Supplemental Information

Contact Angles on Surfaces Using Mean Field Theory: Nanodroplet vs. Nanoroughness

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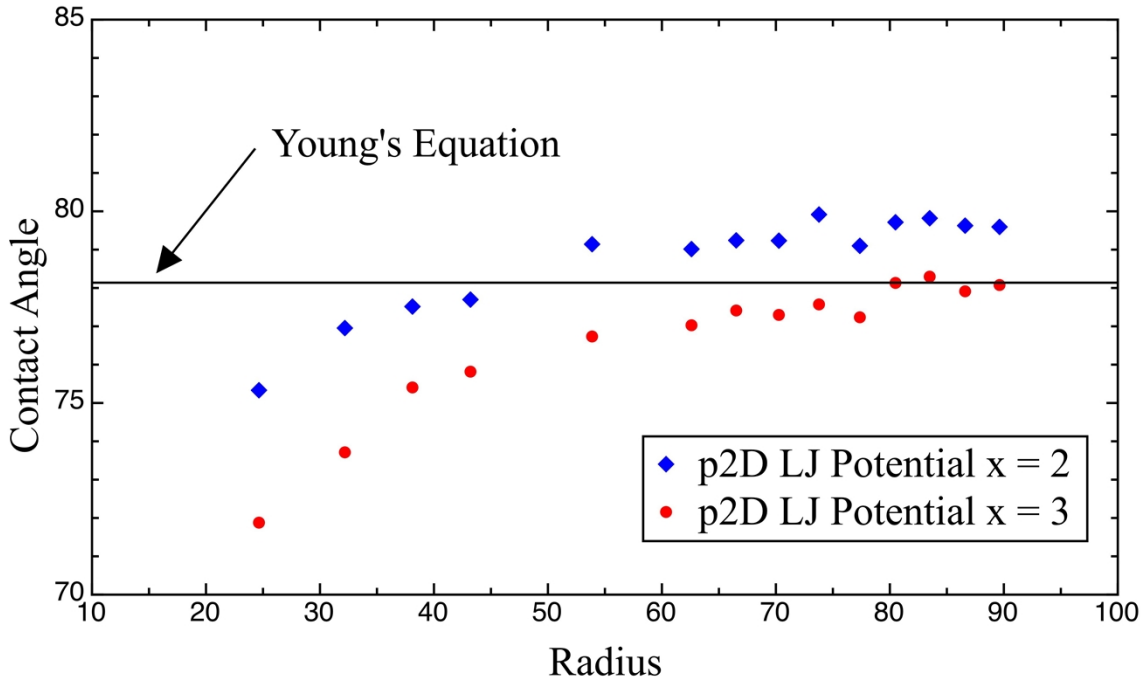
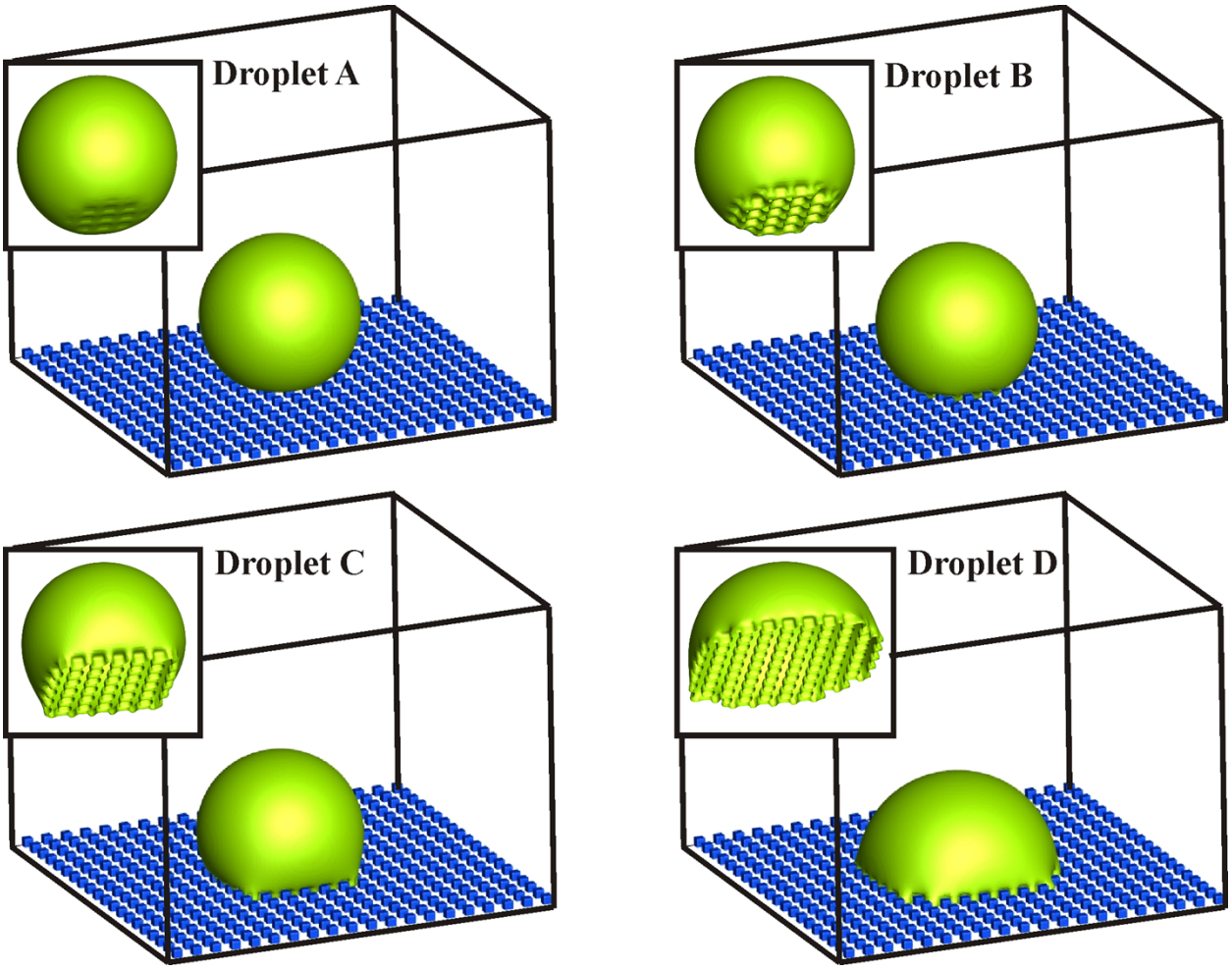
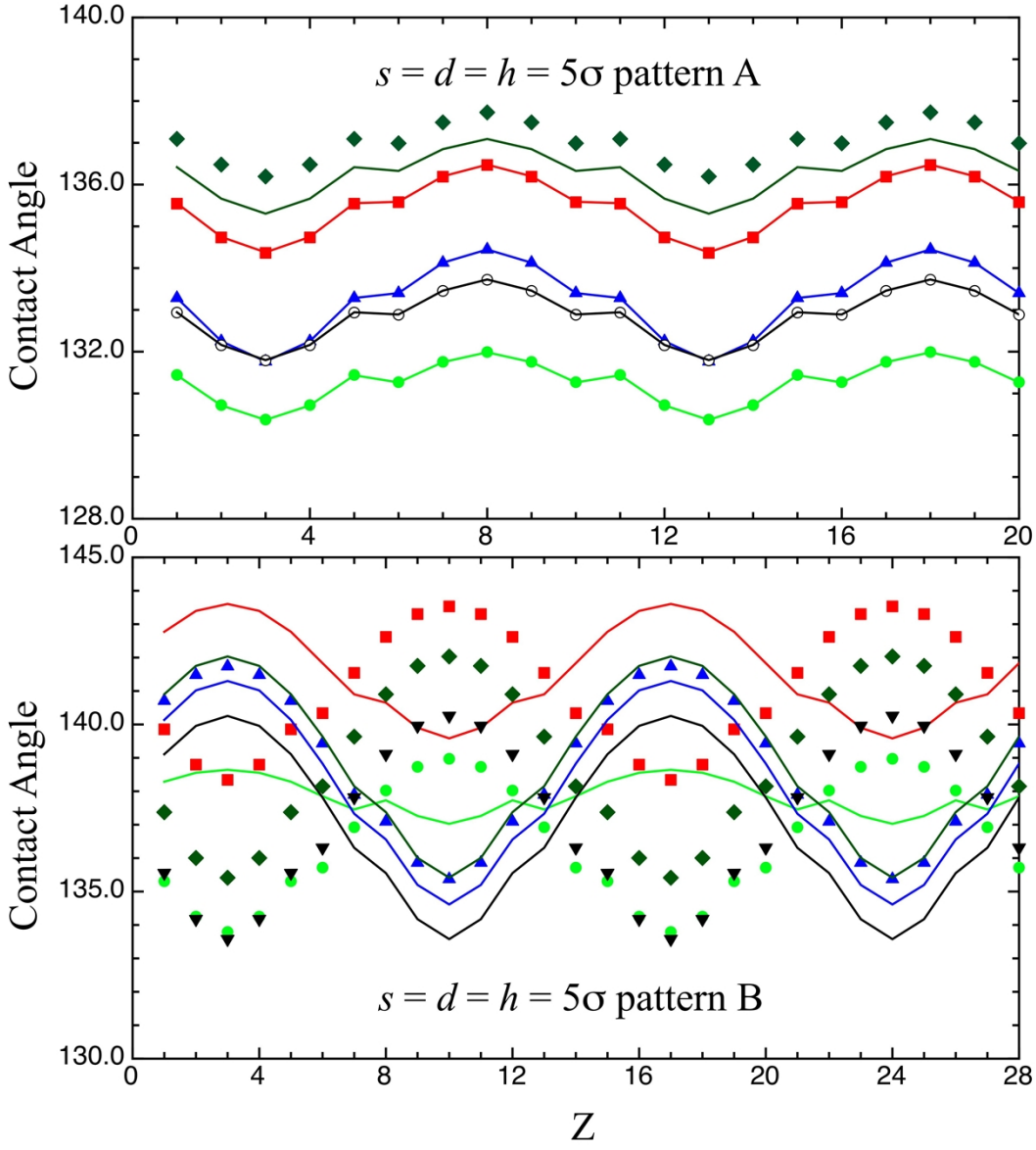
Supplemental Figure S1. For a more wetting surface, contact angle versus the radius of the droplet on a flat surface from p2D droplet DFT solutions with x=3 (diamonds), p2D droplet DFT solutions using the LJ potential with x=2 (circles), and DFT solution free energies with Young's equation (solid line). The value of x is a parameter in the contact angle calculation of droplets.



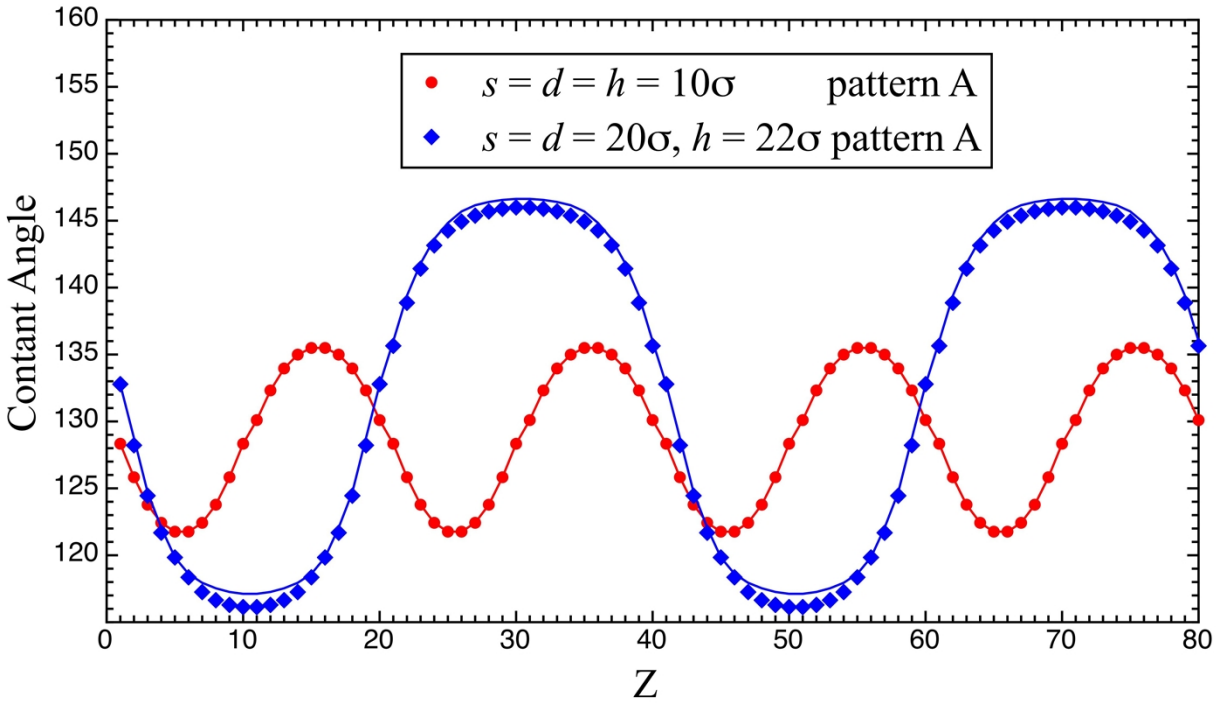
Supplemental Figure S2. Isodensity surfaces (ρ =0.5) for a 3D droplet using LJ potential on a surface with $s = d = h = 5\sigma$. Two views are shown, with and without the pillars rendered. Contact angles are as follows: Droplet A = 146°; Droplet B = 131°; Droplet C = 114°; Droplet D =83°.



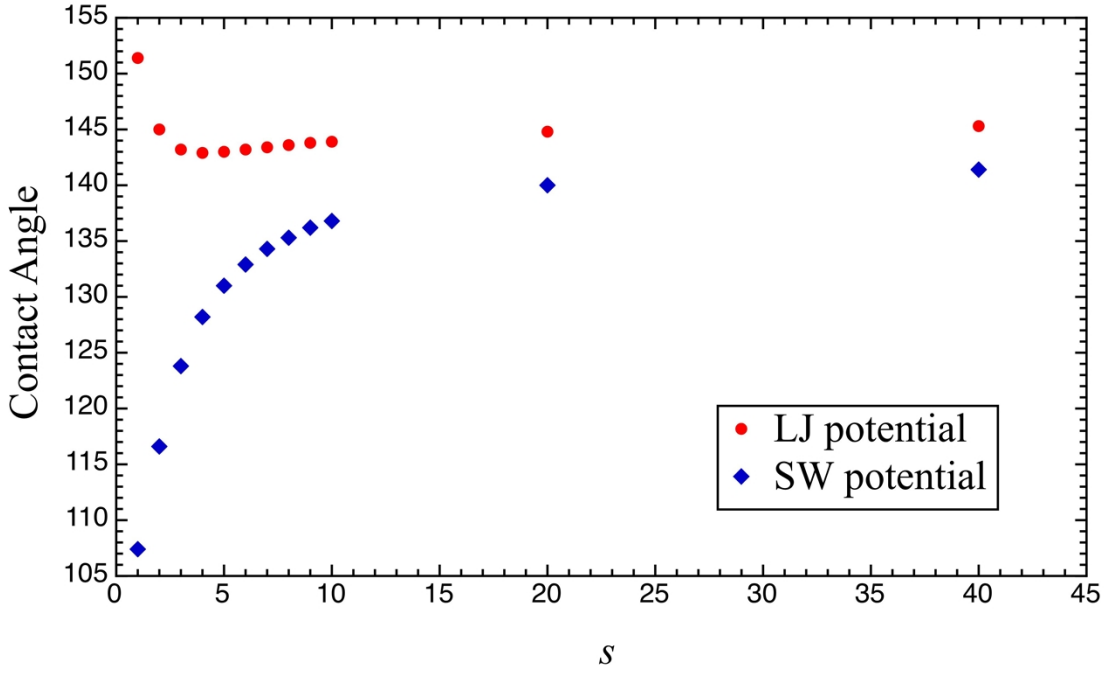
Supplemental Figure S3. Top panel has the local contact angles of a pseudo 2D drop versus Z (the short dimension) for both the left side (points) and right side (lines) of five different droplet simulations using LJ potential where the value of the average fluid density was varied. The droplets are on the pattern in shown in Figure 3A with $s = d = h = 5\sigma$. Bottom panel has the contact angles for droplets on the pattern in Figure 3B.



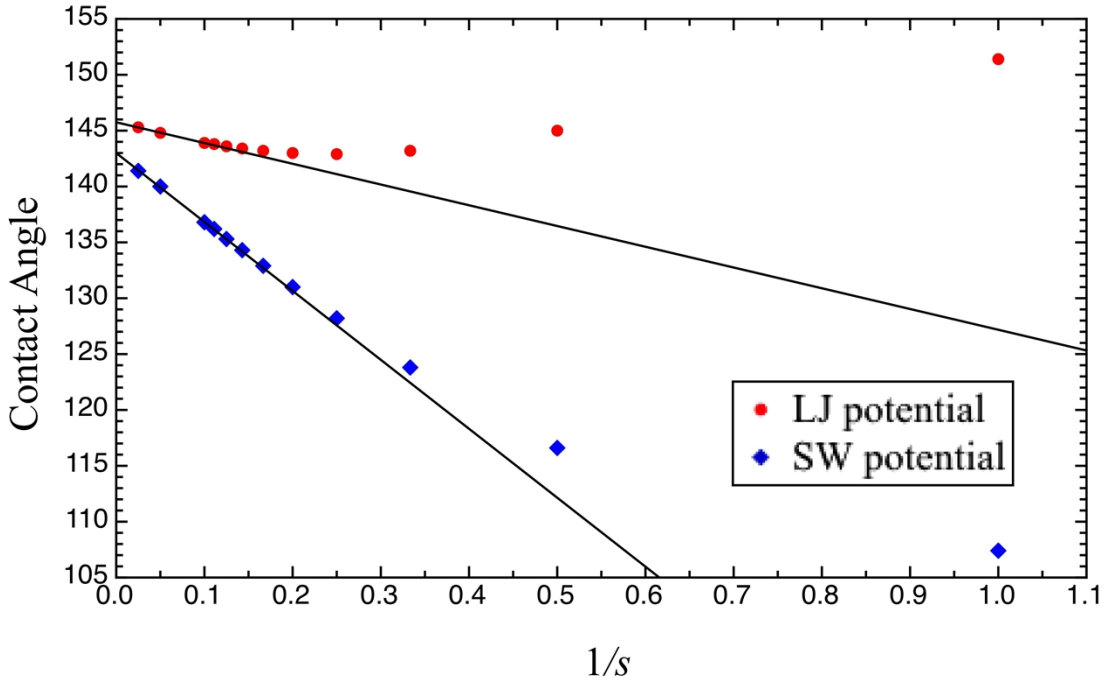
Supplemental Figure S4. Local contact angles of a p2D drop versus Z (the short dimension) for both the left side (points) and right side (lines) on two larger surface patterns using LJ potential.



Supplemental Figure S5A. Tall pillar limit contact angles versus *s*, pillar size, from DFT solution free energies with Young's equation using the two potentials with a low wetting interaction strength.



Supplemental Figure S5B. Tall pillar limit contact angles versus 1/*s* from DFT solution free energies with Young's equation using the two potentials with a low wetting interaction strength.



Supplemental Figure S6. Tall pillar limit contact angles versus *s* for various roughness factors from DFT solution free energies with Young's equation using the two potentials with a higher wetting interaction strength. The lines are the corresponding predictions from the application of the macroscopic Wenzel model.

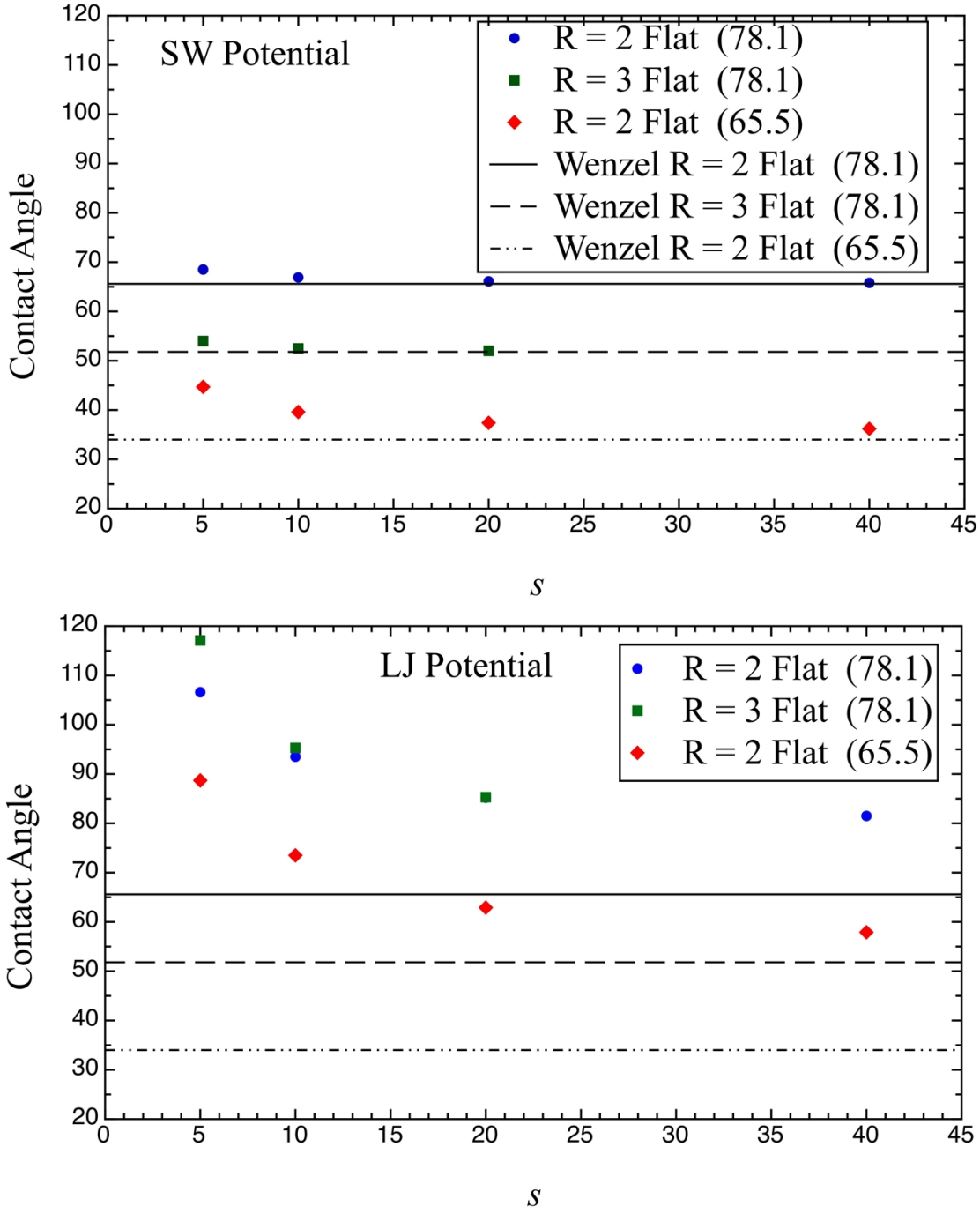


Table S1. Contact angles for low wetting surface using DFT solution free energies and Young's equation

Size	Height	Pattern[a]	Cassie	Wenzel	Contact angle Potential LJ	Contact angle Potential SW
0	0	-	101.7	101.7	101.7	101.9
1	10	A	143.2	180.0	151.3	
1	20	A	143.2	180.0	151.4	107.4
2	10	A	143.2	180.0	144.9	116.5
2	20	A	143.2	180.0	145.0	116.6
3	10	A	143.2	151.5	143.1	123.7
3	20	A	143.2	180.0	143.2	123.8
4	10	A	143.2	135.2	142.8	128.1
4	20	A	143.2	180.0	142.9	128.2
5	1	A	143.2	104.1	113.3	102.6
5	2	A	143.2	106.5	119.7	104.2
5	3	A	143.2	108.9	126.7	106.4
5	4	A	143.2	111.4	134.6	108.8
5	5	A	143.2	113.9	141.6 (143.8)	111.4
5	5	B	143.2	114.4	141.3 (144.6)	
5	6	A	143.2	116.5	142.3	114.2
5	7	A	143.2	119.1	142.6	117.0
5	8	A	143.2	121.8	142.7	119.9 (131.0)
5	9	A	143.2	124.6	142.8	122.8 (131.0)
5	10	A	143.2	127.5	142.8	125.9 (131.0)
5	10	B	143.2	128.4	142.5	
5	20	A	143.2	180.0	142.9	131.0
5	40	A	143.2	180.0	143.0	131.0
6	20	A	143.2	151.5	143.1	132.9
6	40	A	143.2	180.0	143.2	132.9
7	20	A	143.2	141.5	143.4	134.3
7	40	A	143.2	180.0	143.4	134.3
8	20	A	143.2	135.2	143.6	135.3
8	40	A	143.2	180.0	143.6	135.3
9	20	A	143.2	130.8	143.7	130.8
9	40	A	143.2	180.0	143.8	136.2
10	2	A	143.2	104.1	110.9	
10	4	A	143.2	106.5	116.2	
10	6	A	143.2	108.9	121.8	
10	8	A	143.2	111.4	127.6 (143.7)	
10	10	A	143.2	113.9	135.2 (144.4)	113.1 (136.8)
10	12	A	143.2	121.8	140.7 (143.9)	
10	14	A	143.2	124.6	143.9	
10	20	A	143.2	127.5	143.9	127.4 (136.8)
10	40	A	143.2	180.0	143.9	136.8
20	20	A	143.2	113.9	128.2 (144.7)	113.8
20	22	A	143.2	115.2	130.8 (144.7)	
20	26	A	143.2	117.8	136.5 (144.8)	
20	30	A	143.2	120.5	142.9 (144.8)	
20	40	A	143.2	127.5	144.8	127.9 (140.0)
20	60	A	143.2	144.2	144.8	140.0
40	40	A	143.2	113.9	125.4 (145.3)	114.1 (141.4)
40	50	A	143.2	117.1	131.6 (145.2)	117.5 (141.4)
40	100	A	143.2	135.2	145.3	136.6 (141.6)

[a] Patterns are shown in Figure 3. The letter given corresponds to the appropriate panel in the figure.

Table S2. Contact angles for high wetting flat surface using DFT solution free energies and Young's equation

Size	Height	Pattern[a]	Cassie	Wenzel	Contact angle Potential LJ	Contact angle Potential SW
0	0	-	78.1	78.1	78.1	78.0
1	20	A	134.3	0.0	141.4	72.5
2	20	A	134.3	0.0	133.2	66.2
3	20	A	134.3	0.0	131.3	56.1
4	20	A	134.3	0.0	131.2	51.8
5	1	A	134.3	75.7	92.4	77.4
5	2	A	134.3	73.2	97.1	75.7
5	3	A	134.3	70.7	100.6	73.6
5	4	A	134.3	68.2	103.5	71.1
5	5	A	134.3	65.6	106.6	68.5
5	6	A	134.3	63.0	108.3	
5	7	A	134.3	60.3	110.5	
5	8	A	134.3	57.6	112.7	
5	9	A	134.3	54.7	114.9	
5	10	A	134.3	51.8	117.1	54.0
5	20	A	134.3	0.0	131.6	49.0
5	40	A	134.3	0.0	131.6	48.9
6	20	A	134.3	26.7	120.2	47.0
6	40	A	134.3	0.0	132.1	47.0
7	20	A	134.3	37.3	109.2	45.6
7	40	A	134.3	0.0	127.5	45.6
8	20	A	134.3	43.8	102.6	44.6
8	40	A	134.3	0.0	114.4	44.6
9	20	A	134.3	48.4	98.3	49.1
9	40	A	134.3	0.0	106.5	43.7
10	2	A	134.3	75.7	88.3	
10	4	A	134.3	73.2	90.0	
10	6	A	134.3	70.7	90.9	
10	8	A	134.3	68.2	91.6	
10	10	A	134.3	65.6	93.5	66.9
10	12	A	134.3	63.0	92.9	
10	14	A	134.3	60.3	93.5	
10	20	A	134.3	51.8	95.3	52.5
10	40	A	134.3	0.0	101.3	43.0
20	20	A	134.3	65.6	85.2	66.1
20	22	A	134.3	64.3	85.2	
20	26	A	134.3	61.7	85.2	
20	30	A	134.3	59.0	85.2	
20	40	A	134.3	51.8	85.3	52.0
20	60	A	134.3	34.4	85.4	39.9
40	5	A	134.3	76.6	82.9	
40	10	A	134.3	75	83.1	
40	20	A	134.3	72.0	82.1	
40	30	A	134.3	68.8	81.8	
40	40	A	134.3	65.6	81.5	65.8
40	50	A	134.3	62.4	81.1	62.4
40	80	A	134.3	51.8	80.1	51.7
40	100	A	134.3	43.8	79.5	43.5

[a] Patterns are shown in Figure 3. The letter given corresponds to the appropriate panel in the figure.

Table S3. Contact angles for high wetting flat surface using DFT solution free energies and Young's equation

Size	Height	Pattern[a]	Cassie	Wenzel	Contact angle Potential LJ	Contact angle Potential SW
0	0	-	65.5	65.5	65.5	65.8
1	20	A	130.3	0.0	136.3	57.7
2	20	A	130.3	0.0	127.0	50.3
3	20	A	130.3	0.0	124.8	45.2
4	20	A	130.3	0.0	113.1	42.2
5	1	A	130.3	60.2	81.6	64.6
5	2	A	130.3	54.5	85.4	61.3
5	3	A	130.3	48.4	87.4	56.7
5	4	A	130.3	41.8	88.3	51.1
5	5	A	130.3	34.0	88.7	44.7
5	6	A	130.3	24.2	88.8	
5	7	A	130.3	5.6	88.9	
5	8	A	130.3	0.0	88.9	
5	9	A	130.3	0.0	88.8	
5	10	A	130.3	0.0	88.7	40.2
5	20	A	130.3	0.0	88.7	40.2
5	40	A	130.3	0.0	85.7	40.1
6	20	A	130.3	0.0	76.0	38.8
6	40	A	130.3	0.0	64.5	38.8
7	20	A	130.3	0.0	69.9	37.8
7	40	A	130.3	0.0	58.3	37.8
8	20	A	130.3	0.0	66.6	37.0
8	40	A	130.3	0.0	55.3	37.0
9	20	A	130.3	0.0	64.8	36.5
9	40	A	130.3	0.0	53.0	36.4
10	2	A	130.3	60.2	76.4	
10	4	A	130.3	54.5	76.4	
10	6	A	130.3	48.4	75.2	
10	8	A	130.3	41.8	73.7	
10	10	A	130.3	34.0	73.5	39.6
10	12	A	130.3	24.2	70.4	
10	14	A	130.3	5.6	68.8	
10	20	A	130.3	0.0	63.7	36.0
10	40	A	130.3	0.0	51.2	36.0
20	5	A	130.3	58.8	71.4	61.2
20	10	A	130.3	51.5	69.8	54.2
20	20	A	130.3	34.0	62.9	37.4
20	22	A	130.3	29.4	61.7	
20	26	A	130.3	17.5	59.2	
20	30	A	130.3	0.0	56.7	
20	40	A	130.3	0.0	50.0	33.7
20	60	A	130.3	0.0	43.4	33.7
40	40	A	130.3	34.0	57.9	36.2
40	50	A	130.3	21.1	54.2	32.5
40	80	A	130.3	0.0	41.8	32.5
40	100	A	130.3	0.0	31.6	23.2

[a] Patterns are shown in Figure 3. The letter given corresponds to the appropriate panel in the figure.

Table S4. Contact angles for low wetting flat surface using DFT solution free energies and Young's equation; fixed *s* changing *d*

Size	Height	Pattern[a]	Cassie	Wenzel	Contact angle Potential LJ
0	0	-	101.7	101.7	101.7
5	5	A	143.2	113.9	141.6 (143.8)
5	5	B	155.7	100.4	118.6
5	5	C	165.5	93.7	107.5
5	5	D	169.7	119.1	104.6
5	5	E	171.2	121.8	103.5
5	10	A	143.2	127.5	142.8
5	10	B	155.7	105.7	135.0 (155.3)
5	10	C	165.5	95.6	112.6 (165.0)
5	10	D	169.7	92.8	107.2 (169.4)
5	10	E	172.0	91.7	105.0 (171.2)
5	20	A	143.2	180.0	142.9
5	20	B	155.7	116.8	155.4
5	20	C	165.5	99.3	123.1 (165.3)
5	20	D	169.7	94.7	112 (169.4)
5	20	E	172.0	92.9	108.0 (171.7)
5	40	A	143.2	180.0	142.9
5	40	B	155.7	144.2	155.4
5	40	C	165.5	107.0	150.7 (165.3)
5	40	D	169.7	98.6	122.9 (169.5)
5	40	E	172.0	95.2	114.1 (171.8)
5	80	A	143.2	180.0	142.9
5	80	B	155.7	180.0	155.4
5	80	C	165.5	123.5	165.3
5	80	D	169.7	106.3	151.1 (169.5)
5	80	E	172.0	99.8	127.6 (171.8)

[a] Patterns are shown in Figure 3 and Supplemental Figure S7. The letter given corresponds to the appropriate panel in the figure.

Supplemental Figure S7. Patterns C, D, and E show the unit cell of Figure 3A repeated 24 times in the y-direction and 4 in the z-direction with different arrangements of pillars with two different fluid interaction energies.