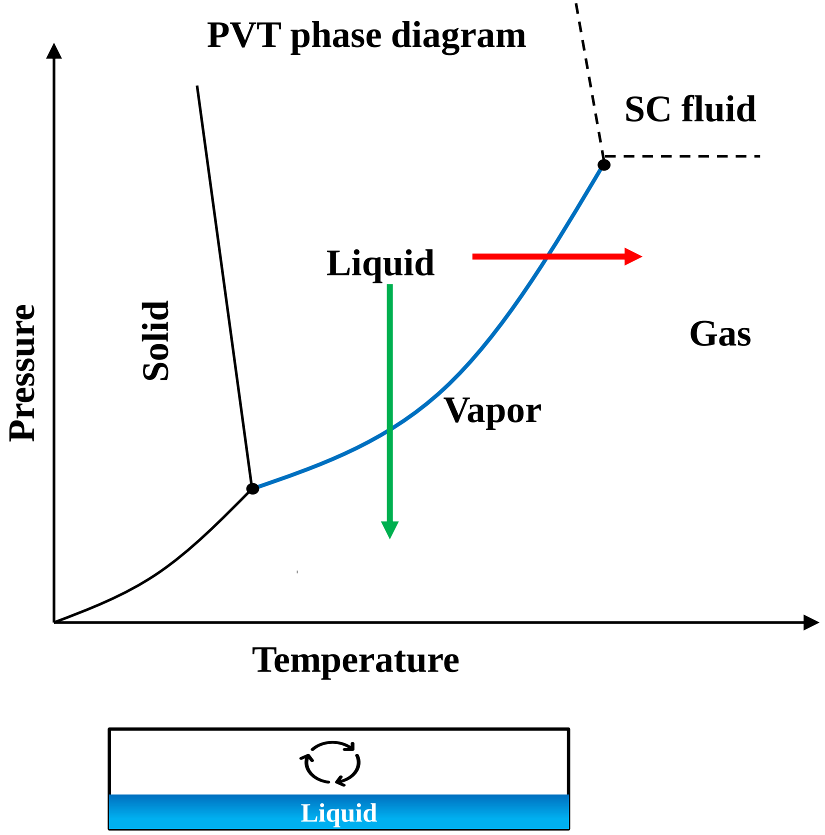
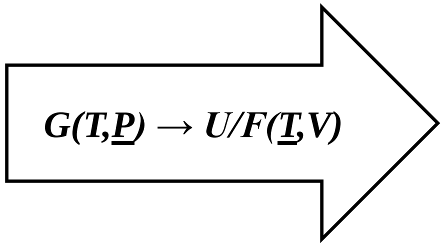
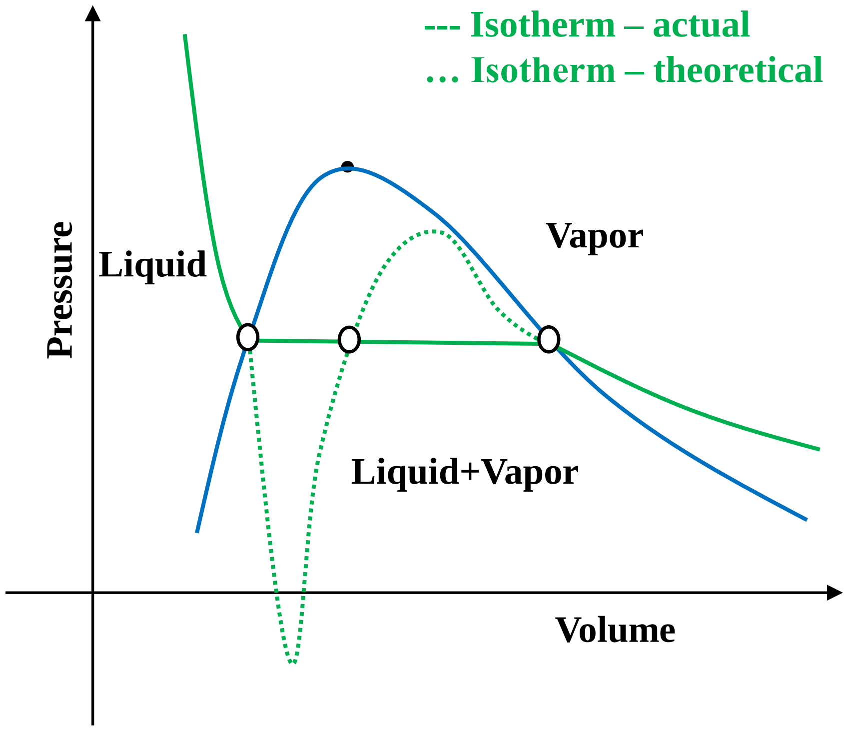
Cavitation in Nanoconfinements

Vapor pressure, boiling and cavitation

Definition

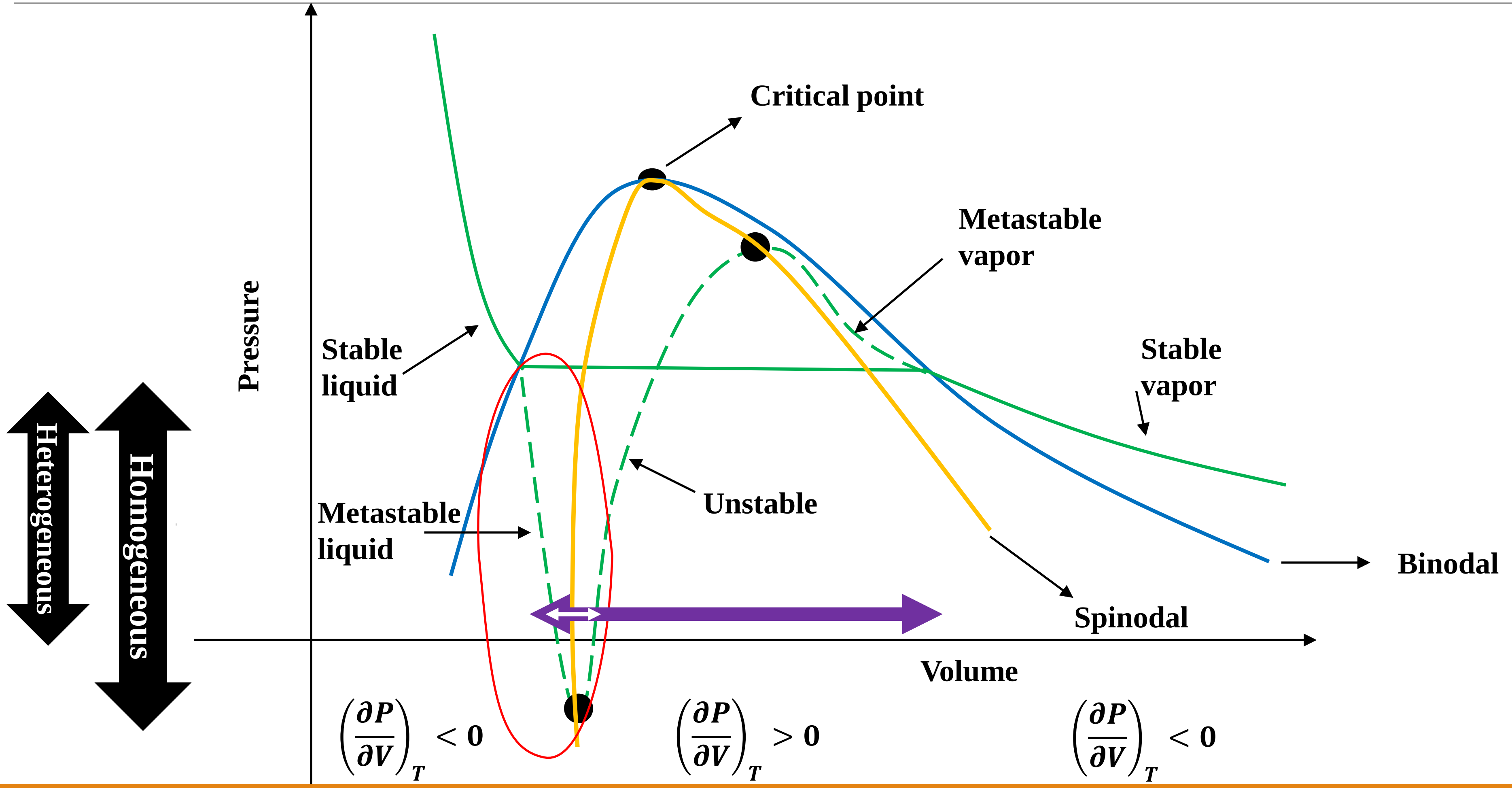






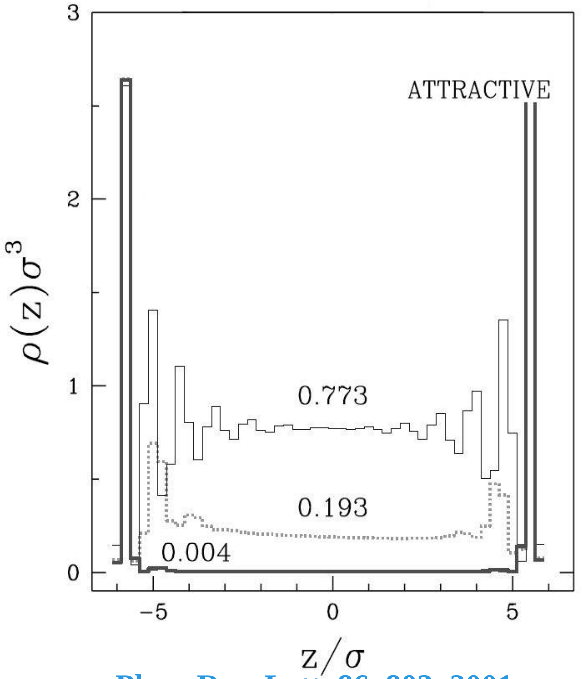
P/T–V diagram

Inclusive of confinement

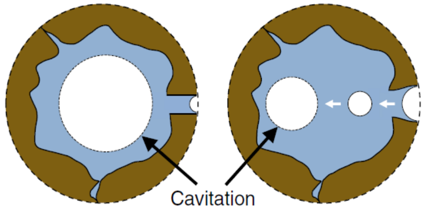


Cavitation

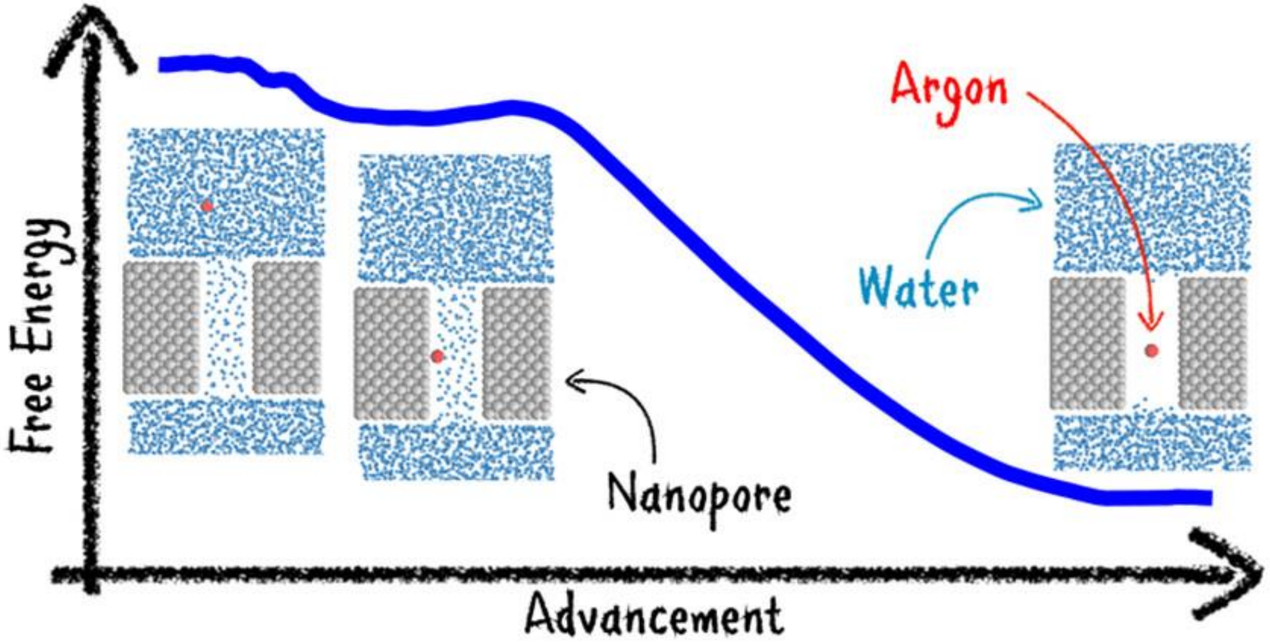
Examples



Phys. Rev. Lett. 86, 803, 2001



J. Geotech. Geoenviron. Eng., 2021, 147(8): 04021079



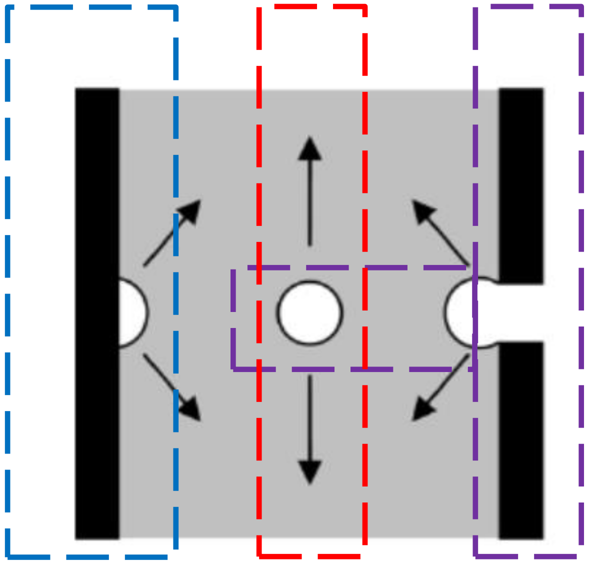
J. Phys. Chem. Lett. 2020, 11, 21, 9171–9177

Cavitation

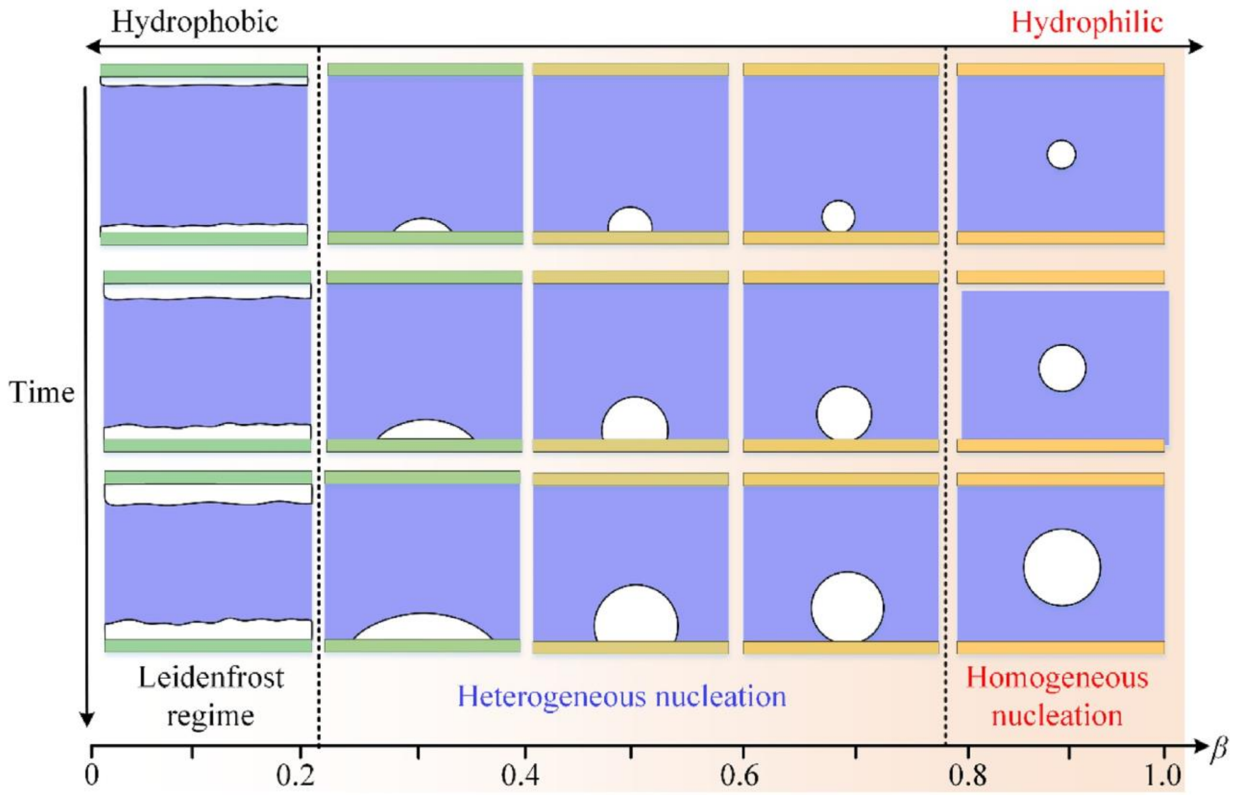
Recapping what's known

1. Velocity slippage
2. Solid-Liquid affinity

Cohesive forces



Imperfections:
Entrapped bubbles,
Surface texture,
Edge/Defects,
Contaminations,
Etc.



C. R. Physique 7 (2006) 1018–1026

International Journal of Thermal Sciences 145 (2019) 106033

Experimental Specs

Observations and simulation motives

Silica frits pore diameter: **1 – 10 microns**

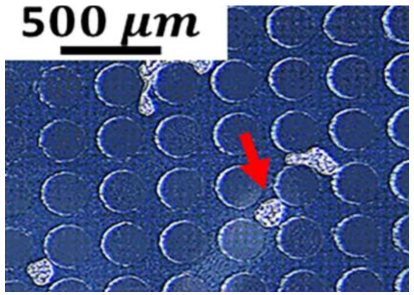
Silica frits thickness: **3.3 – 4 millimeter**

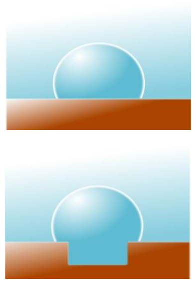
Hydrophilic internal surface (Silica frits and glass Pyrex)

Pressure dropdown / flow induced via **continuous evaporation**

Interruptions in flow / evaporation rate / bubbles

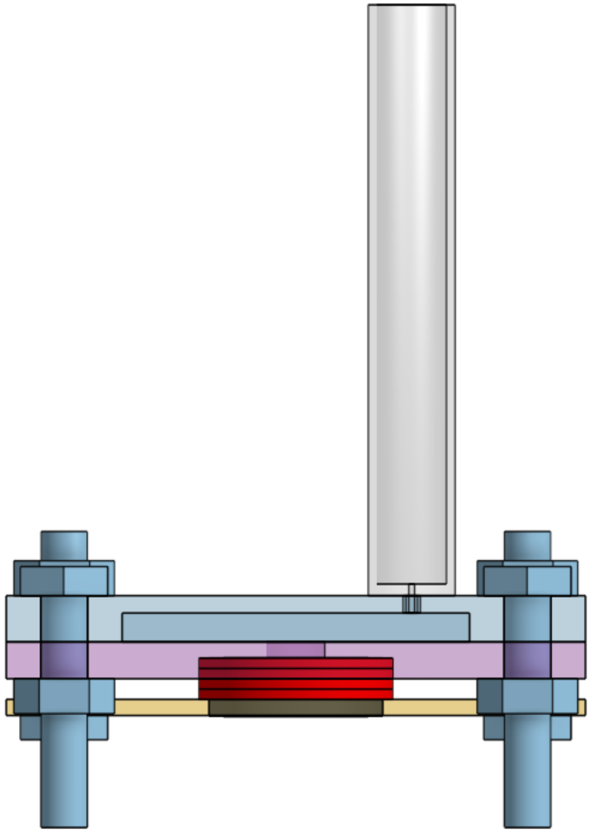
Properties of evaporation front





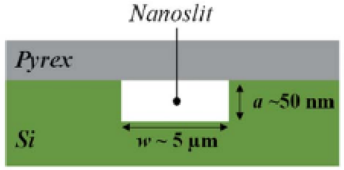
Morphology:

1. **Frits internally**
2. **Frits/Frits**
3. **Frits/Pyrex**



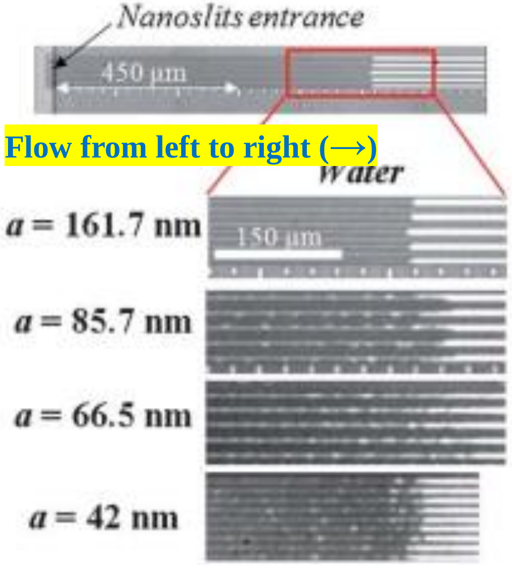
Flow Interruption

Where confinement loss effect



Chemically Homogeneous Surface
(Uniform Solid-Liquid Affinity)

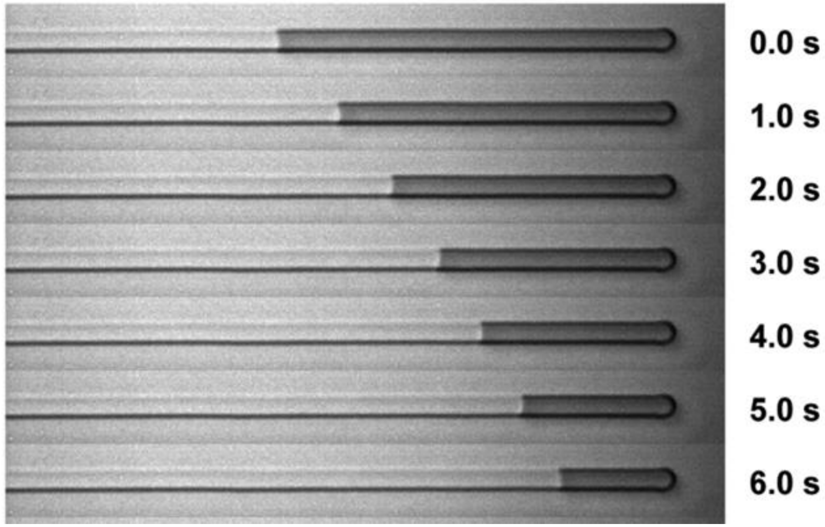
Silicon glass = hydrophilic



Flow from left to right (⟶)

[Soft Matter, 2012,8, 10738-10749]

Silicon nanochannels: *L*=1000µm, *W*=3µm, *H* > 115 nm

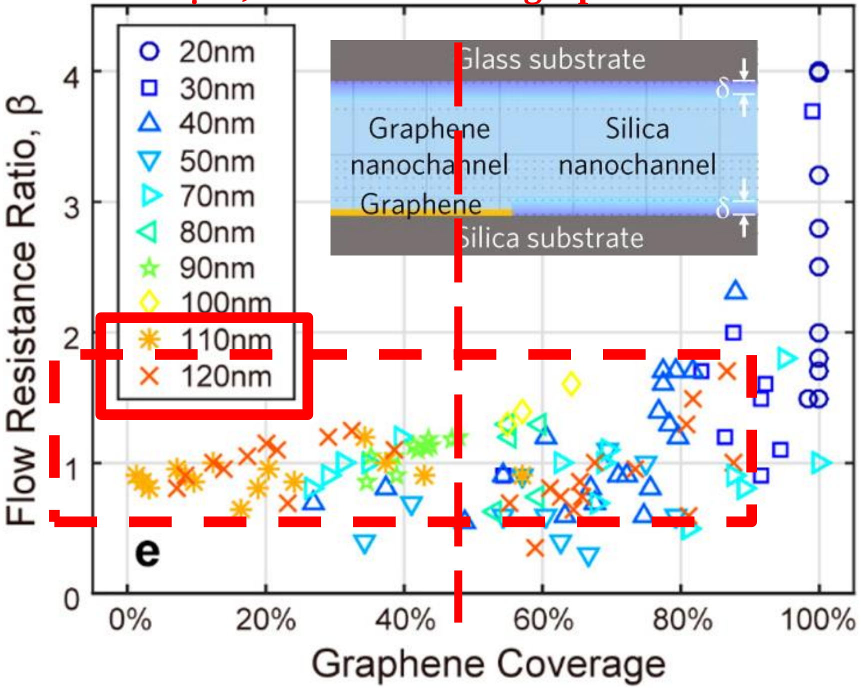


Flow from right to left (⟵)

[Langmuir 2017, 33, 8395−8403]

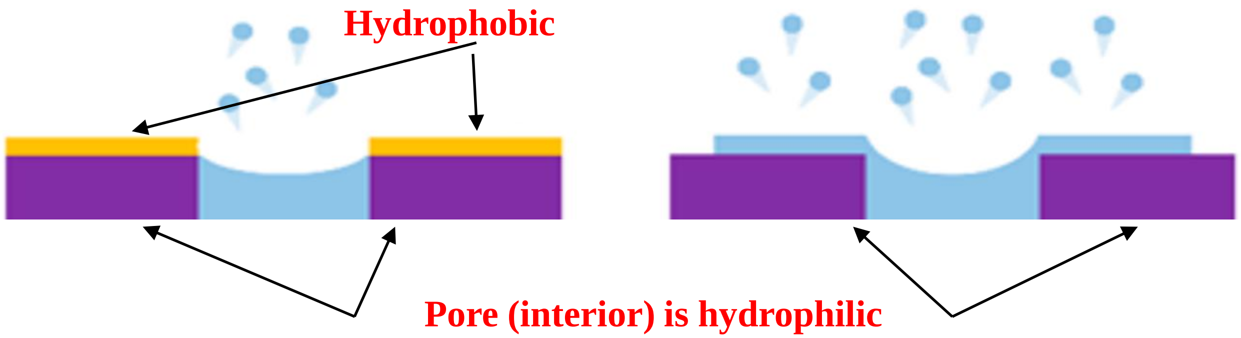
Chemically Heterogeneous Surface
(Nonuniform Solid-Liquid Affinity)

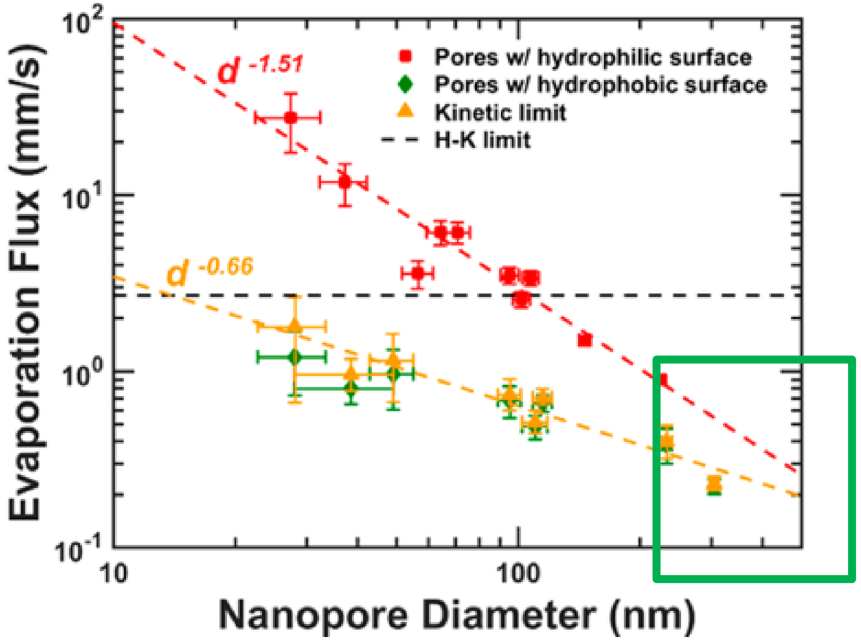
As in left; leftmost bottom% is graphene
L=400µm, *W*=*H*= labels on graph



[Nature Nanotechnology, 2018, 13, 238–245]

Chemical Heterogeneity
Evaporation Zone

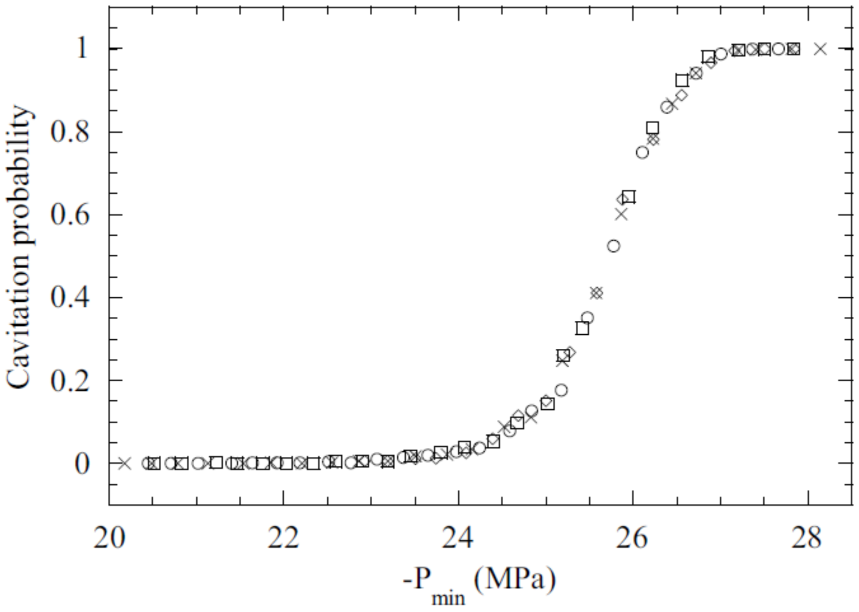




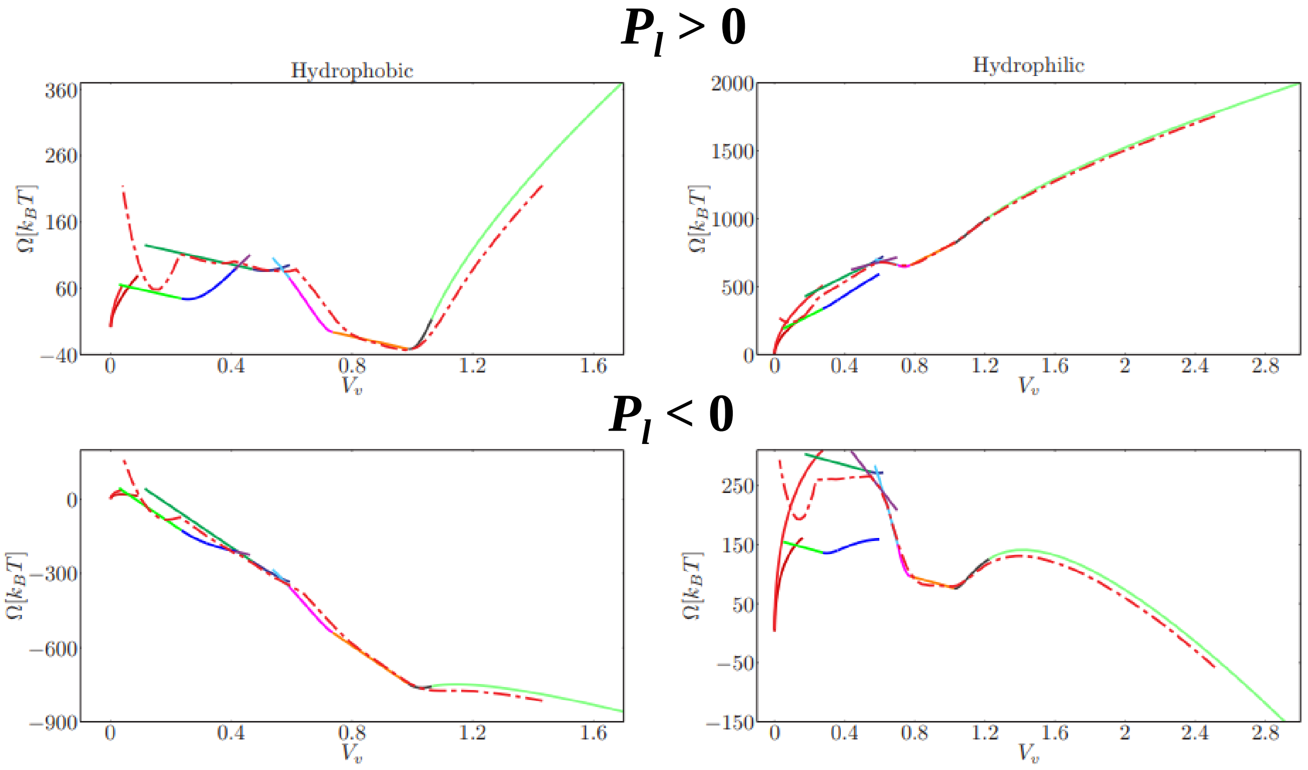
[ACS Nano 2019, 13, 3363−3372]

Chemical/Physical Heterogeneity

Liquid response



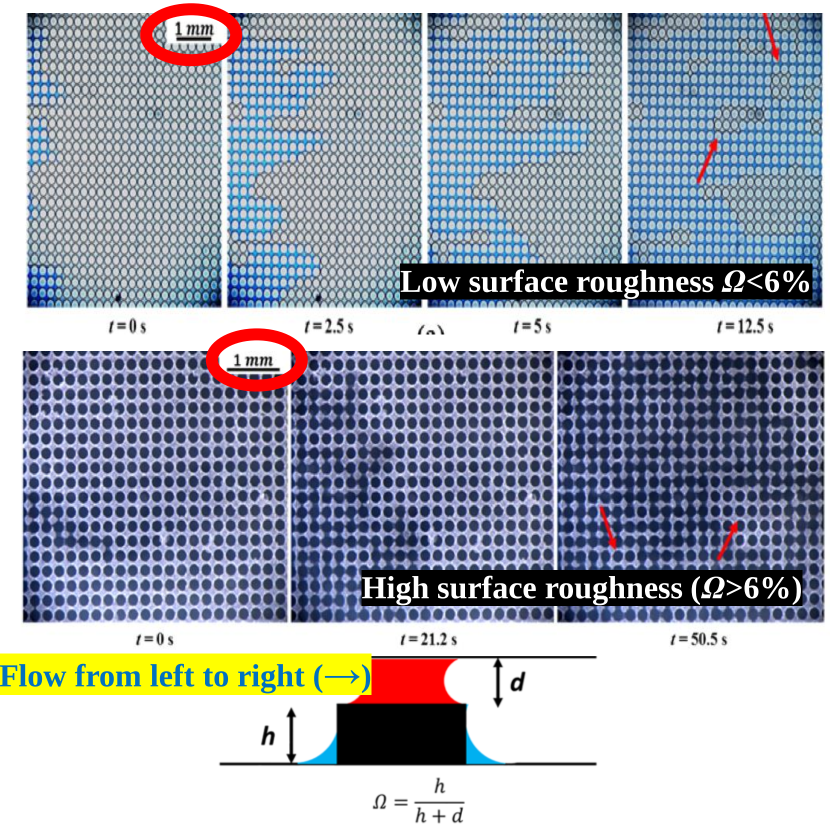
J. Chem. Phys. 133, 134505 (2010)

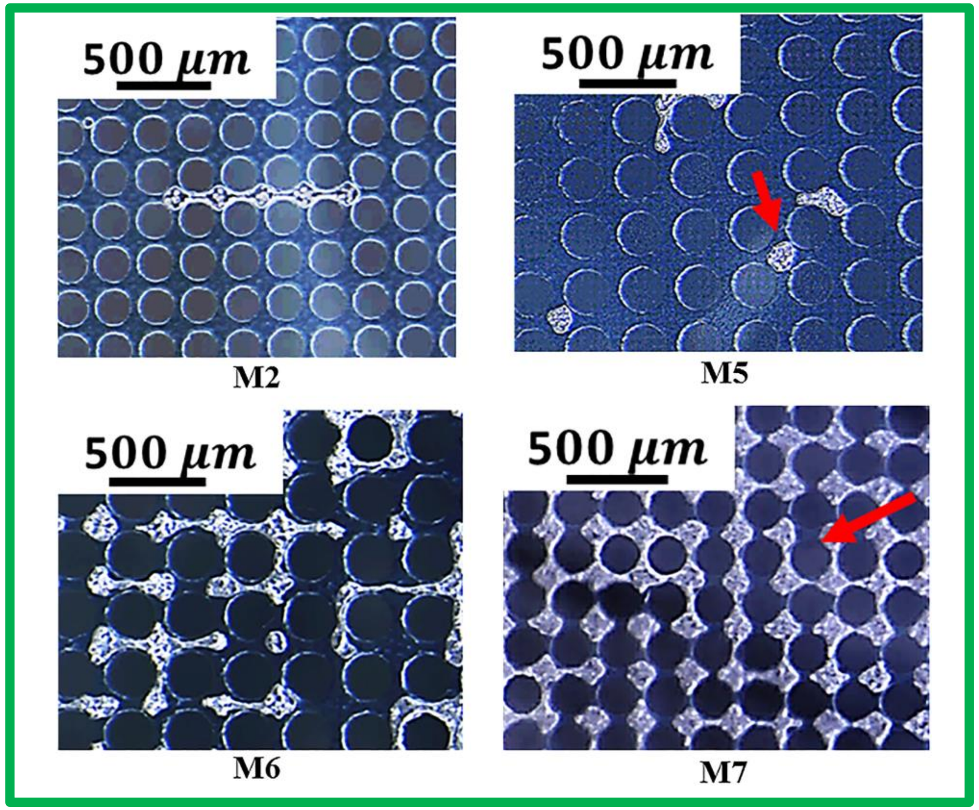


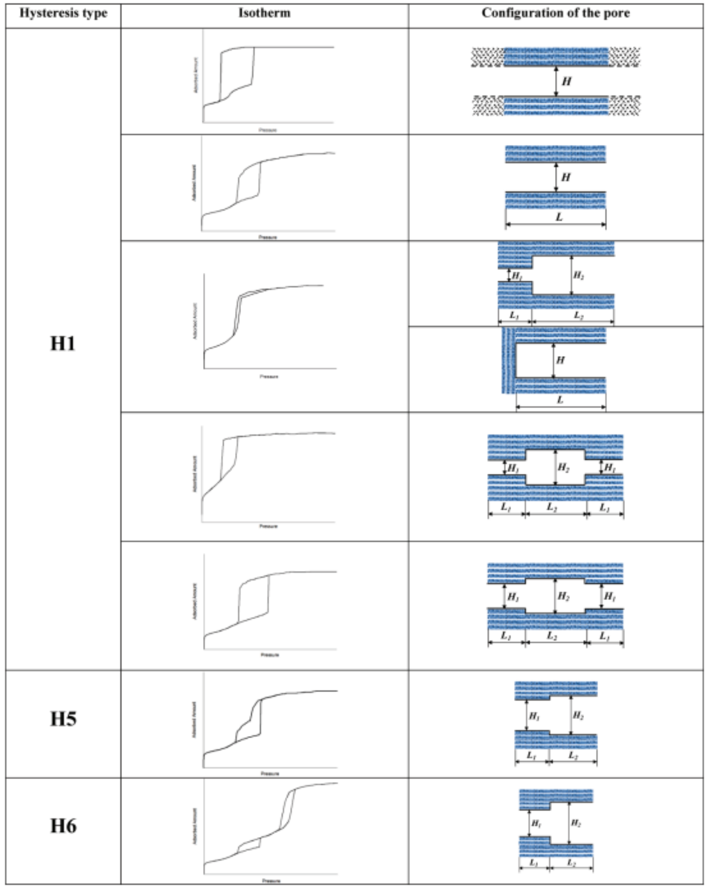
Soft Matter, 2016,12, 3046-3055

Chemical/Physical Heterogeneity

Morphology/Microstructure





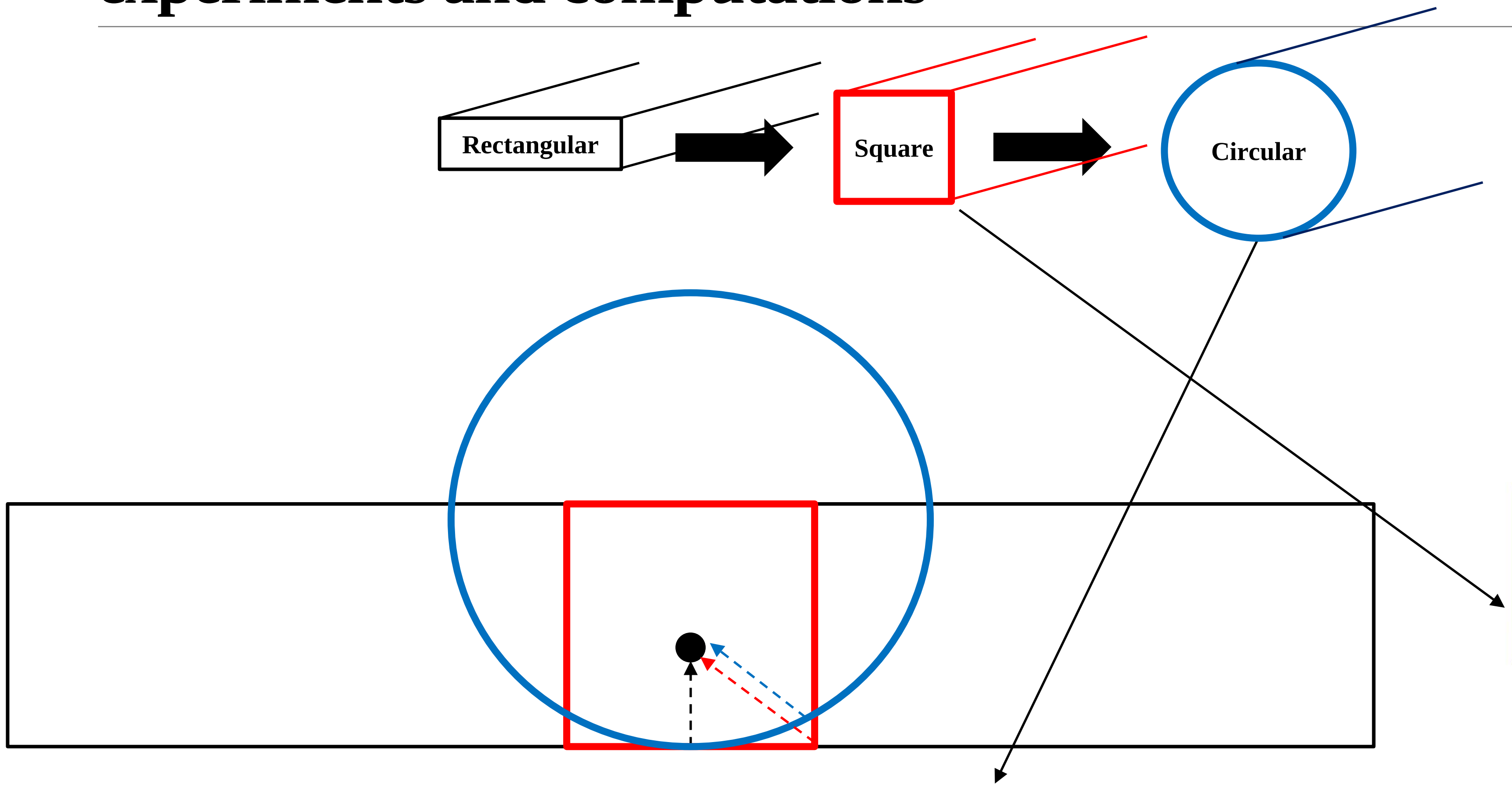


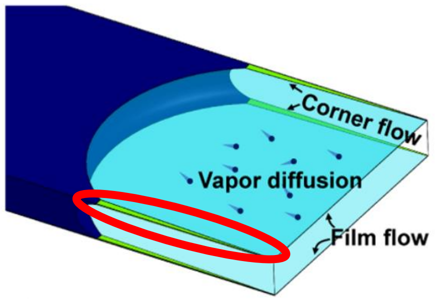
[Water Resources Research, 55, 9905–9925, 2019]

[Langmuir 2011, 27, 7, 3511–3526]

Pore Geometry Preferred

experiments and computations



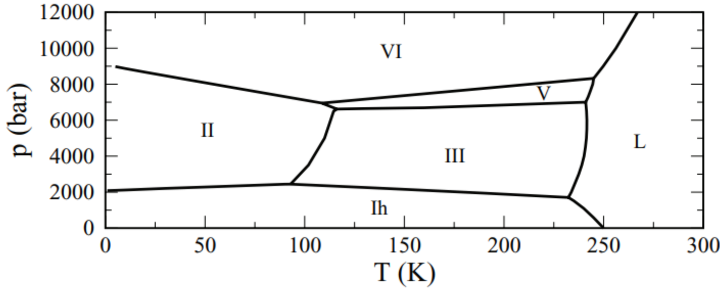


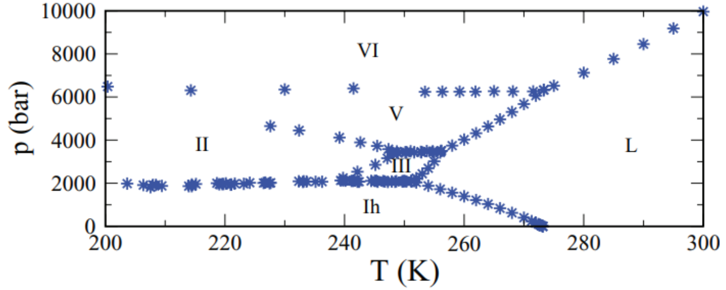
Langmuir 2017, 33, 8395−8403

Site-averaged interatomic potential

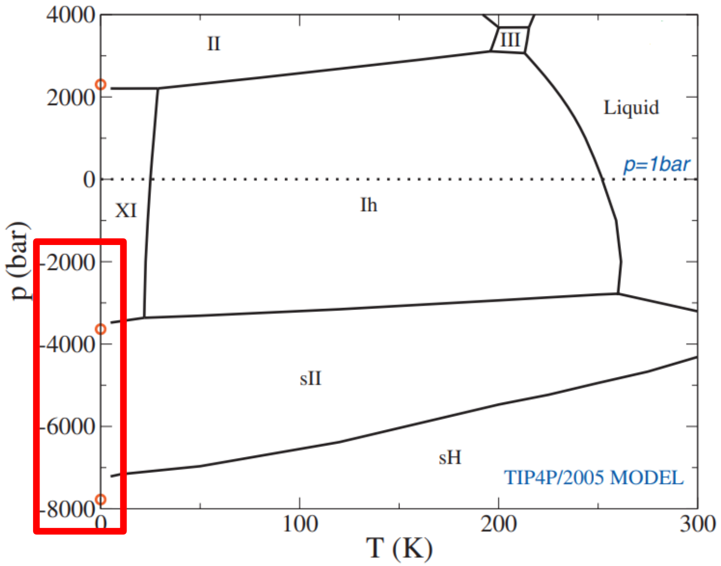
Water model

The **TIP4P/2005** (*NIST*) model (a LJ site for the O, and three charge sites).

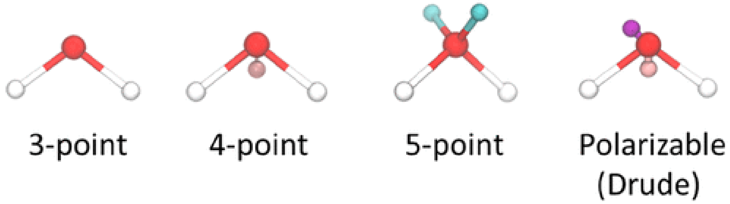




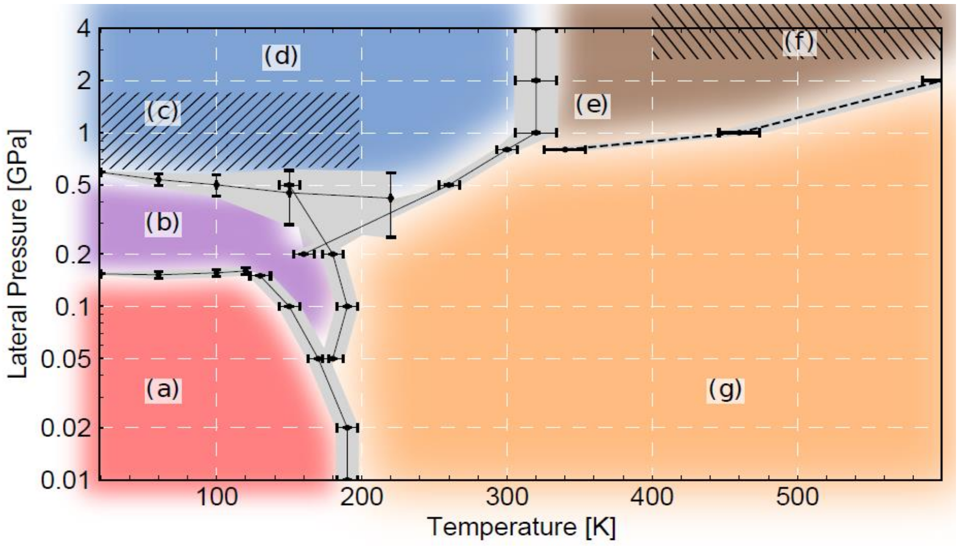
J. Chem. Phys. 139, 154505 (2013).

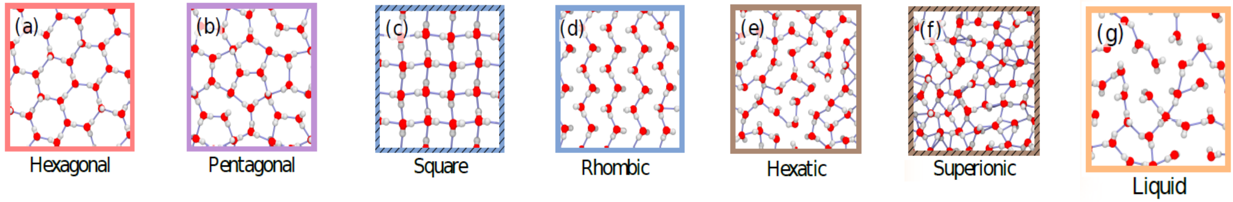


J. Chem. Phys. 131, 034510 (2009).



J. Chem. Inf. Model. 2021, 61, 9, 4521–4536





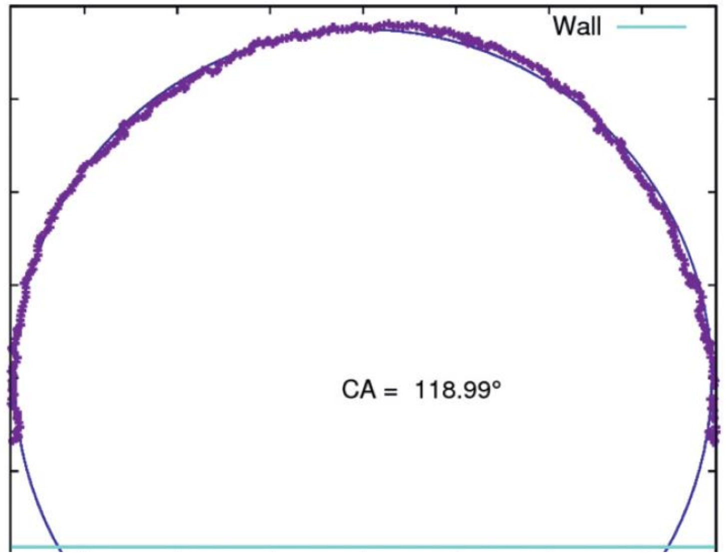
arXiv:2110.14569v1 [cond-mat.mtrl-sci]

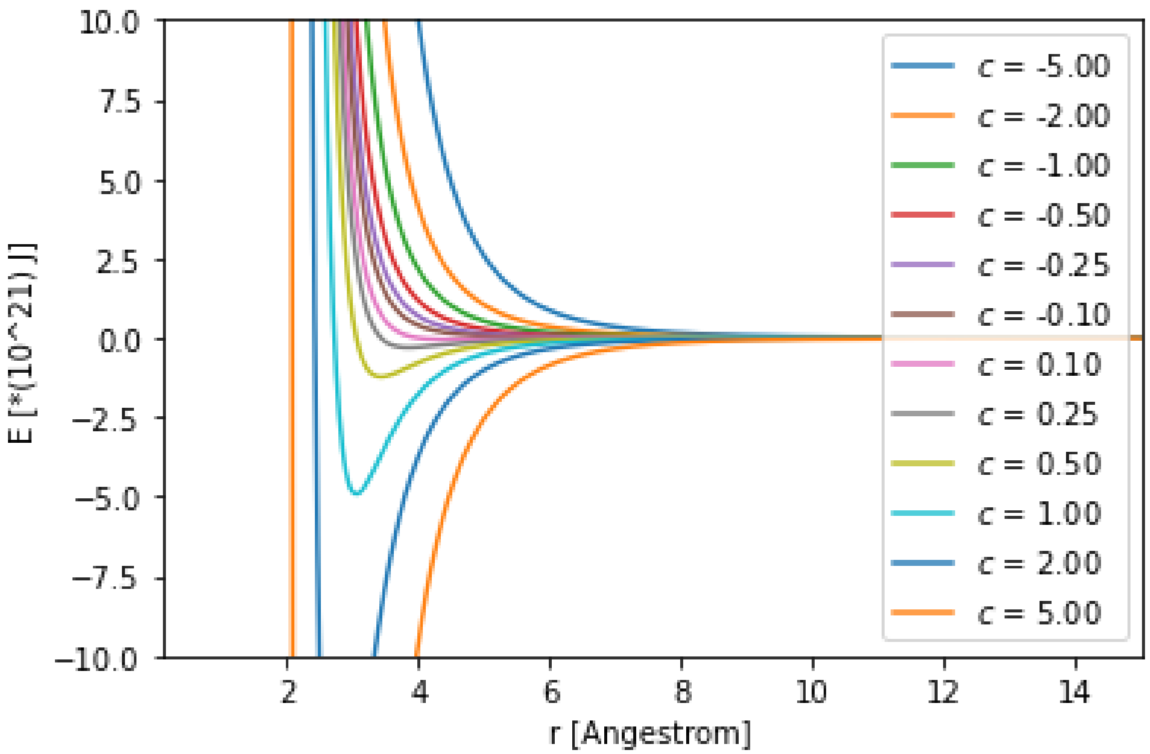
Surface model

The **TIP4P/2005** model in (hydrophobic/hydrophilic) pore / nano-confinement

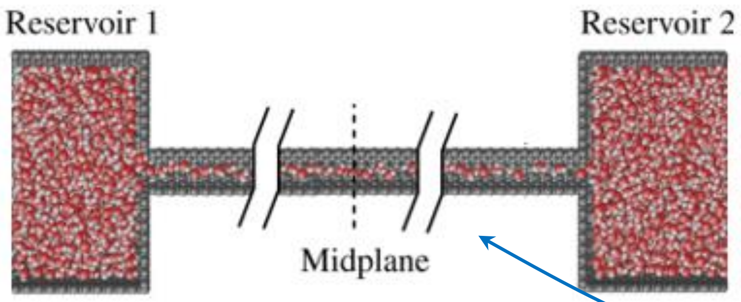
$$V(r_{ij}) = 4\epsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - c\left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

PNAS November 28, 2017 114 (48) E10266-E10273

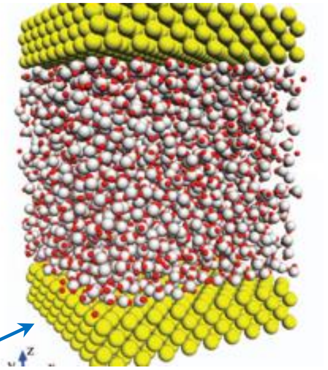




Inducing pressure dropdown/flow



Pore geometry:
1. Remains fixed
2. Changes



Phys. Rev. Lett. 102, 184502

J. Chem. Phys. 136, 134104 (2012)

Creating a pressure drop over pore:

1. Removing (directing to the other) particles (*N*) from one reservoir
2. Applying a piston on left/rightmost side of reservoirs
3. Fixing *P* via NPT and letting chambers *V* change (pseudo piston)

Creating flow (in addition to above):

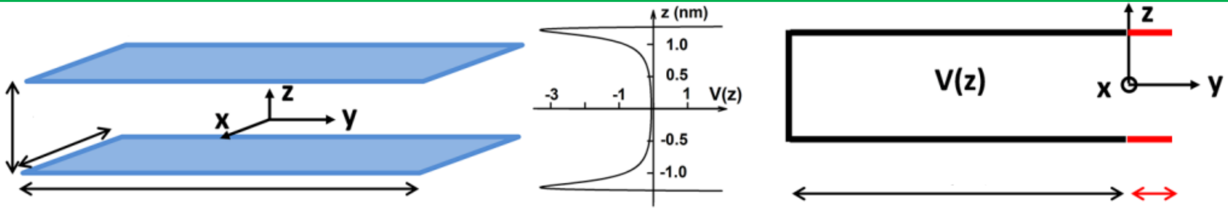
1. Applying fixed force to all particle in the pore w/out reservoirs

Creating a pressure drop:

1. Moving both or one of the walls vertically
2. Removing particles (*N*) from one side
3. Adding an acceptable long empty part for evaporation and vapor diffusion

Creating flow (in addition to above):

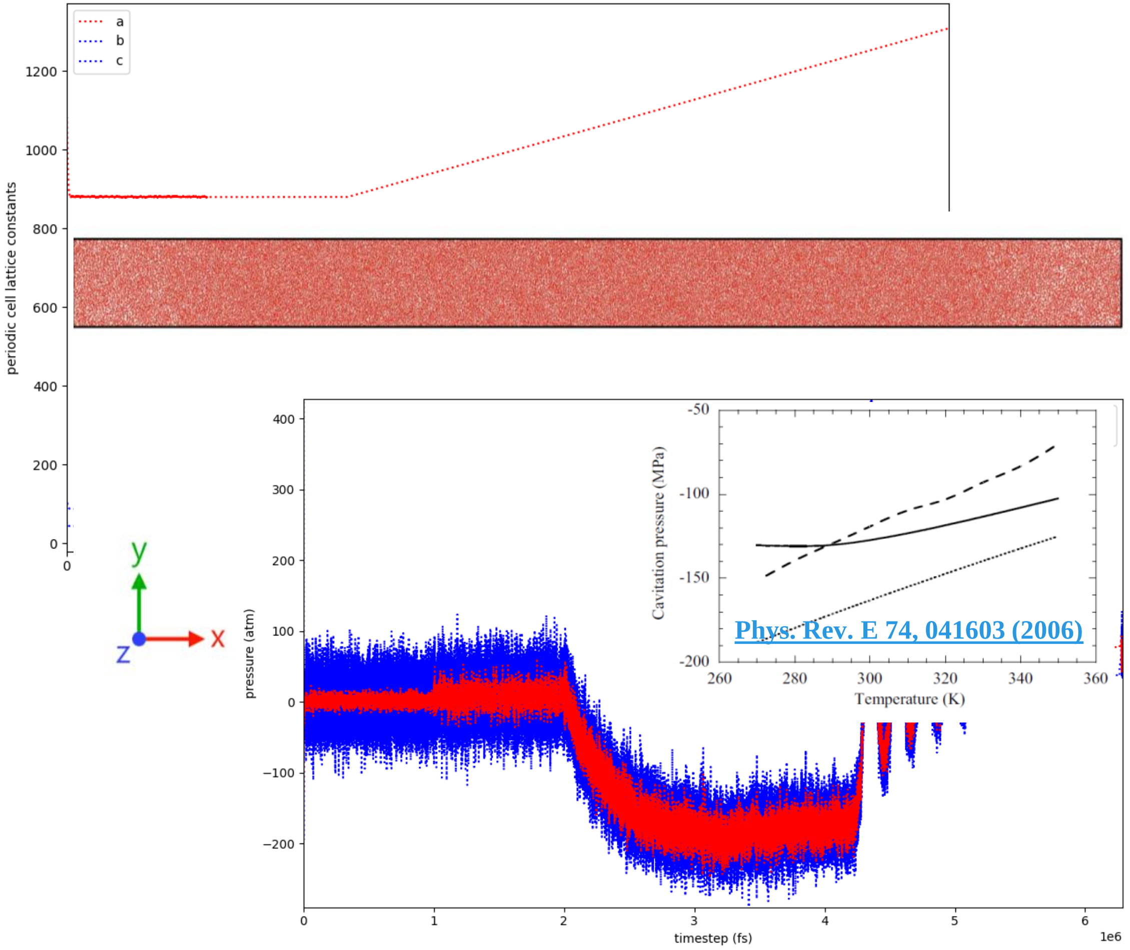
1. Applying fixed force to all particle



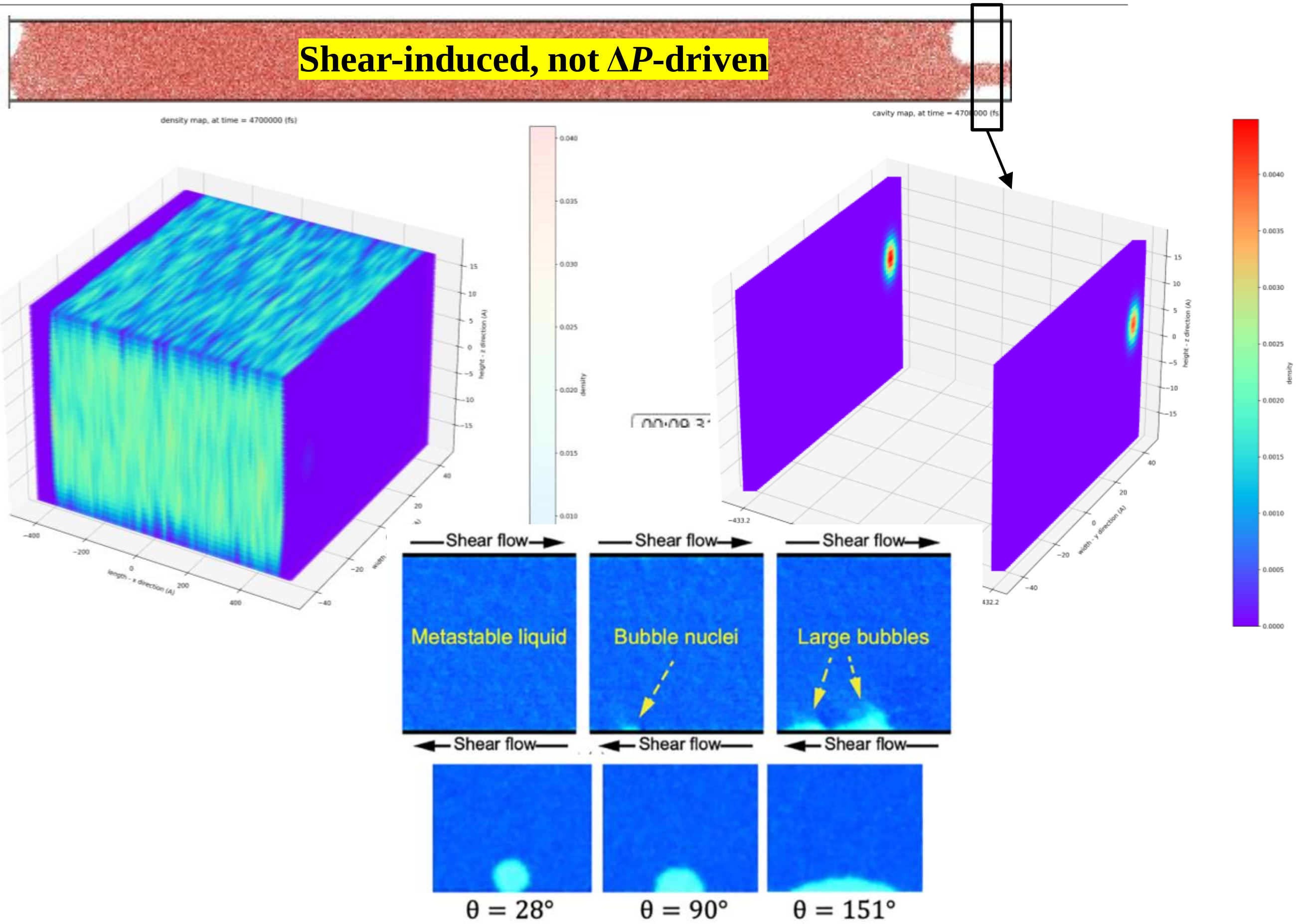
AIP Advances 11, 095311 (2021)

Pressure dropdown/Flow

inducing via expansion ! (OK in bulk)



[Phys. Rev. E 74, 041603 (2006)]



[Sci Adv. 2020;6, eaaz0504.]