

Lattice Gas models: interaction of water with surfaces

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1 Model

We study the interaction of water and surfaces using Monte Carlo simulations in the grand canonical ensemble.

$$H = -\epsilon \sum_{\langle i,j \rangle} c_i c_j - b_s \sum_{i \in \mathcal{S}} c_i - \mu \sum_i c_i \quad (1)$$

We use periodic boundary conditions and a von Neumann neighborhood for the interaction between water-water and water-surface.

Parameter	Value
General parameters	
Temperature, T	298 K
Water-water, ϵ	3
AFM tip simulations	
Number lattice sites horizontal, w	100
Number lattice sites vertical, h	100
Tip radius R	10 nm
Tip surface distance y_0	0-5 l
Relative humidity, s	0.30-0.65
Icosahedral virus simulations	
Virus radius, R	50 nm
Virus shell thickness, t	3 nm

Table 1: Simulation parameters.

General and simulation specific parameters

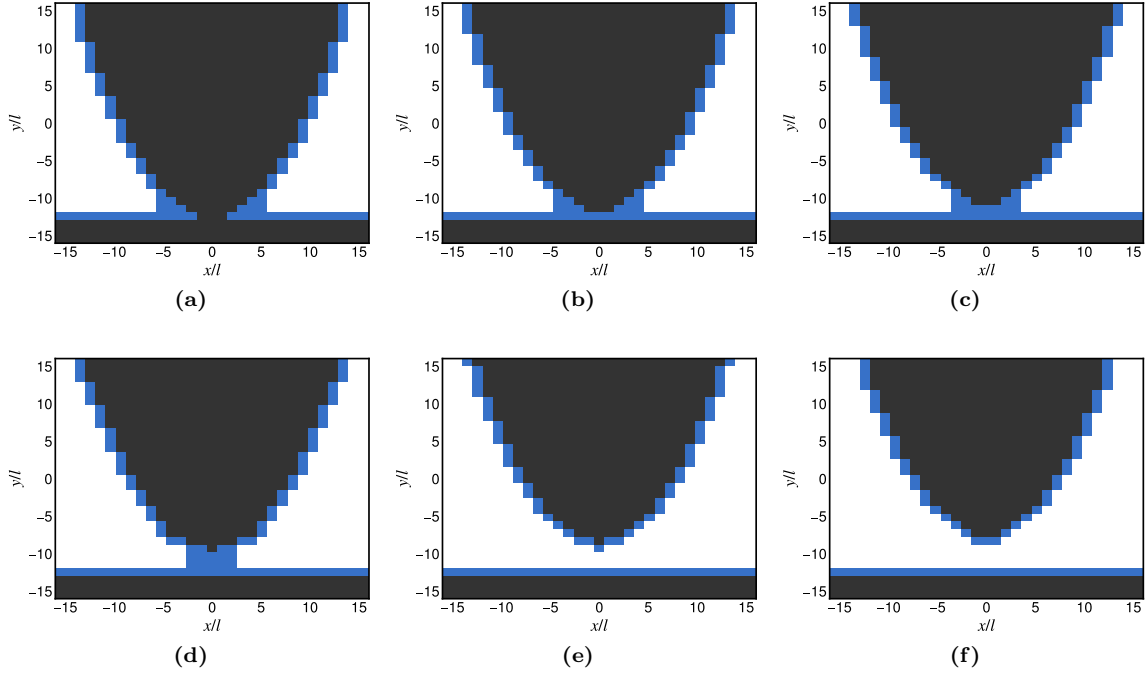


Figure 1: Water meniscus depending on the distance to surface

Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of l ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.30$.

2 Meniscus between surface and AFM tips

We consider the AFM tip as the values above the parabola given by $y(x) = ax^2 + y_0$, where y_0 is the distance to the surface and $a = \frac{1}{2R}$, with R the desired radius of the tip.

Minimisation proceeds by randomly selecting lattice locations and comparing the energy change following the Metropolis criterion.

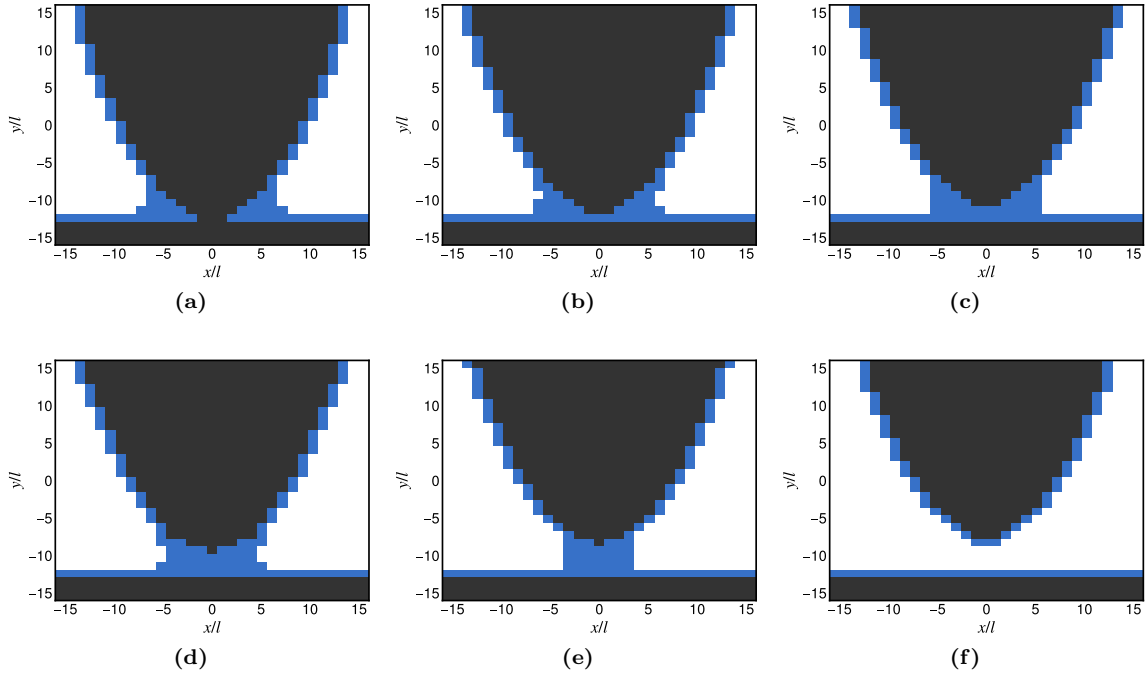


Figure 2: Water meniscus depending on the distance to surface

Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of l ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.50$.

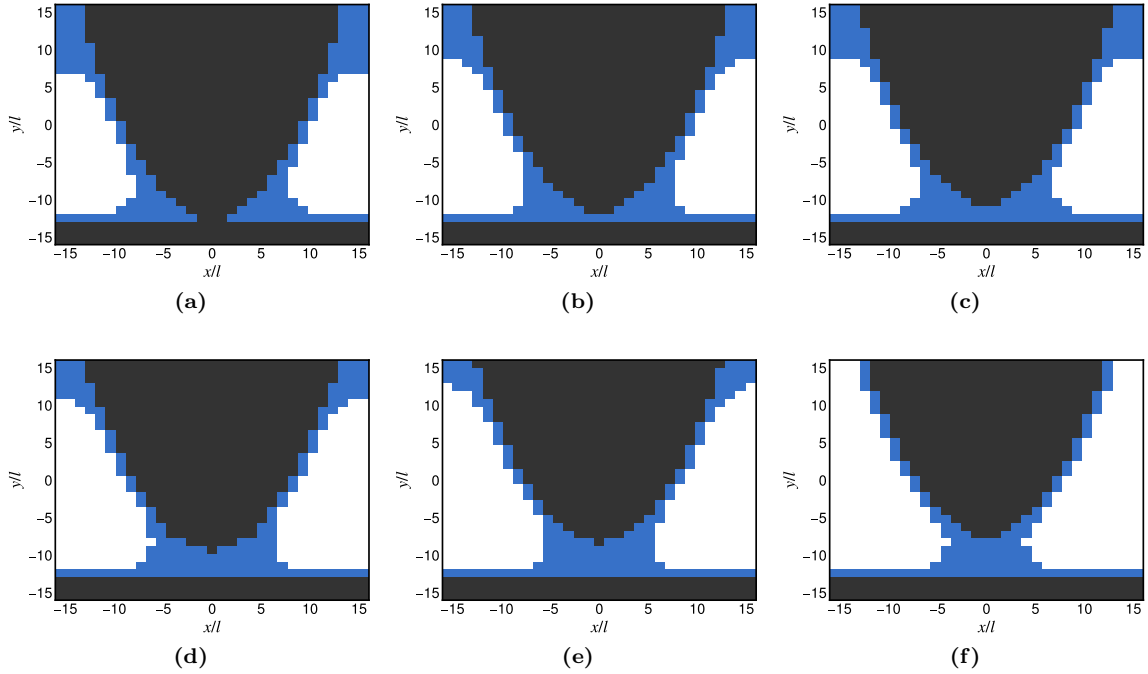


Figure 3: Water meniscus depending on the distance to surface

Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of l ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.65$. Note the artifact on the upper part due to the limited size of the mesh in the horizontal direction.

3 Icsaohedral viruses

References