_{eq} (Å)
Water	O-H			1.000
Ethanol	C-C	536		1.529
	C-H	680		1.090
	C-O	640		1.410
	O-H	1106		0.945
Molecule	Bond bending	k_θ (kcal mol^{-1} rad^{-2})		θ_{eq} (deg.)
Water	H-O-H			109.47
Ethanol	H-C-C	75		110.7
	C C O	100		109.5
	H-C-H	66		107.8
	H-C-O	70		109.5
	C-O-H	70		109.5
Molecule	Dihedral	V_1 (kcal mol^{-1})	V_2 (kcal mol^{-1})	V_3 (kcal mol^{-1})
Ethanol	H-C-C-O	0.0	0.0	0.468
	H-C-C-H	0.0	0.0	0.318
	C-C-O-H	0.356	0.174	0.492
	H-C-O-H	0.0	0.0	0.450

[a]In the case of ethanol, C1and C2 stand for carbon atom of $–CH_2–$ and $–CH_3$ group respectively. H1, H2 and OH are the hydrogen atom of $–CH_2–$, $–CH_3$, and –OH group respectively.

Table S2: System size of the droplets, microscopic and macroscopic contact angle, and the line tension as a function of ethanol concentration on smooth surface.

Wt% of ethanol	System size		Microscopic contact angle (θ^{o})	Macroscopic contact angle (θ_{∞}^{o})	$\tau \times 10^{-11}(\mathrm{N})$
	Number of ethanol molecules	Number of water molecules			
0	-	-	-	83.0 ± 2.0	3.0 ± 0.3[6]
10	87	2000	83.9	68 ± 3	5.2 ± 0.3
	131	3000	82.3		
	174	4000	80.5		
	261	6000	79.1		
20	196	2000	79.0	75 ± 3	6.4 ± 0.2
	294	3000	76.3		
	392	4000	74.0		
	588	6000	72.3		
30	336	2000	74.8	34 ± 2	9.4 ± 0.2
	504	3000	70.3		
	672	4000	65.8		
	1008	6000	61.0		

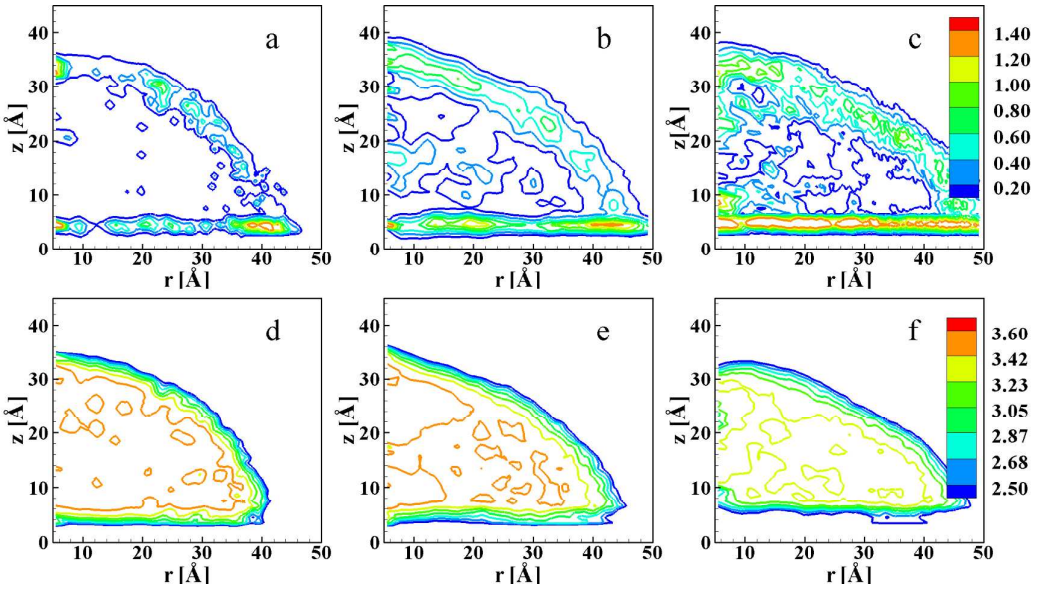

Figure S3: Average number of hydrogen bonds per ethanol (a–c) and water (d–e) molecules in ethanol-water droplet on a smooth surface for 10, 20, and 30 wt% of ethanol respectively.

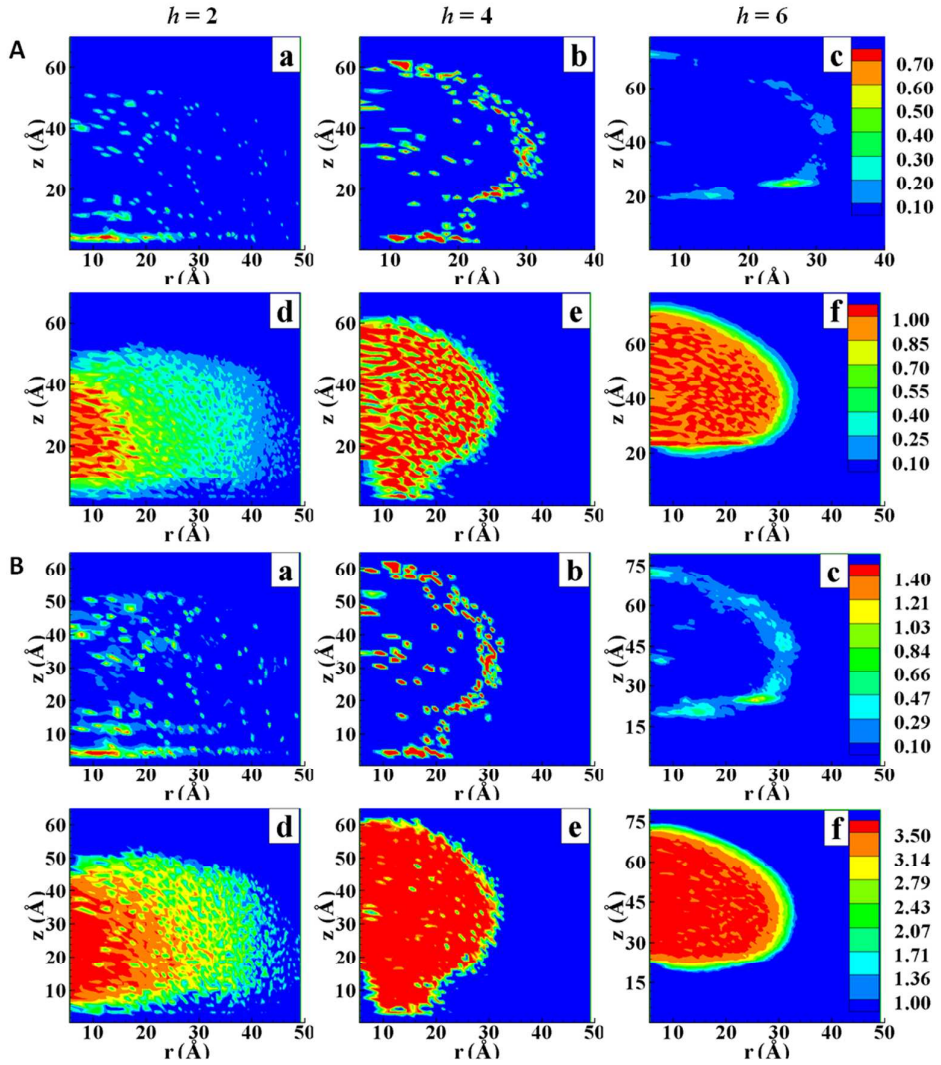

Figure S4: Density profile (A), and average number of HB distribution (B) of ethanol (a–c) and water (d–f) of 10 wt% ethanol solution, $\alpha = 0.25$ with h = 2, 4, 6.

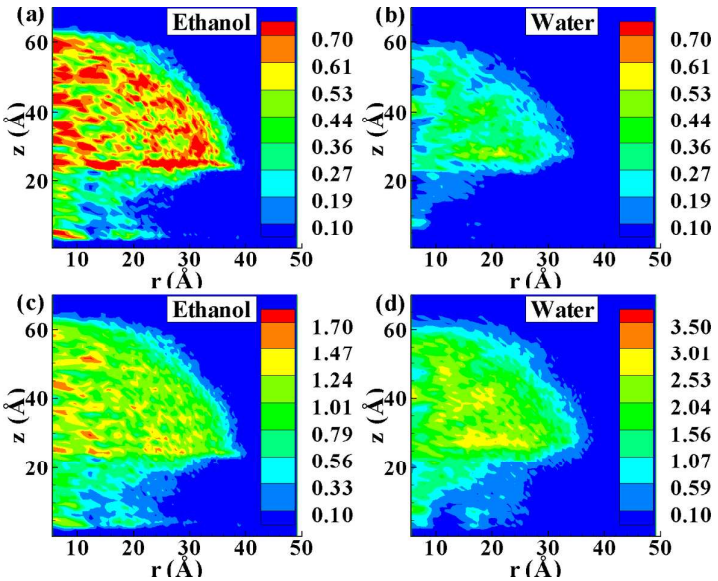

Figure S5: Density profile (a and b) and HB distribution (c and d) of ethanol and water molecules for 75 wt% ethanol solution at $h = 6$ and $\alpha = 0.25$

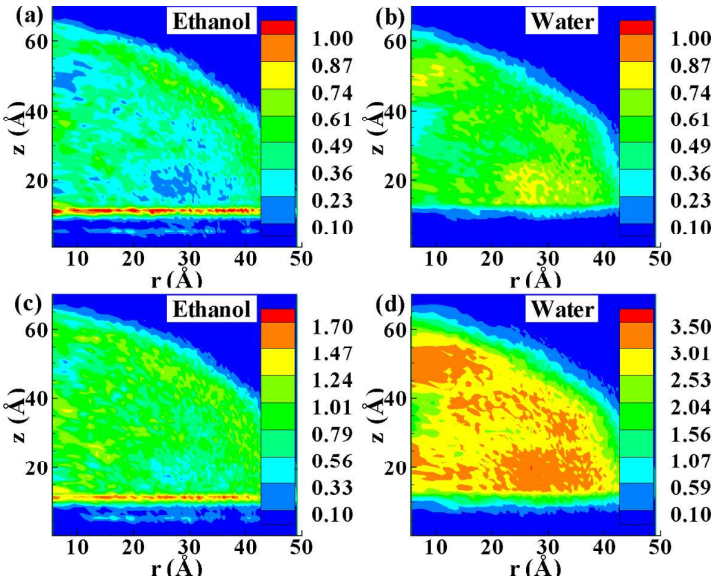

Figure S6: Density profile (a and b) and HB distribution (c and d) of ethanol and water molecules for 50 wt% ethanol solution at pillar height, $h = 2$ and $\alpha = 0.51$.

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