

Article

What is the Value of Water Contact Angle on Silicon?

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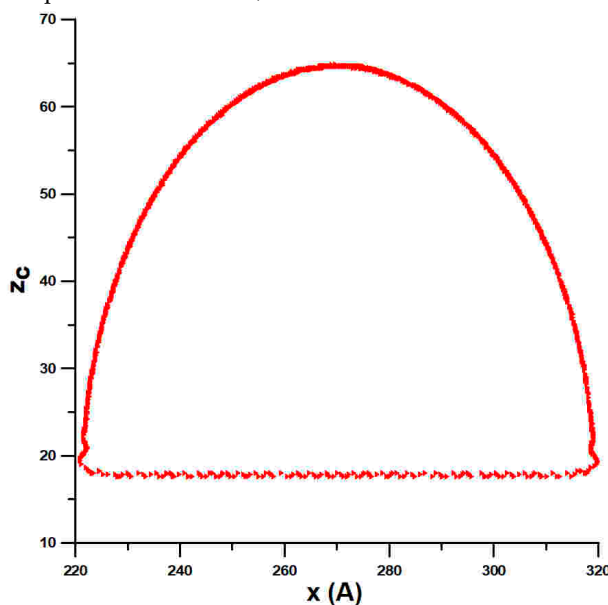


Figure S1. The cylindrical droplet contour calculated for the water- bare silicon surface system with $k_d = 0.147$. The x_c and z_c . Cartesian coordinates denote the position of the water density profile with value $0.5 \pm 0.03 \text{ g/cm}^3$.

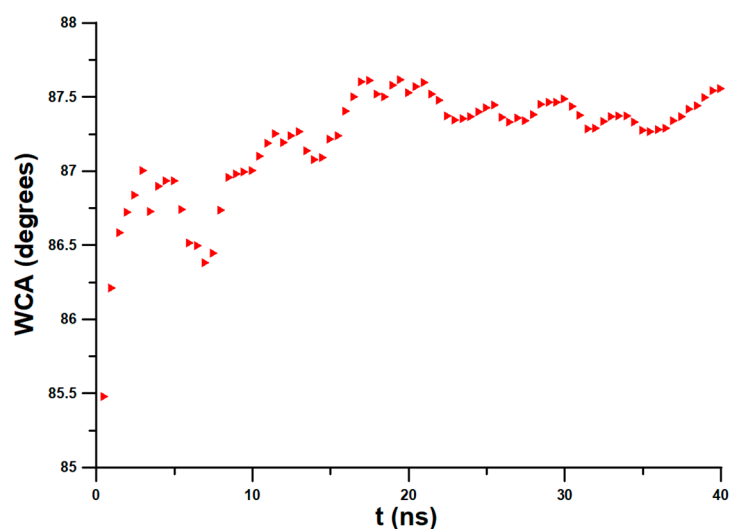


Figure S2. Time dependence of the simulated water contact angle for the system with $k_d = 0.147$.

Table S1. Forcefield parameters applied during simulations of n-decane.

Parameter	Value
σ_C	3.5 Å
ϵ_C	0.276144 kJ/mole
q_C^{CH2}	-0.12e
q_C^{CH3}	-0.18e
q_H	0.06e
ϵ_H	0.125520 kJ/mole
l_{CC}	0.1535 nm
k_{CC}	224262.4 kJ/(mole nm ²)
l_{CH}	0.10930 nm
k_{CH}	284512.0 kJ/(mole nm ²)
Θ_{HCH}	1.88146493 rad
Θ_{HCC}	1.93207984 rad
Θ_{CCC}	1.96698607 rad
k_{HCH}	276.144 kJ/(mole rad ²)
k_{HCC}	313.800 kJ/(mole rad ²)
k_{CCC}	488.273 kJ/(mole rad ²)
$c_{HCCC}^{(0)}$	0.6276 kJ/mole
$c_{HCCC}^{(1)}$	1.882800 kJ/mole
$c_{HCCC}^{(2)}$	0.0000 kJ/mole
$c_{HCCC}^{(3)}$	-2.510400 kJ/mole
$c_{HCCCH}^{(0)}$	0.6276 kJ/mole
$c_{HCCCH}^{(1)}$	1.882800 kJ/mole
$c_{HCCCH}^{(2)}$	0.0000 kJ/mole
$c_{HCCCH}^{(3)}$	-2.510400 kJ/mole
$c_{CCCC}^{(0)}$	2.9288 kJ/mole
$c_{CCCC}^{(1)}$	-1.4644 kJ/mole
$c_{CCCC}^{(2)}$	0.2092 kJ/mole
$c_{CCCC}^{(3)}$	-1.6736 kJ/mole