Electronic Supplementary information for

Controlling States of Water Droplets on Nanostructured Surfaces by Design

Chongqin Zhu[1, 2†], Yurui Gao[3†], Yingying Huang[4], Hui Li[2], Sheng Meng[5,6], Joseph S. Francisco[1], Xiao Cheng Zeng[1, 2*]

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Table S1. Calculated probabilities P_w of the Wenzel state on a surface with a trapezoid base angle of $\varphi = 45^{\circ}$, given different downward velocities v_d of the droplet and various intrinsic contact angles (θ_{in}).

Table S2. Calculated probabilities P_w of the Wenzel state on a surface with a trapezoid base angle of $\varphi = 60^{\circ}$, given different downward velocities v_d of the droplet and various intrinsic contact angles (θ_{in}).

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Figure S5. Side and top views of the initial configuration with the water droplet in the Wenzel state on a modelled surface with trapezoidal nanostructures.

Figure S6. Enlarged snapshots of systems at t = 2.0 ns after MD simulations with initial configurations with the water droplet in the Wenzel state. The intrinsic contact angles of the surfaces are θ_{in} = 137.7° (a) and θ_{in} = 135.9° (b), respectively, and the trapezoid base angle is $\varphi = 120^{\circ}$.

Figure S7. Variations in potential energy with intrinsic contact angle for water droplets on modelled surfaces with $\varphi = 45^{\circ}$(a), $\varphi = 60^{\circ}$(b), $\varphi = 90^{\circ}$(c) and $\varphi = 120^{\circ}$(d) after equilibrium when the droplet is in the Wenzel state in the initial configuration.

Figure S8. Snapshots of a water droplet (with 24256 water molecules) in a constrained equilibrium state above the surface (a), in the Cassie state (b), and in the Wenzel state (c) after the droplet has collided with a surface with trapezoidal nanostructures.

Table S1. Calculated probabilities P_w of the Wenzel state on a surface with a trapezoid base angle of $\varphi = 45^{\circ}$, given different downward velocities v_d of the droplet and various intrinsic contact angles (θ_{in}).

θ_{in} (deg)	v_d (m/s)	e_k (kJ/mol)	Cassie	Wenzel	P_w
60	70	0.044	100	20	0.167
	80	0.057	93	27	0.225
	90	0.073	85	35	0.292
	100	0.090	47	73	0.608
	110	0.109	25	95	0.792
	120	0.129	9	111	0.925
75	90	0.073	116	4	0.033
	100	0.090	104	16	0.133
	110	0.109	92	28	0.233
	120	0.129	75	45	0.375
	130	0.152	33	87	0.725
	140	0.176	7	113	0.942
90	120	0.129	105	15	0.125
	130	0.152	90	30	0.250
	140	0.176	45	75	0.625
	145	0.189	33	87	0.725
	150	0.202	18	102	0.850
	155	0.216	9	111	0.925
	160	0.230	5	115	0.958
105	150	0.202	106	14	0.117
	160	0.230	83	37	0.308
	165	0.244	73	47	0.392
	170	0.259	43	77	0.642
	175	0.275	30	90	0.750
	180	0.291	13	107	0.892
	190	0.324	2	118	0.983
120	200	0.359	112	8	0.067
	205	0.377	102	18	0.150
	210	0.396	90	30	0.250
	220	0.435	56	64	0.533
	230	0.475	19	101	0.842
	235	0.496	19	101	0.842

Table S2. Calculated probabilities P_w of the Wenzel state on a surface with a trapezoid base angle of $\varphi = 60^{\circ}$, given different downward velocities v_d of the droplet and various intrinsic contact angles (θ_{in}).

θ_{in} (deg)	v_d (m/s)	e_k (kJ/mol)	Cassie	Wenzel	P_w
90	86	0.066	112	8	0.067
	94	0.079	110	10	0.083
	102	0.093	102	18	0.150
	110	0.109	86	34	0.283
	118	0.125	59	61	0.508
	126	0.143	37	83	0.692
100	142	0.181	116	4	0.033
	150	0.202	111	9	0.075
	158	0.224	94	26	0.217
	166	0.247	79	41	0.342
	174	0.272	60	60	0.500
	182	0.297	24	96	0.800
110	142	0.181	116	4	0.033
	150	0.202	111	9	0.075
	158	0.224	94	26	0.217
	166	0.247	79	41	0.342
	174	0.272	60	60	0.500
	182	0.297	24	96	0.800
	190	0.324	9	111	0.925

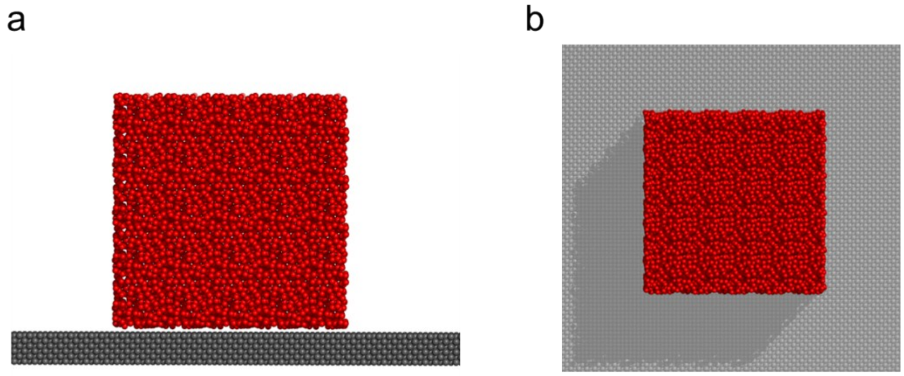

Figure S1. Side and top views of the initial water droplets in MD simulations of a water droplet on a flat surface.

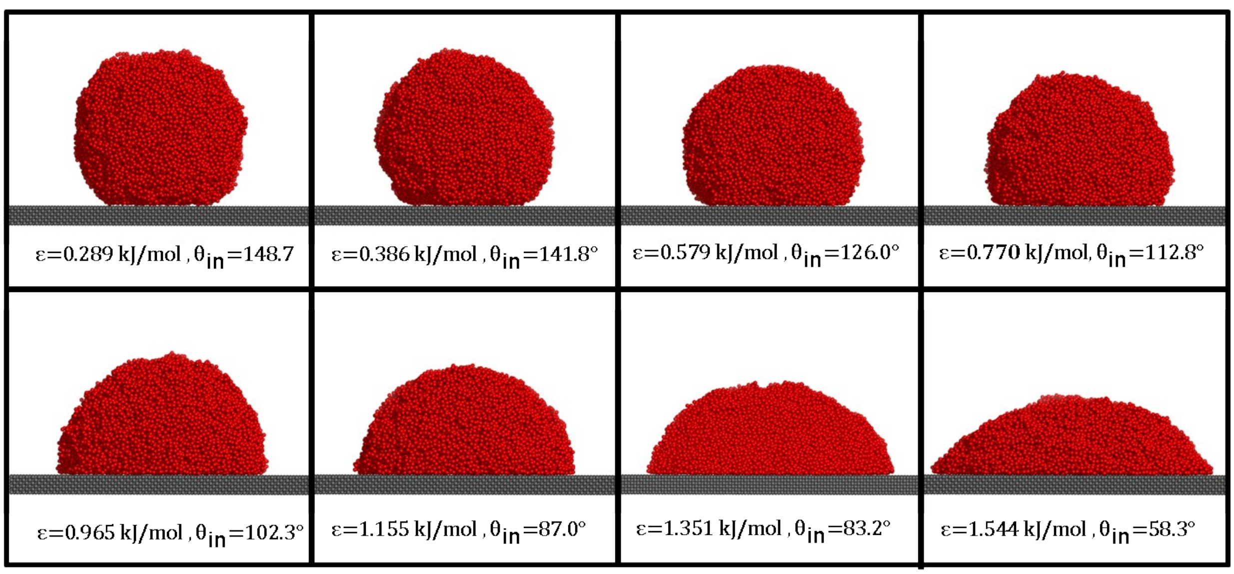

Figure S2. Snapshots of water nanodroplets on flat modelled surfaces at the end of MD simulations with ε values varying from 0.289 kJ/mol to 1.544 kJ/mol.

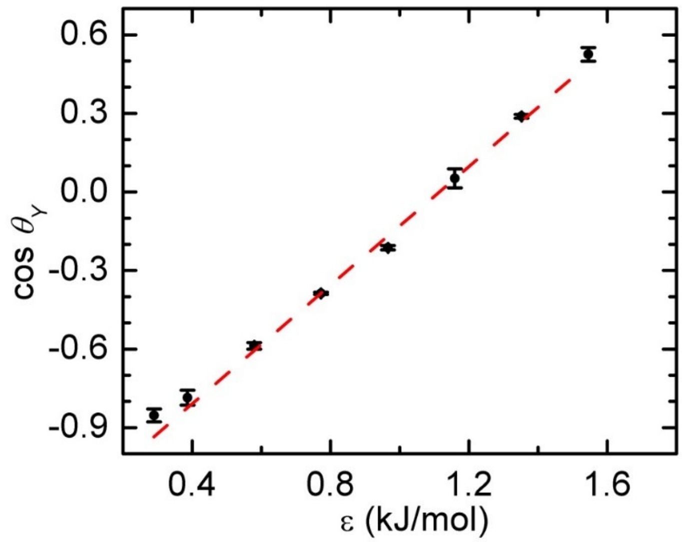

Figure S3. Cosine of the intrinsic contact angle of a water droplet on a modelled surface as a function of the interaction parameter ε between a water molecule and an atom of the solid surface.

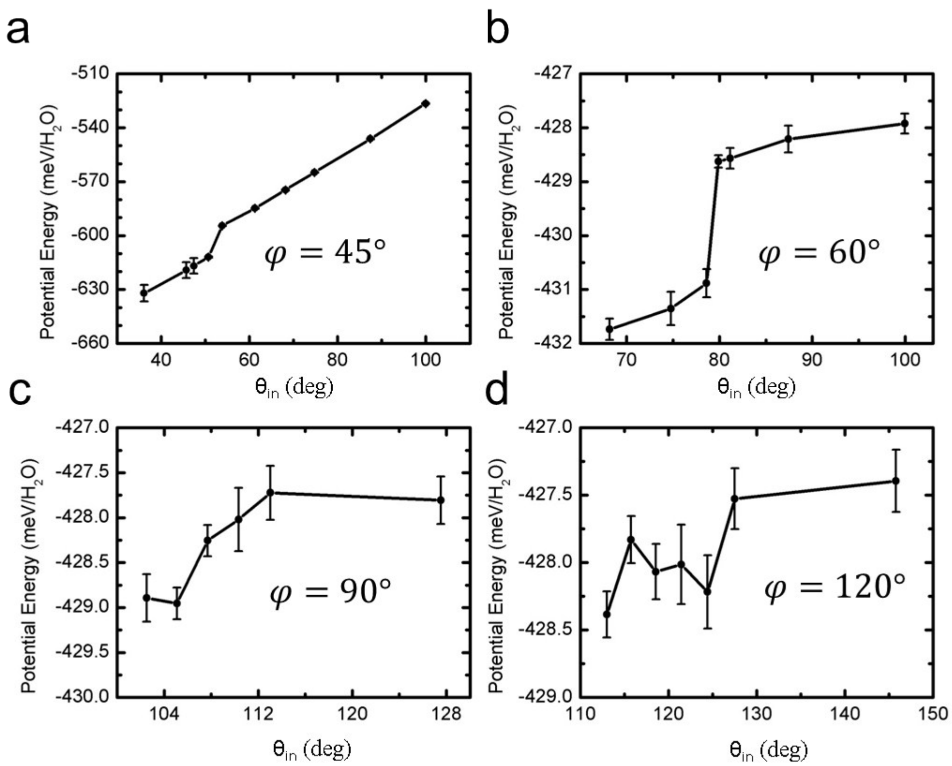

Figure S4. Variations in potential energy (which includes both water-water interaction energy and water-surface interaction energy) with intrinsic contact angle for water droplets on modelled surfaces with $\varphi = 45^\circ$(a), $\varphi = 60^\circ$(b), $\varphi = 90^\circ$(c) and $\varphi = 120^\circ$(d) after equilibrium when the droplet is in the Cassie state in the initial configuration.

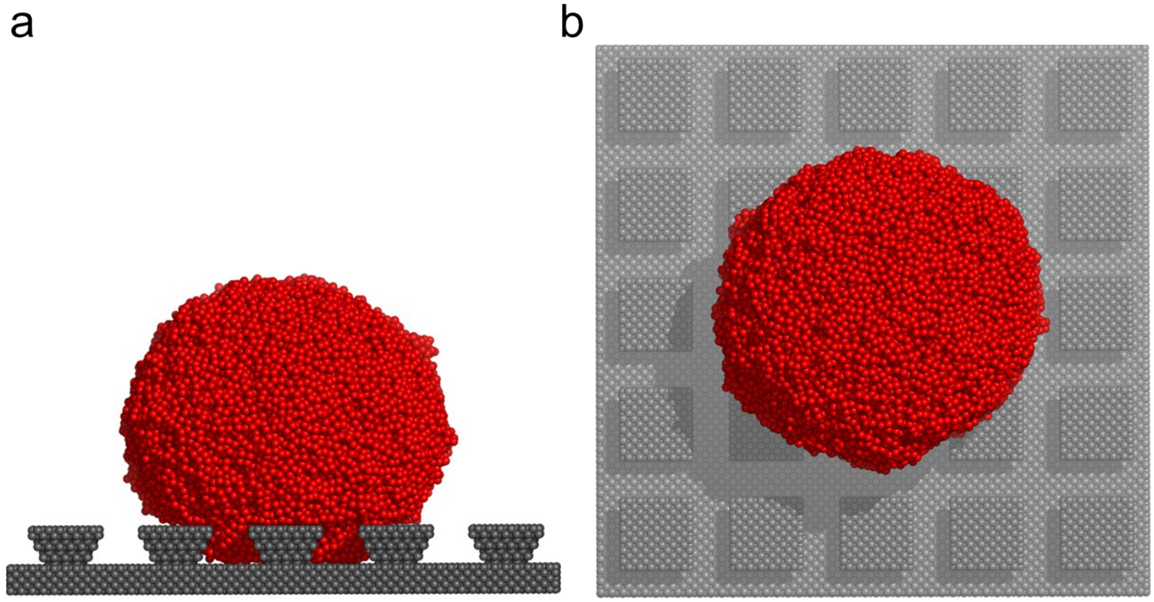

Figure S5. Side and top views of the initial configuration with the water droplet in the Wenzel state on a modelled surface with trapezoidal nanostructures.

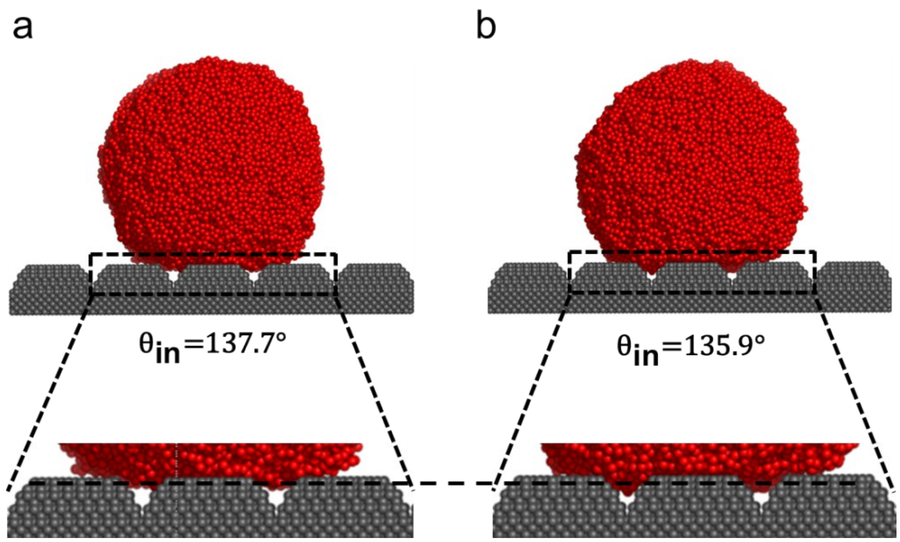

Figure S6. Enlarged snapshots of systems at t = 2.0 ns after MD simulations with initial configurations with the water droplet in the Wenzel state. The intrinsic contact angles of the surfaces are θ_{in} = 137.7° (a) and θ_{in} = 135.9° (b), respectively, and the trapezoid base angle is φ = 120°.

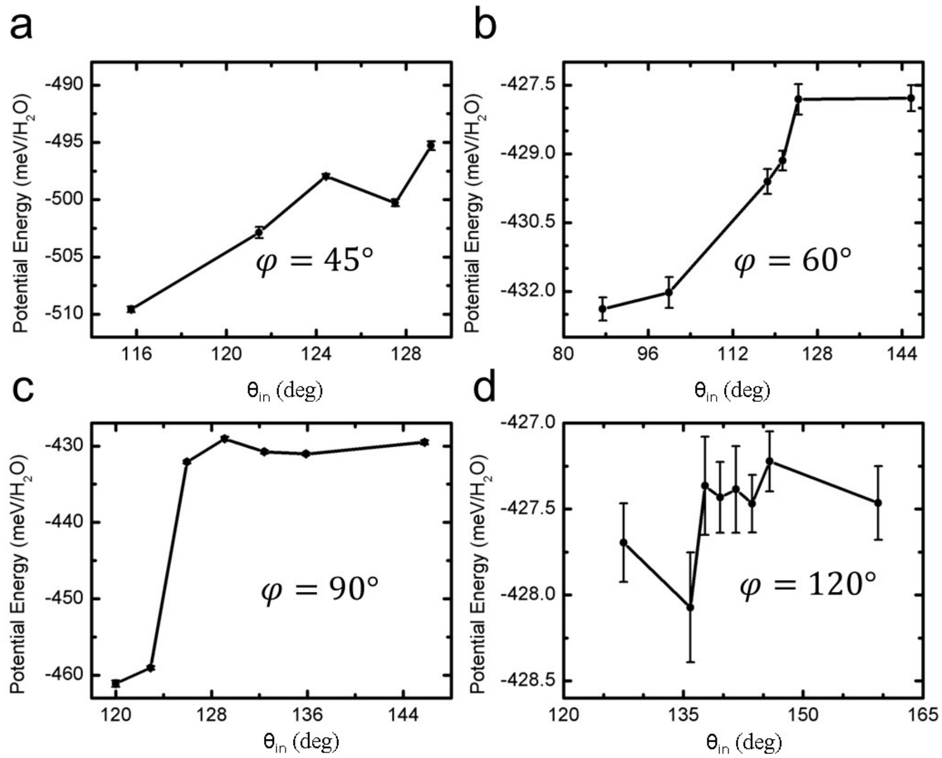

Figure S7. Variations in potential energy with intrinsic contact angle for water droplets on modelled surfaces with $\varphi = 45^\circ$ (a), $\varphi = 60^\circ$ (b), $\varphi = 90^\circ$ (c) and $\varphi = 120^\circ$ (d) after equilibrium when the droplet is in the Wenzel state in the initial configuration.

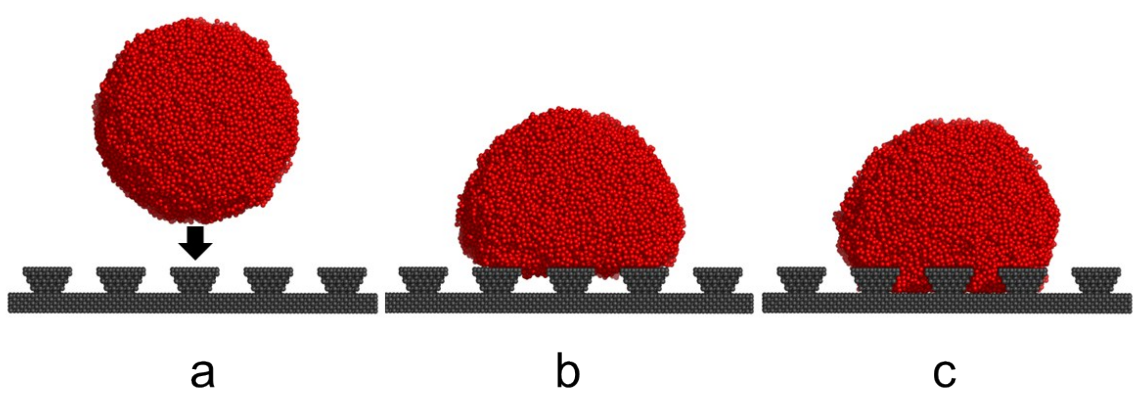

Figure S8. Snapshots of a water droplet (with 24256 water molecules) in a constrained equilibrium state above the surface (a), in the Cassie state (b), and in the Wenzel state (c) after the droplet has collided with a surface with trapezoidal nanostructures.

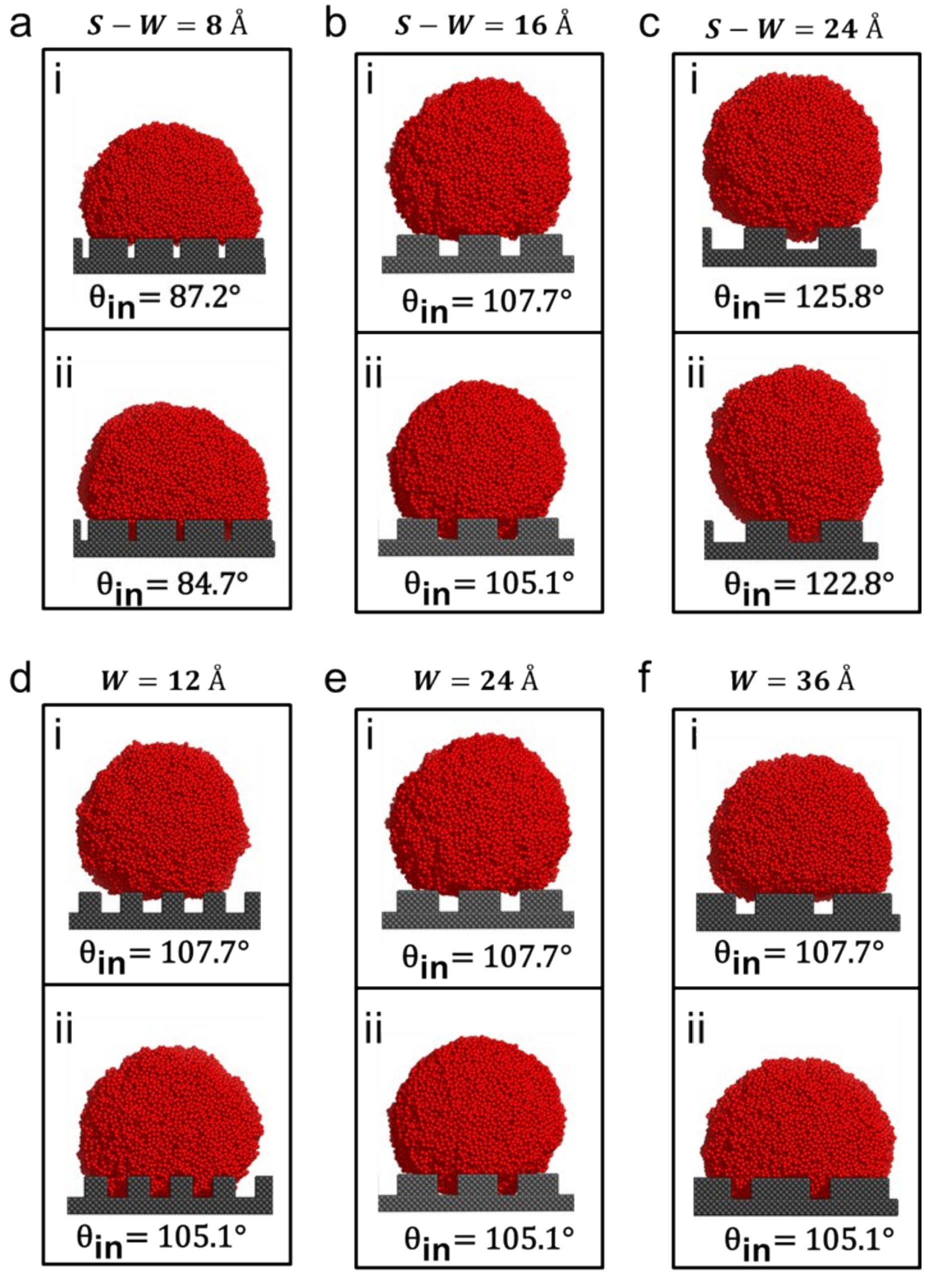

Figure S9. Snapshots of systems at t = 2.0 ns from MD simulations with fixed W = 24 Å (a, b and c) and fixed S-W = 16 Å (d, e and f). The intrinsic contact angle of the surface, θ_{in}, is shown below each snapshot. Trapezoid base angle is fixed at φ = 90°. For W = 24 Å, three different S-W values, i.e., S-W = 8 Å (a), S-W = 16 Å (b), and S-W = 24 Å (c) were selected for the MD simulations. While for S-W = 16 Å, three W values, i.e., W = 12 Å (d), W = 24 Å (e), W = 36 Å (a) were selected for the MD simulations.