Lattice Gas models: interaction of water with surfaces

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Abstract

1 Model

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

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

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

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.

3 Icsaohedral viruses