

Molecular Origin of Contact Line Friction in Dynamic Wetting

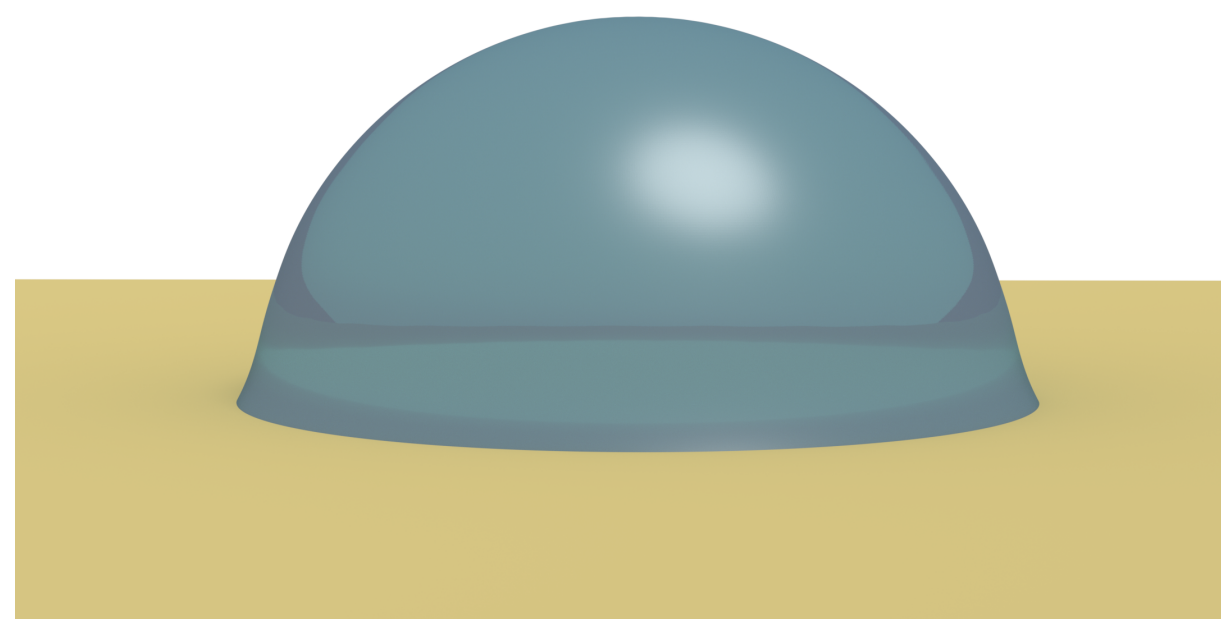
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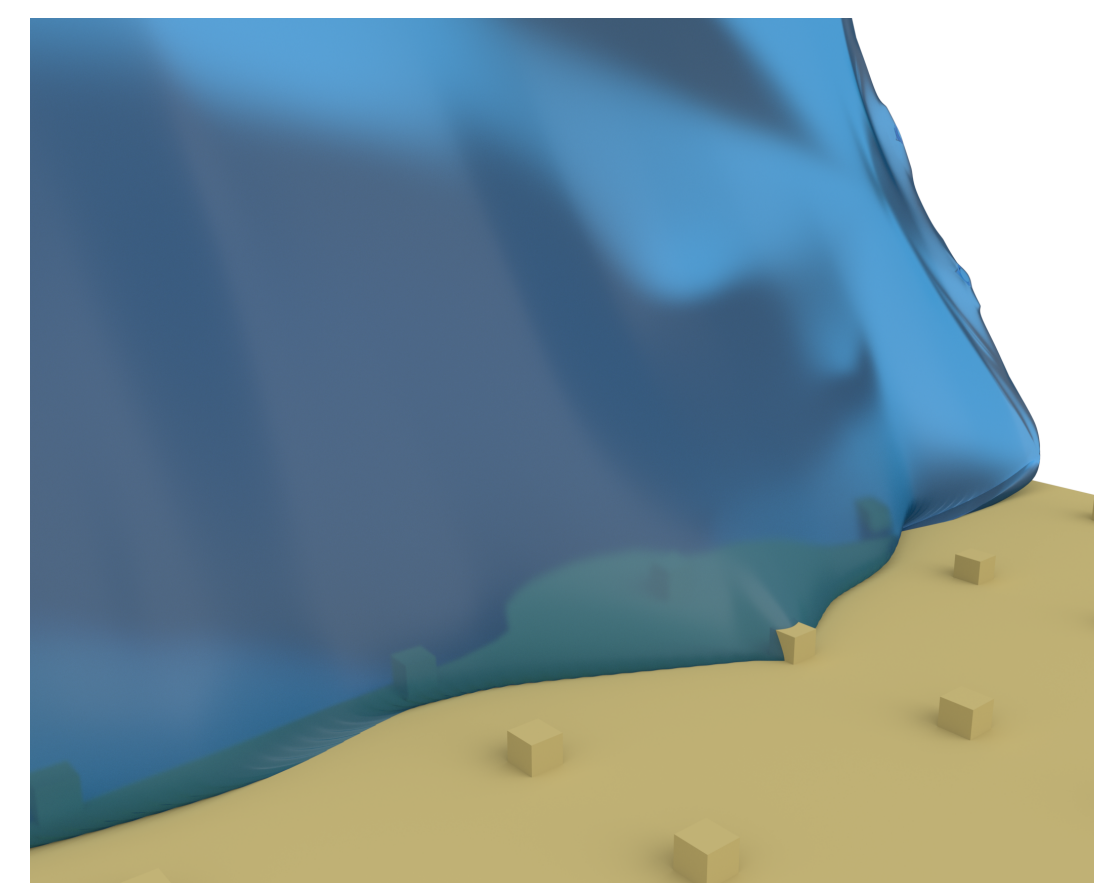
Macroscopic Wetting

Dynamics are well described by Navier-Stokes with supplied boundary conditions (eg. slip, contact line friction).



PROBLEM:

- Parameters are fitted to match dissipation rates.
- Contact line friction needed to replicate experiments.
- Unknown nature of this boundary condition.



Mesoscopic

Wetting on microstructured substrates inform how surface structure affect boundary conditions.

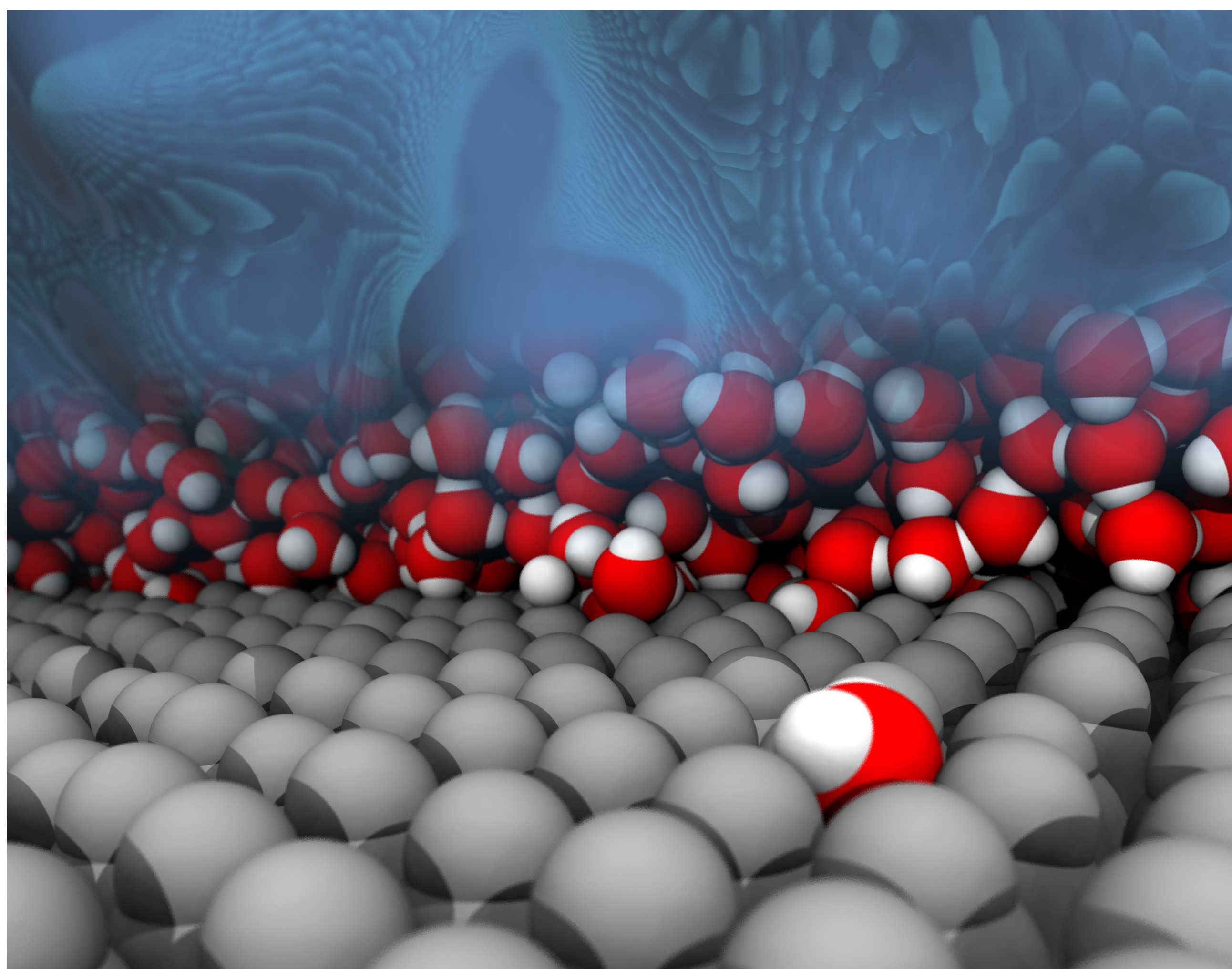
PROBLEM:

- Still does not answer origin question.

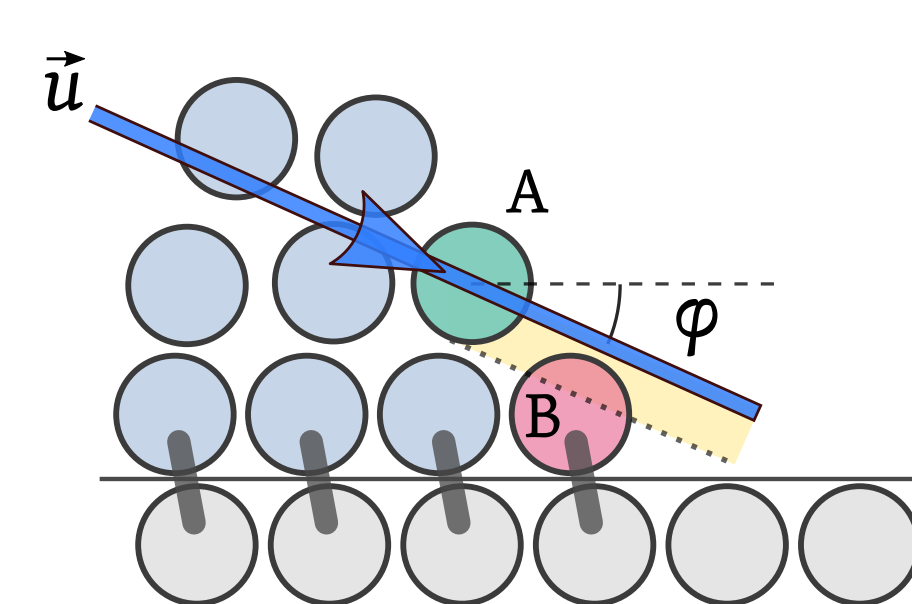
Molecular Scale Dynamics

Use molecular dynamics simulations to probe wetting dynamics in a large scale, realistic molecular system. A large system size enables longer investigation time scales. Water forms hydrogen bonds with the substrate molecules which occurs in realistic systems and results in a no-slip condition.

- Enables a detailed study of contact line friction.
- Friction is related to how molecules advance the contact line.



Molecular modes of contact line advancement

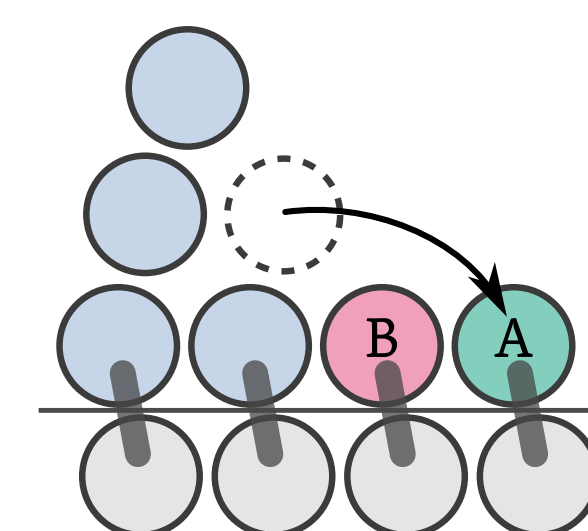


$\vec{u}$ is the average local flow in the contact line region and makes an angle φ to the substrate.

The bottom layer of liquid molecules is bonded to the substrate.

Bonded molecules $\rightarrow$ No-slip condition

MODE 1: ROLLING



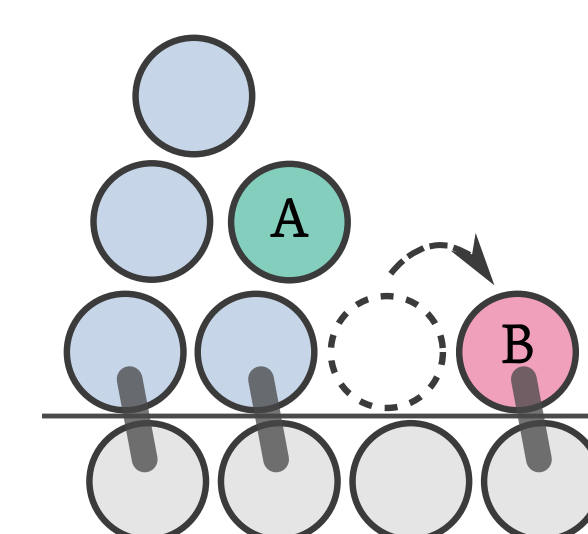
Molecule A has to cross an energy barrier ΔE through a thermal fluctuation to advance.

Molecule B acts as an *obstacle* which increases the barrier height. The obstacle "size" is related to the angle φ of approach.

After advancement, the energy is dissipated. In effect, *friction*.

Small $\varphi \rightarrow$ High barrier
High barrier $\rightarrow$ High dissipation

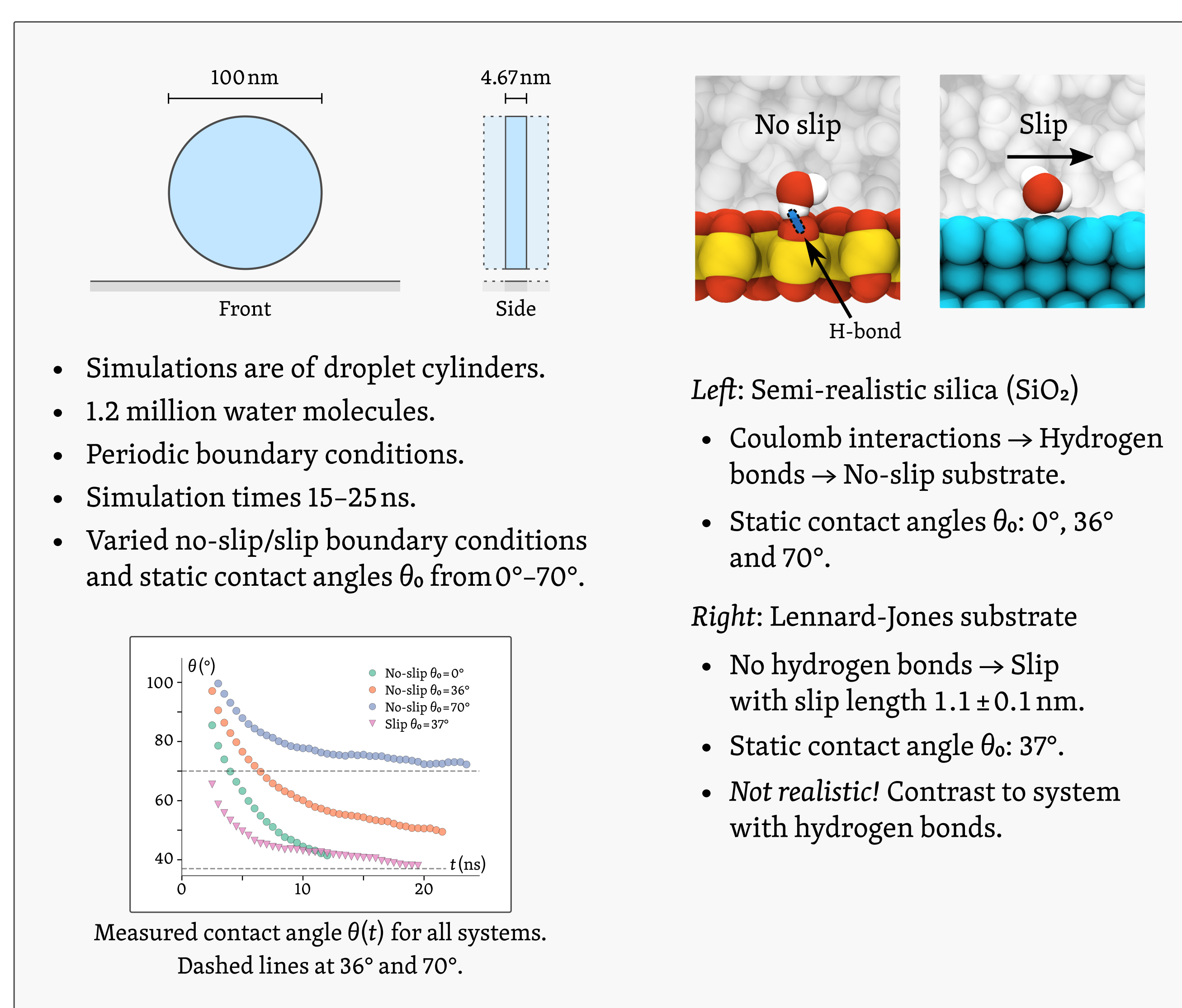
MODE 2: JUMPING (MKT)



Molecule B jumps to an adjacent lattice site through a thermal fluctuation (molecular kinetic theory).

Barrier (mostly) related to *energetics*, not dynamics.

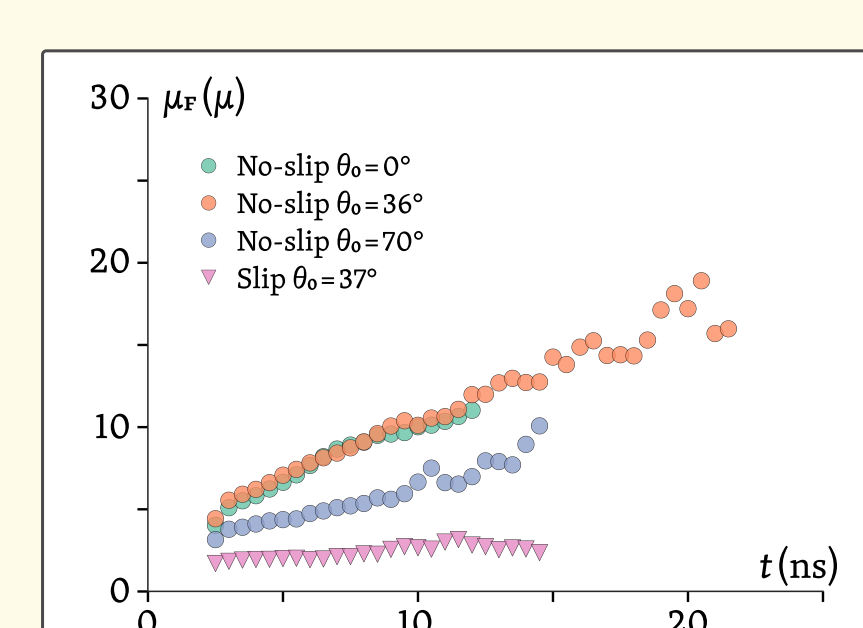
These modes contribute equally to advancement in late stage wetting



Contact line friction accounts for dissipation in the contact line region.

The dissipation rate is characterized by a parameter μ_F in units of viscosity.

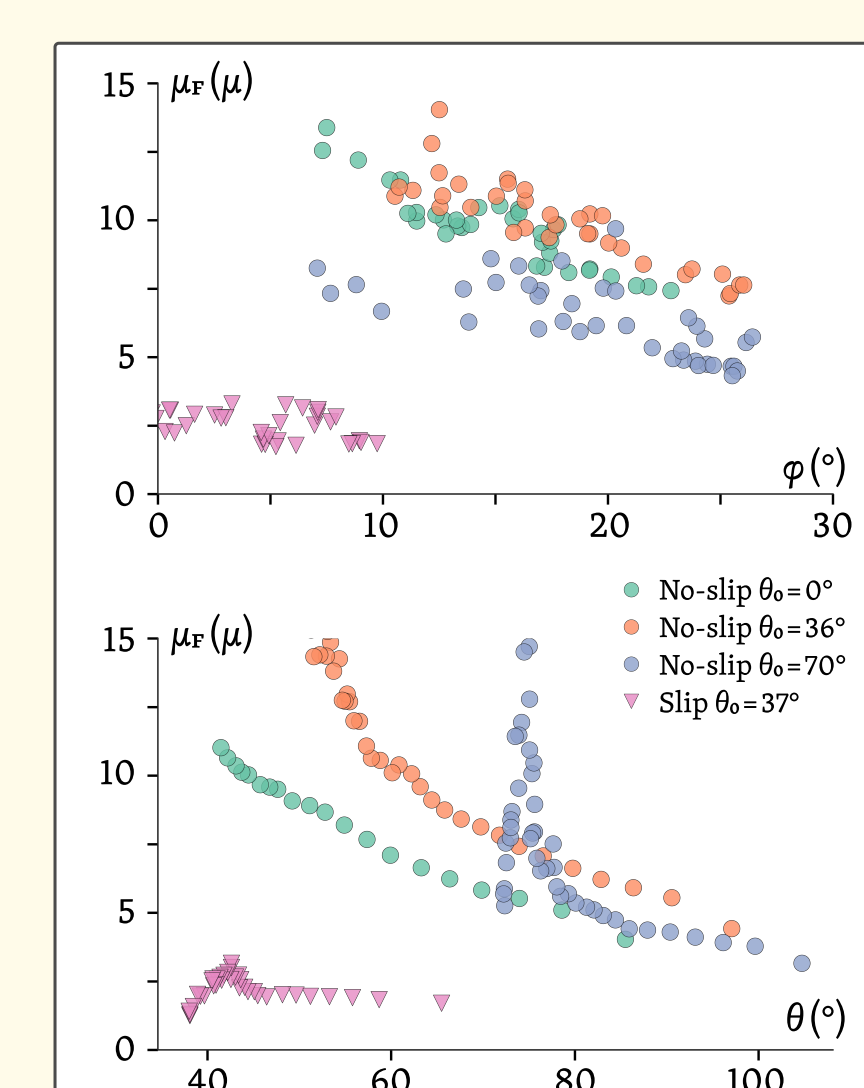
Measuring μ_F shows that it is constant when the liquid can slip but otherwise for no-slip systems.



The measured flow angle φ is a good predictor of the μ_F change. This suggests that contact line friction is related to the difficulty in advancing through MODE 1: A purely molecular effect.

A liquid which slips opens up another mode of advancement, consistent with this data.

Other parameters cannot describe the change as well.



$\dot{E}_\mu$: Rate of contact line dissipation.

$\dot{E}_\gamma$: Rate of free energy gain from wetting.

Measuring the two rates and comparing them shows that contact line friction accounts for a substantial part of the total dissipation.

We thus assert that contact line friction is important to consider when modeling realistic wetting dynamics.

