Institute of Physics
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Steering fluid motion with gradient substrates

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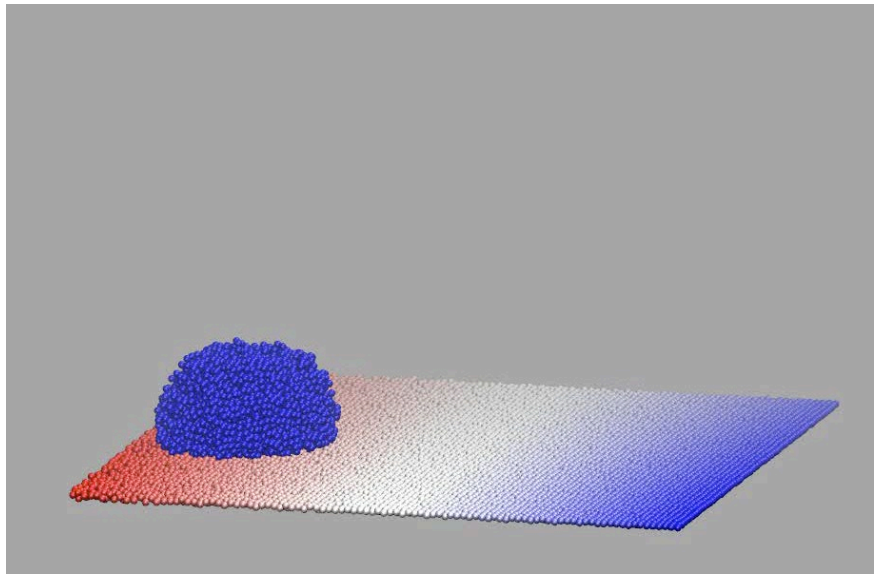


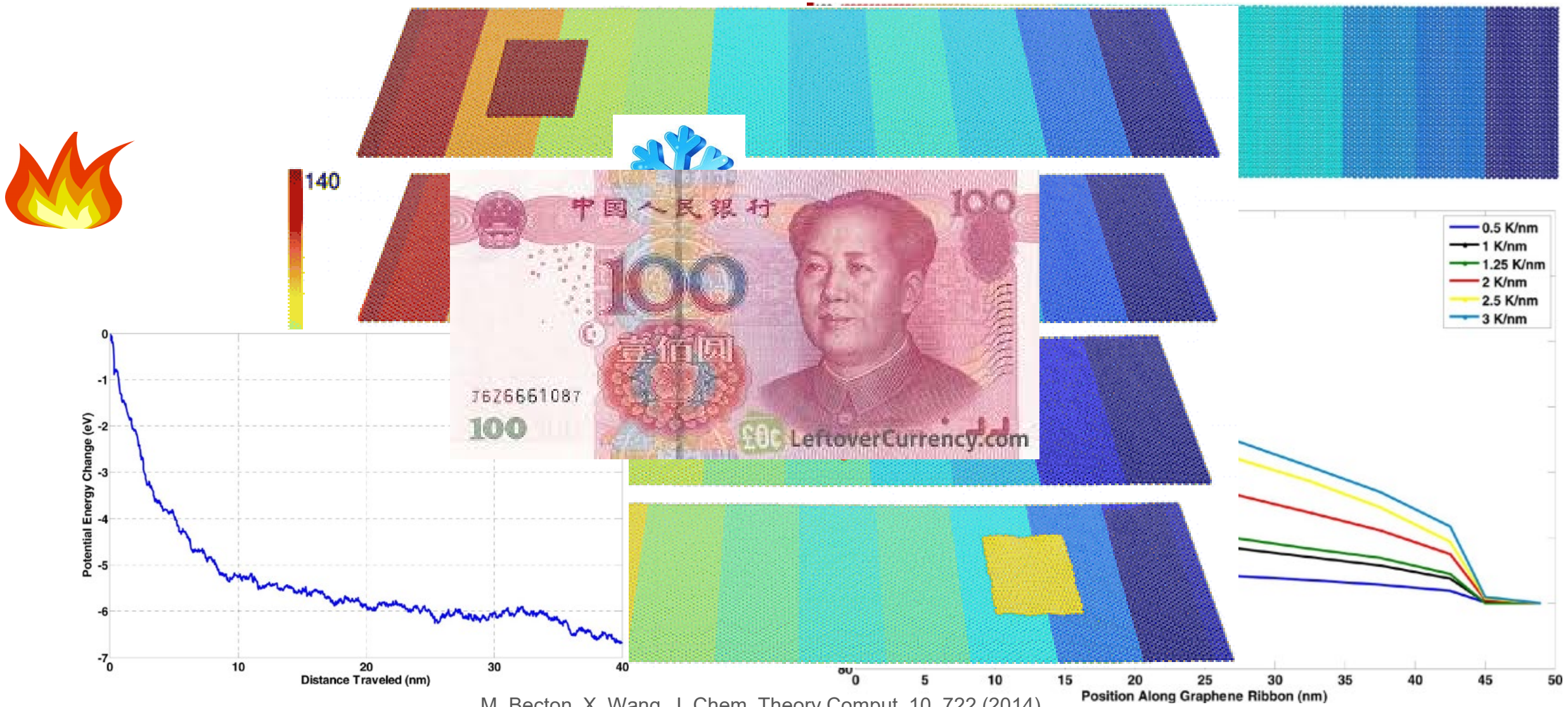
Durotaxis

THE JOURNAL OF CHEMICAL PHYSICS **146**, 244705 (2017)

Stiffness-guided motion of a droplet on a solid substrate

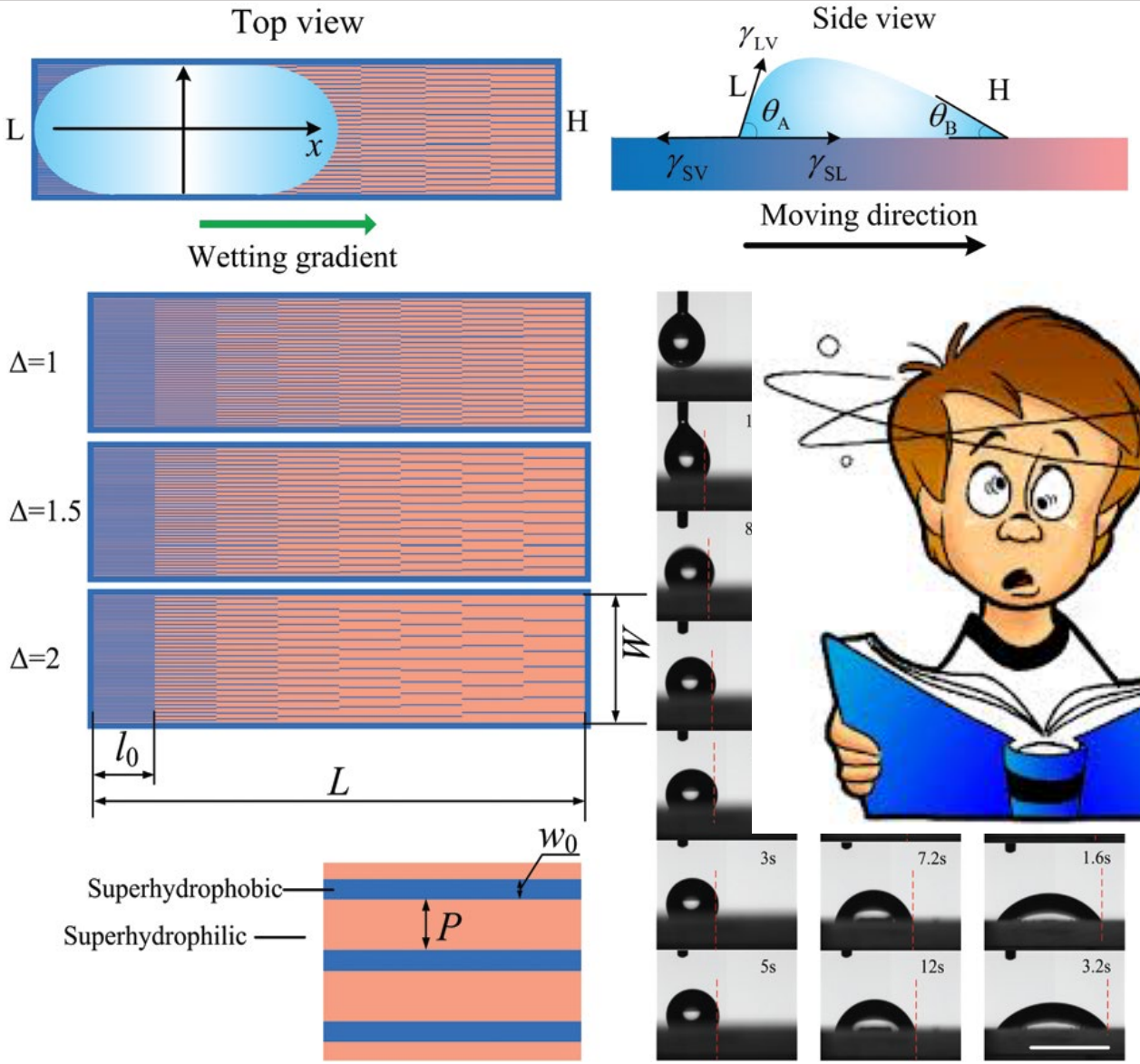
Panagiotis E. Theodorakis,[1,a)] Sergei A. Egorov,[2,3,b)] and Andrey Milchev[4,c)]

Thermotaxis



M. Becton, X. Wang, J. Chem. Theory Comput. 10, 722 (2014)

Wettability gradient



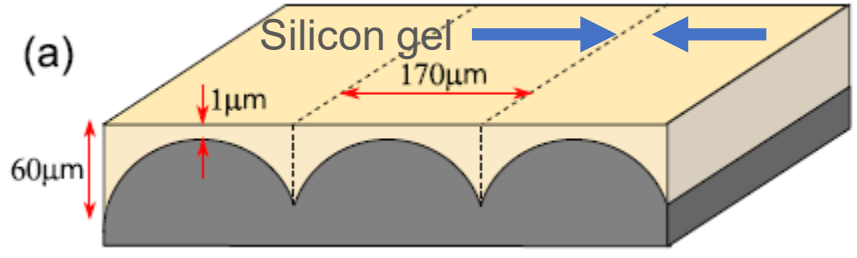
Gradient induced by tuning the parameters:

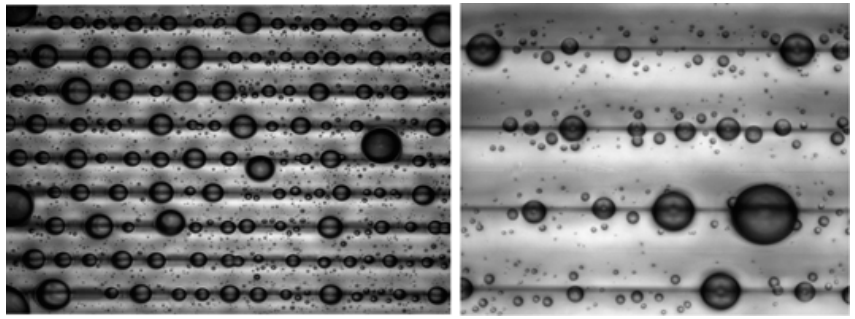
- Distance P
- Distance l_0
- Distance L
- Distance w_0

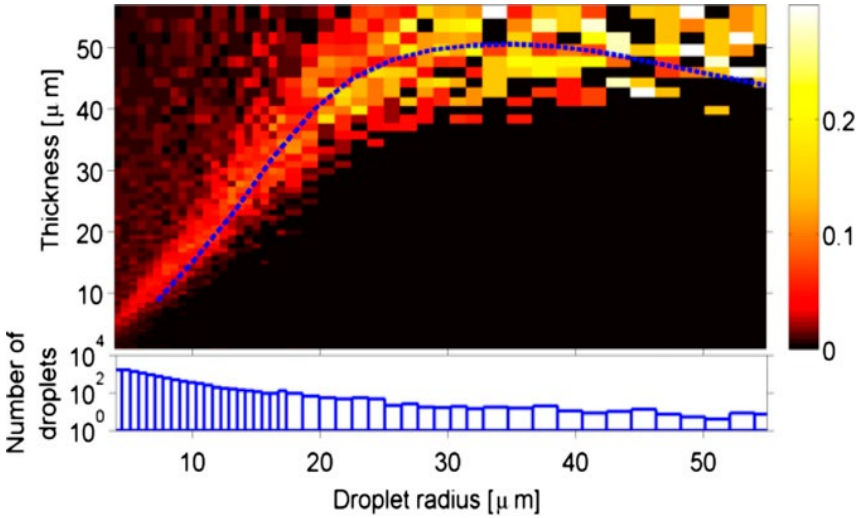
onversion from *super-hydrophobic* *super-hydrophilic* when the TiO_2 atings were modified with tri methoxy octadecyl silane (TMOS) were exposed to ultraviolet light.

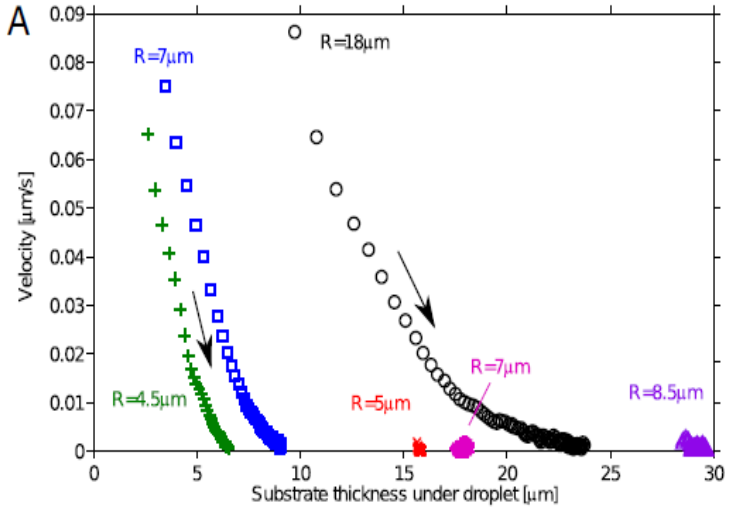
Wu et al.Soft Matter 13, 2995 (2017)

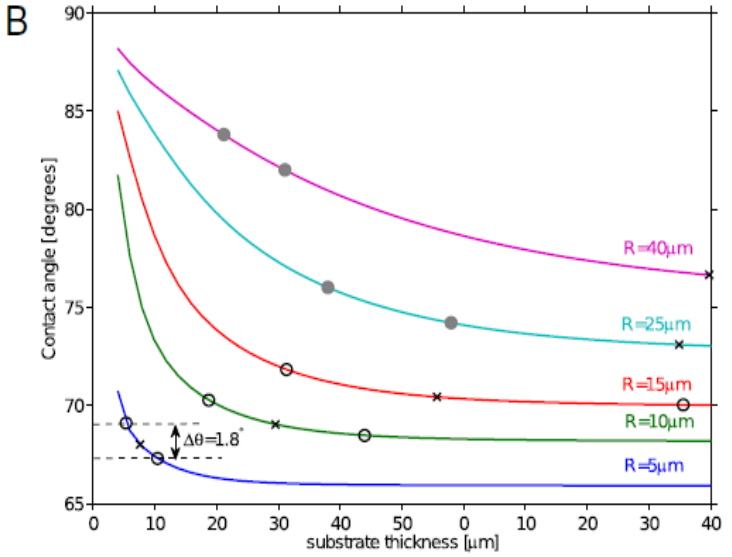
Durotaxis (Experiment)









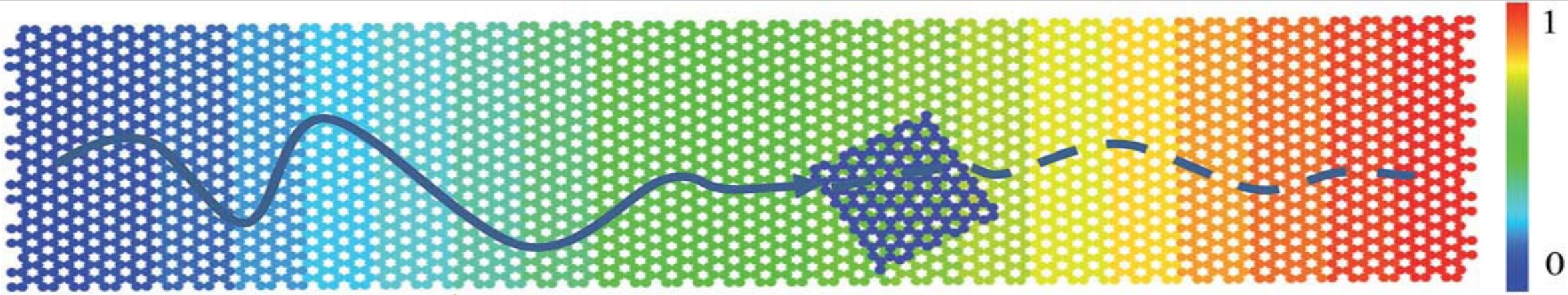


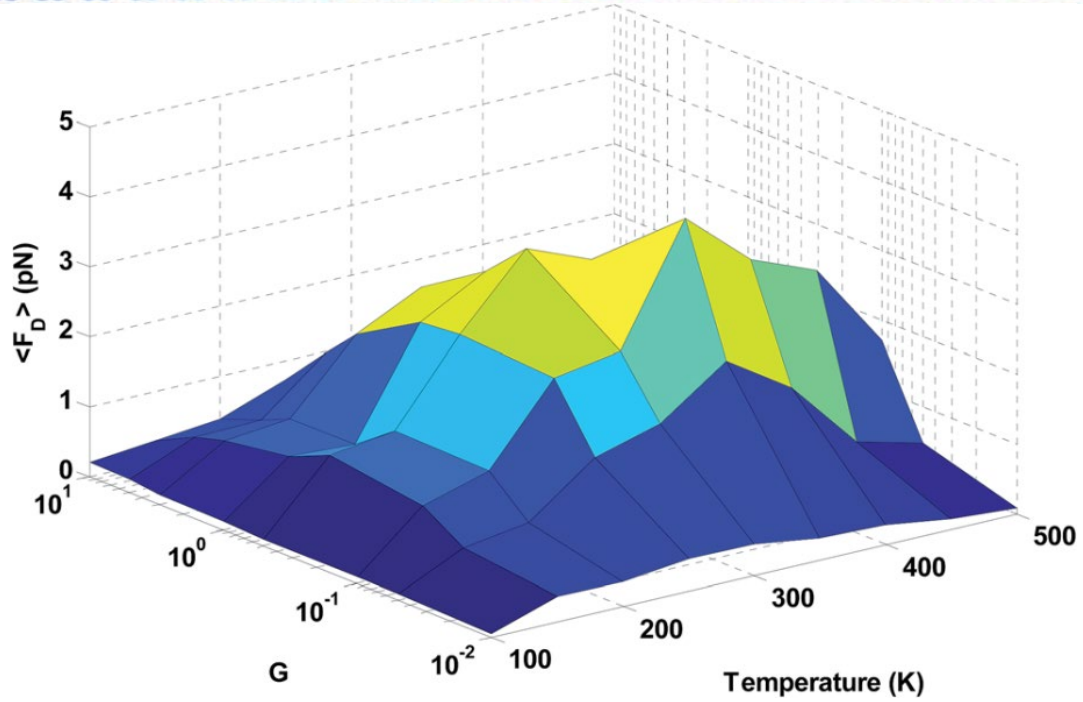
1. Droplets move from stiff to soft regions of the substrate!

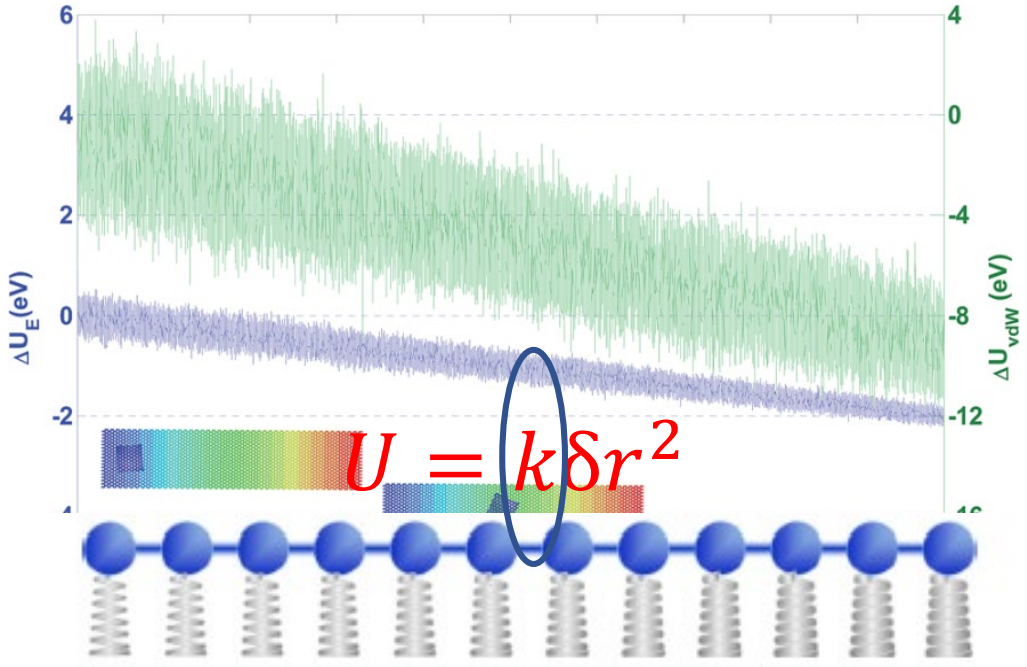
2. Larger droplets ⟹ better durotaxis!

R. W. Style et al. PNAS 110, 12541 (2013)

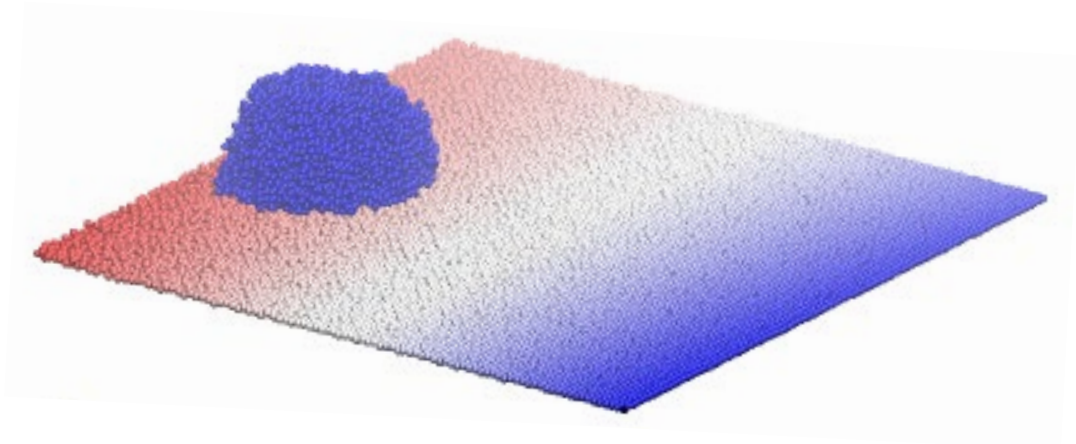
Durotaxis (simulation)







Our model



Parameters to consider:

- The stiffness gradient
- Affinity of droplet to the substrate
- Droplet size
- Viscosity of the droplet

Molecular Dynamics Simulations (Langevin Thermostat)

$$m\frac{d\vec{v}_i}{dt} = \vec{F}_i(t) - \xi\vec{v}_i(t) + \vec{F}_i^{\,R}(t)$$

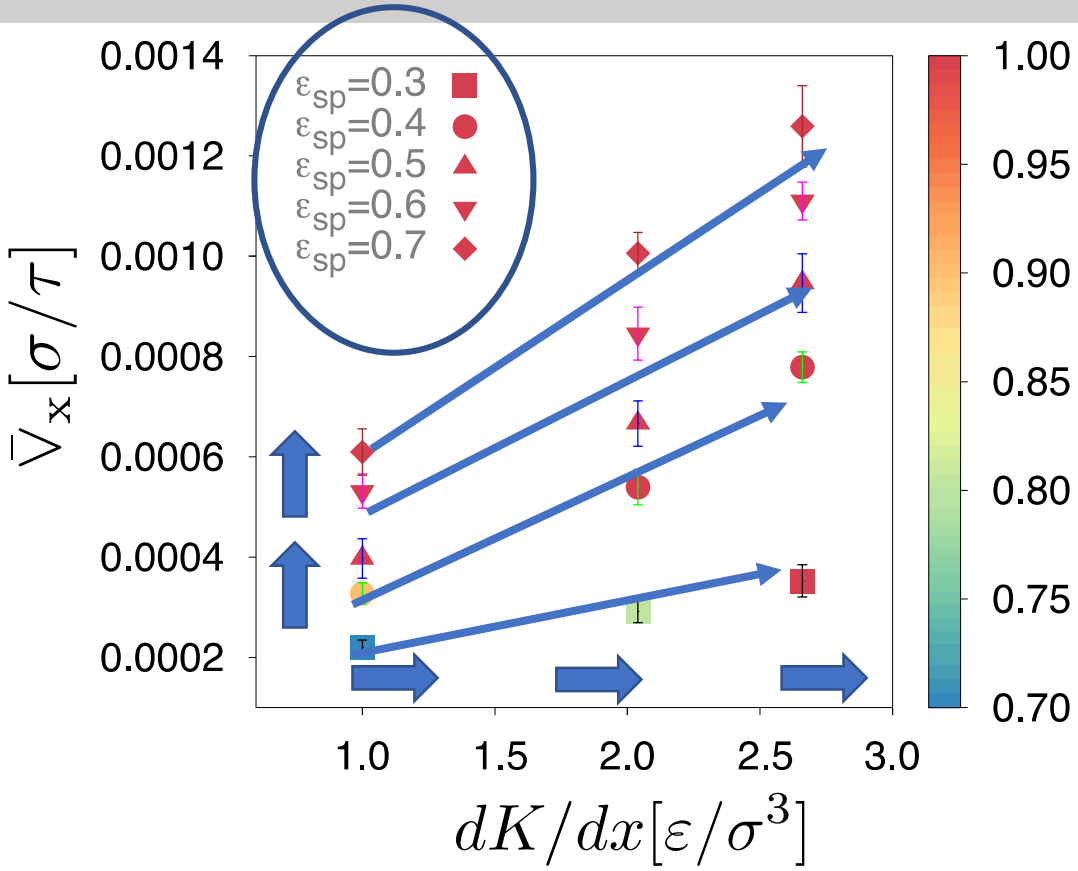
$$U_{LJ} = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right]$$

$$\left\langle \vec{F}_i^{\,R}(t)\vec{F}_i^{\,R}(t')\right\rangle = 6\xi k_B\delta(t-t')$$

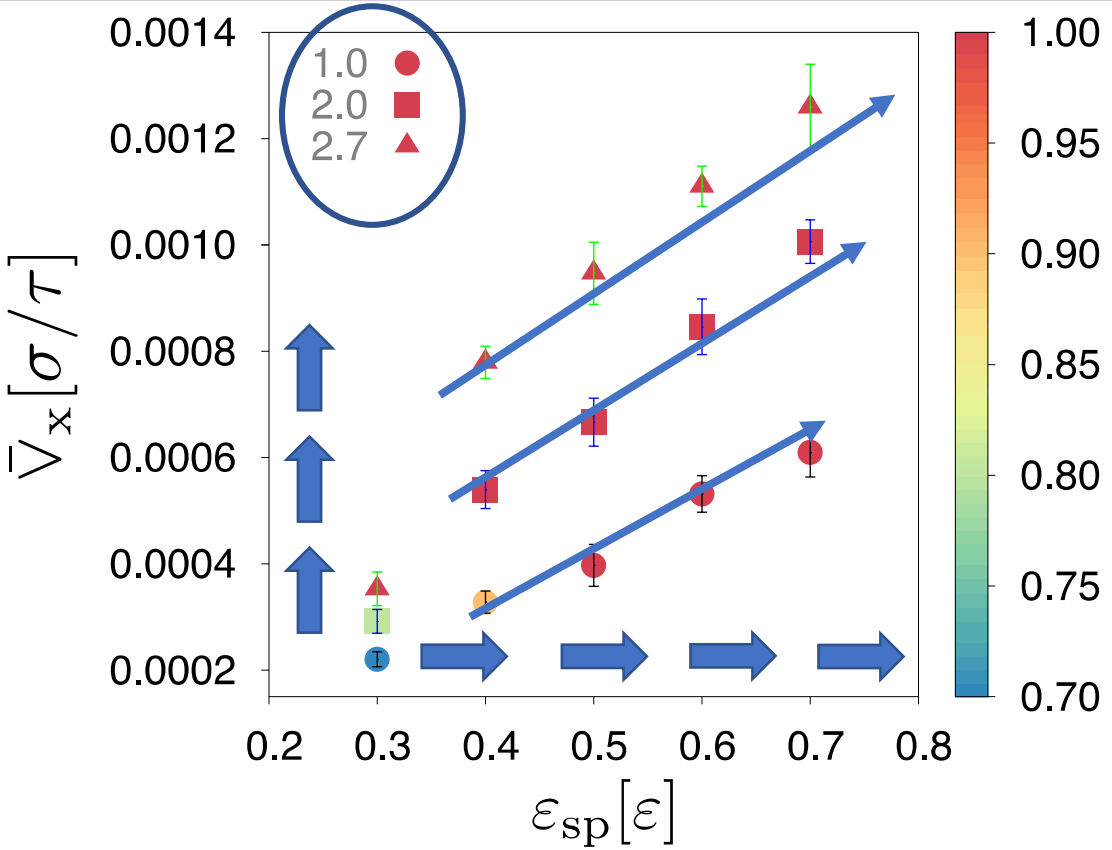
$$\left\langle \vec{r}_i(t)\right\rangle = 0$$

$$U_{FENE} = -k_{FENE}\frac{R_0^2}{2}\ln\left[1-\left(\frac{r}{R_0}\right)^2\right]$$

Effect of the stiffness gradient and the substrate wettability

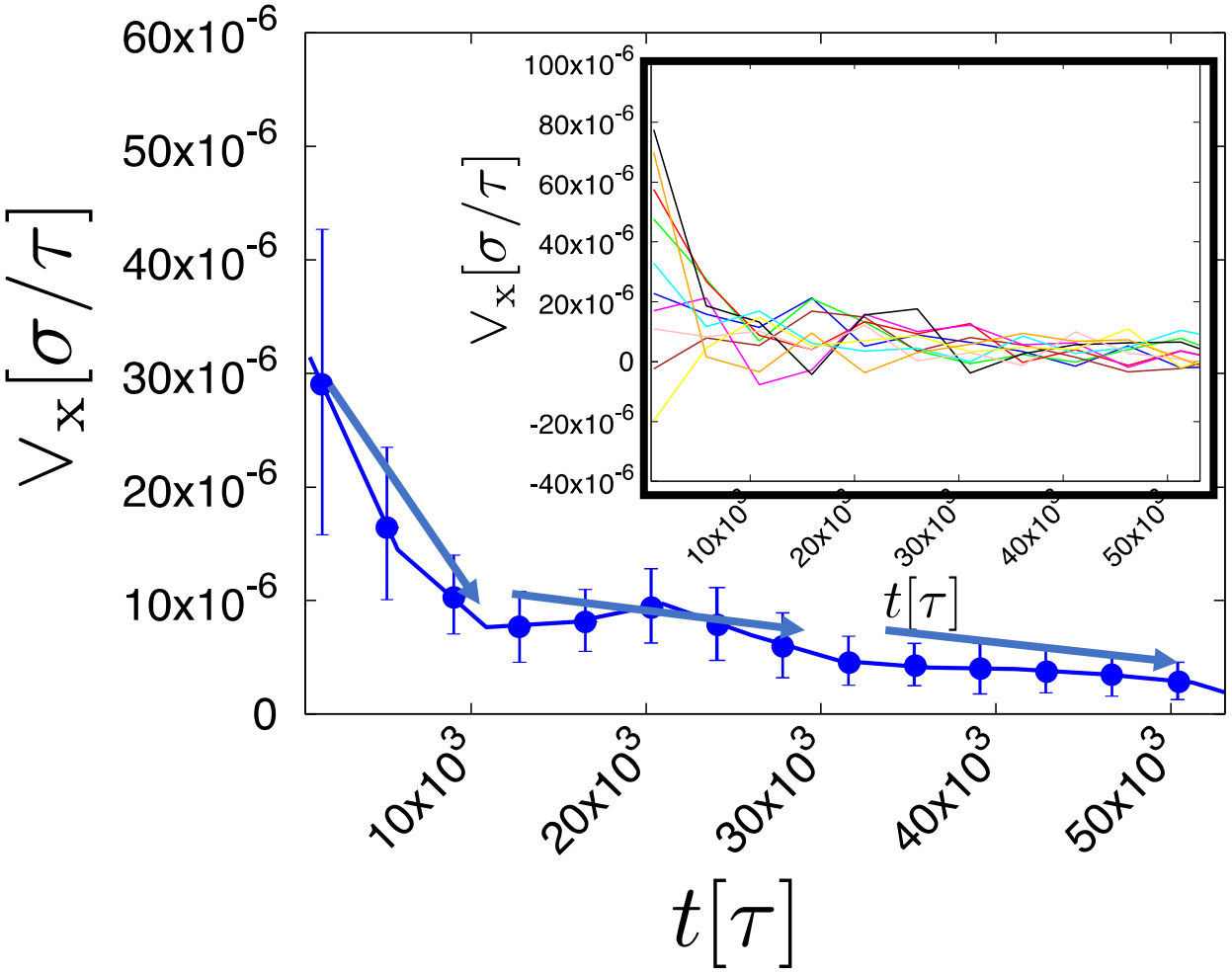


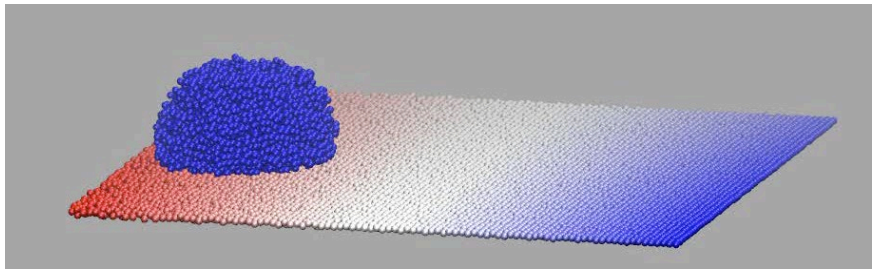
Larger gradient ⟹ better durotaxis for all substrate – droplet affinities (tuned by ε_{sp})



Higher affinity between the substrate and the droplet ⟹ better durotaxis for all substrate – droplet affinities (tuned by ε_{sp})

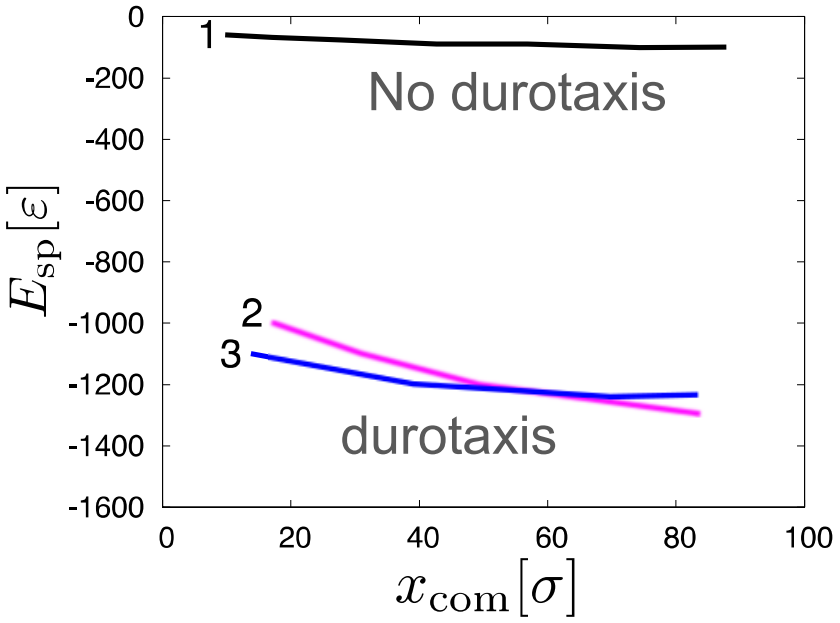
Instant velocity during durotaxis

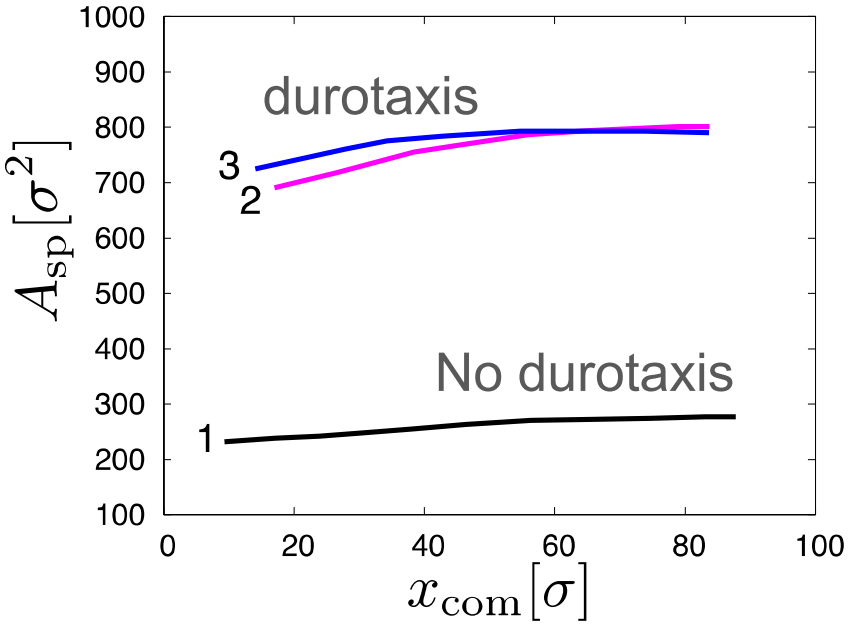


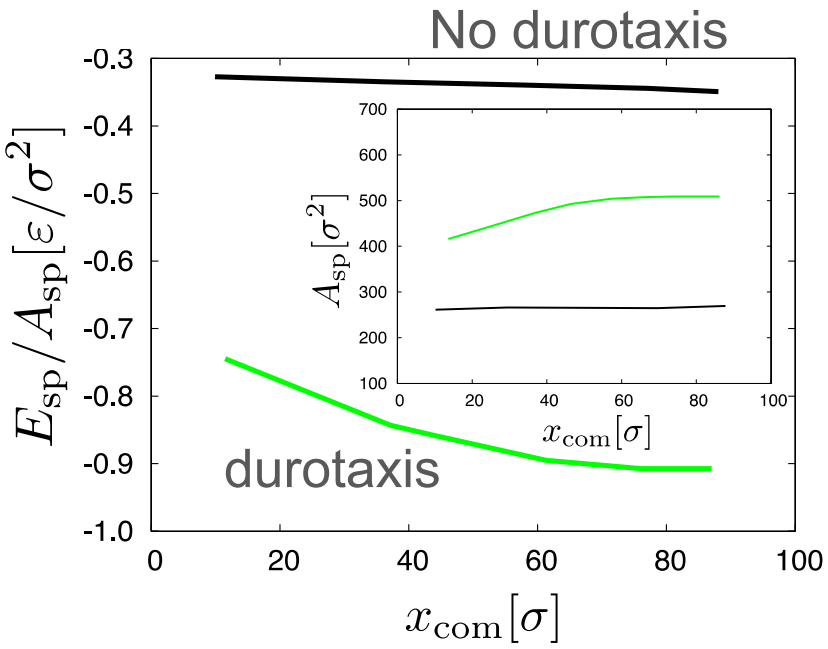


- Local velocity during durotaxis isn't linearly correlated with the stiffness gradient
- Droplet diffusion due to thermal fluctuations affect the durotaxial motion of the droplet

Driving force of durotaxis





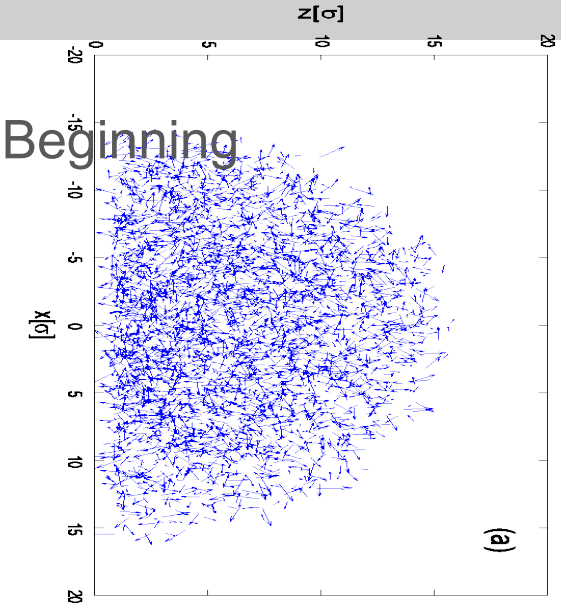


Comparison between durota
force of durotaxis is the gra
direction, $\frac{dE_{sp}}{dx}$

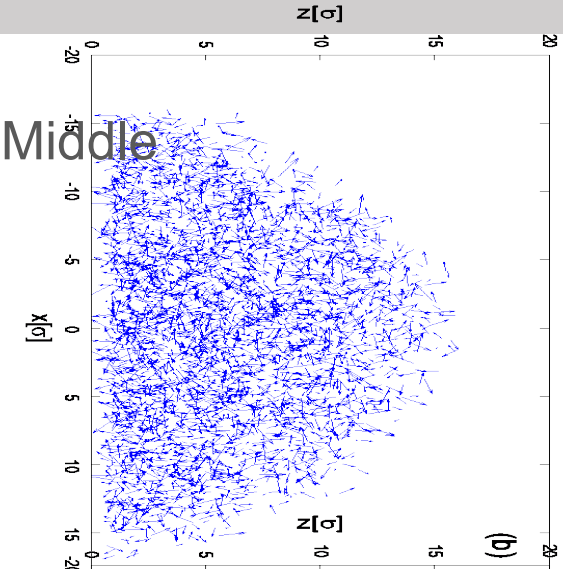
show that the driving
stiffness gradient

No intertial movement

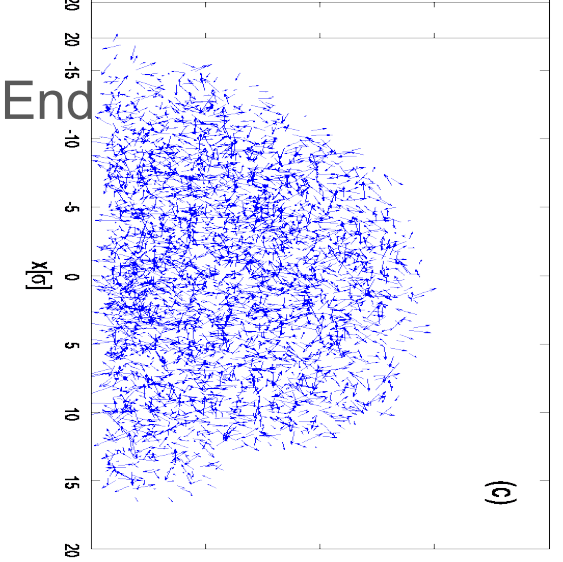
Beginning



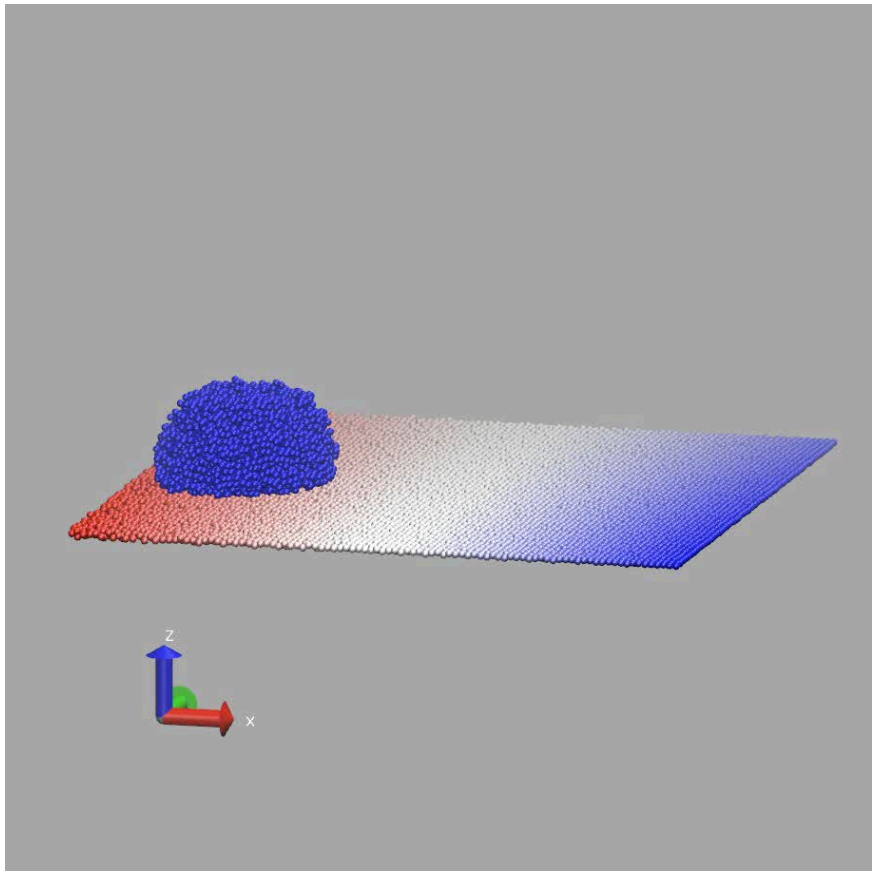
Middle



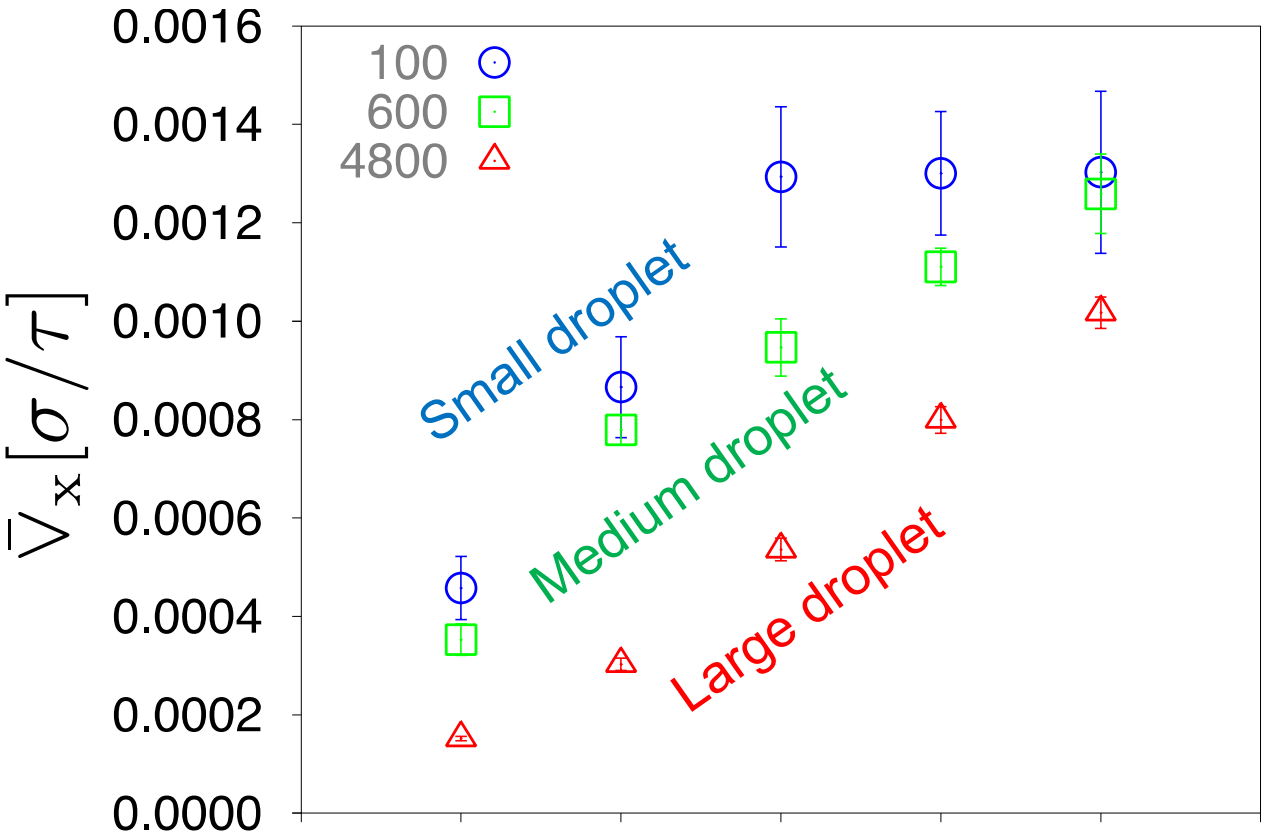
End



No indication of inertial movement, carpet motion, etc.

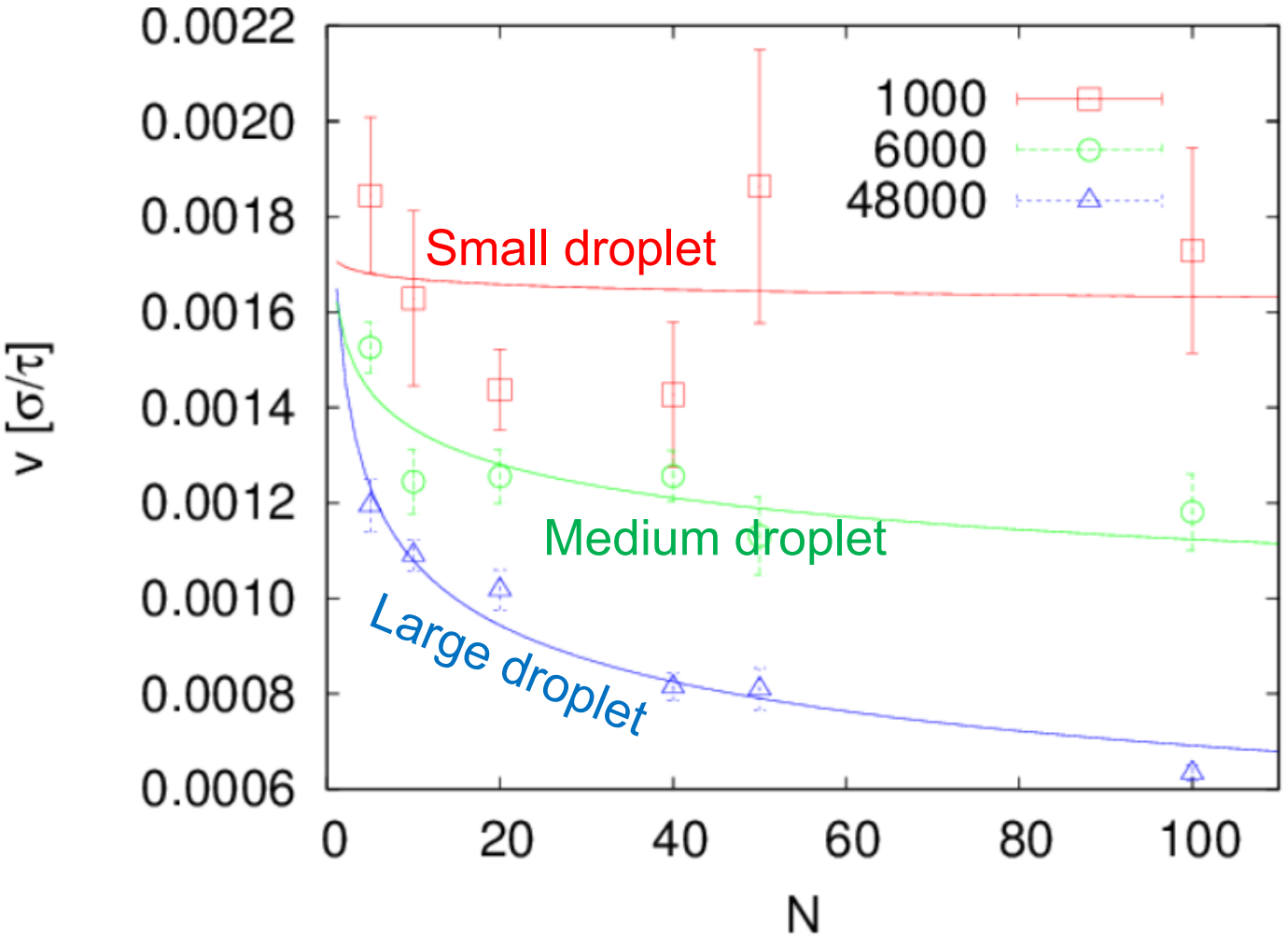


Effect of droplet size



Smaller droplet ⟹ better durotaxis for all droplet - substrate affinities up to a threshold value

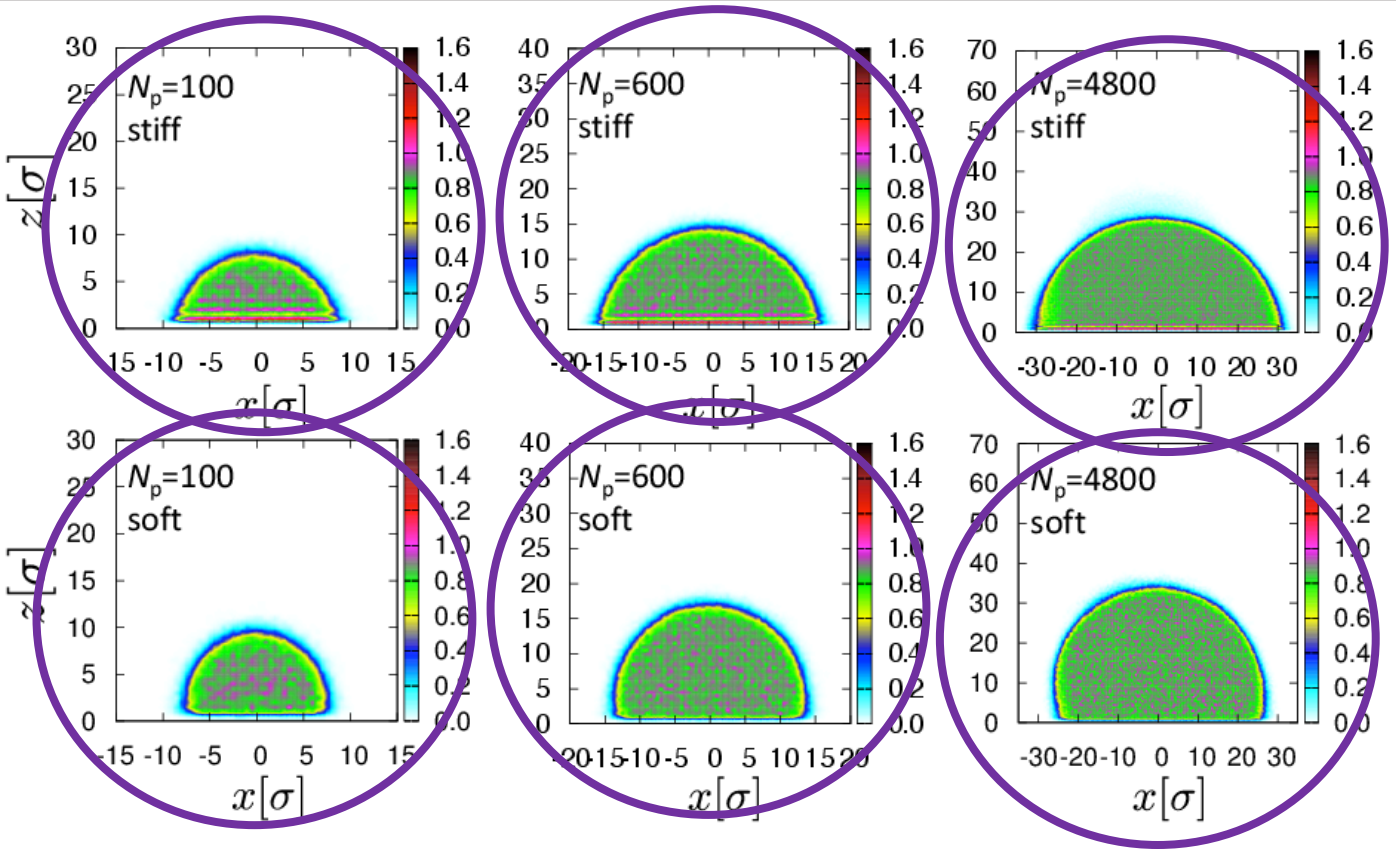
Effect of droplet viscosity

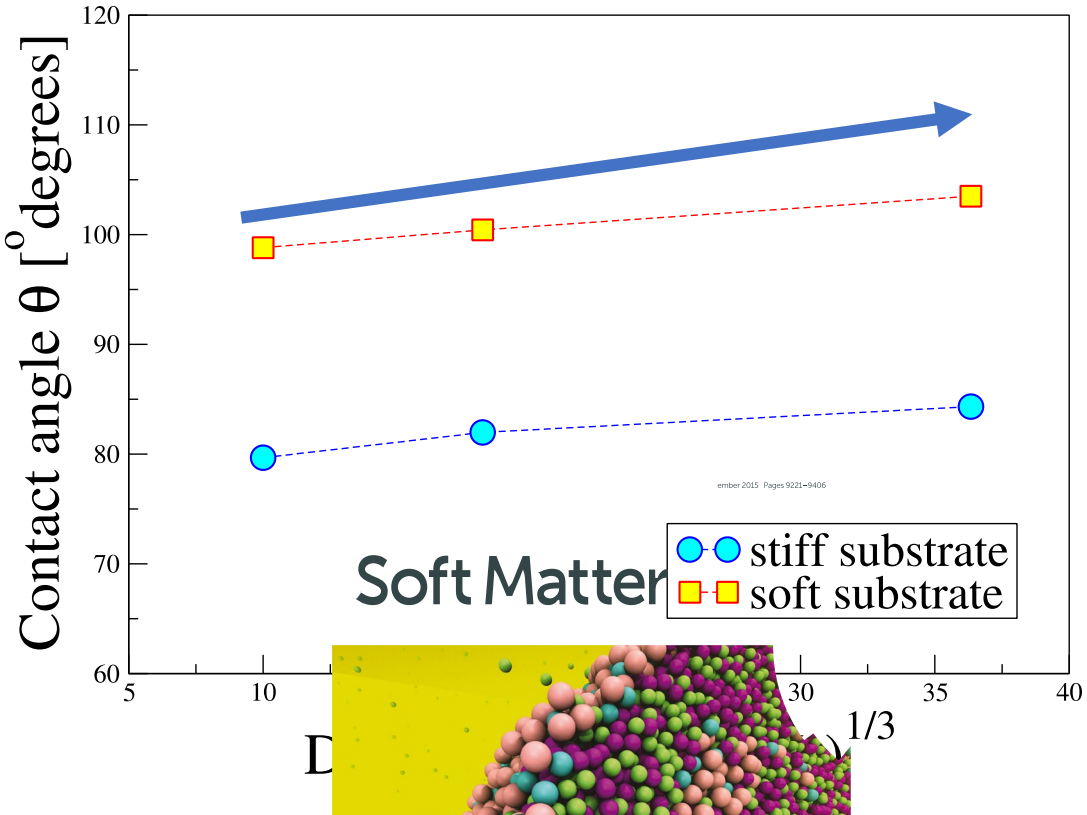


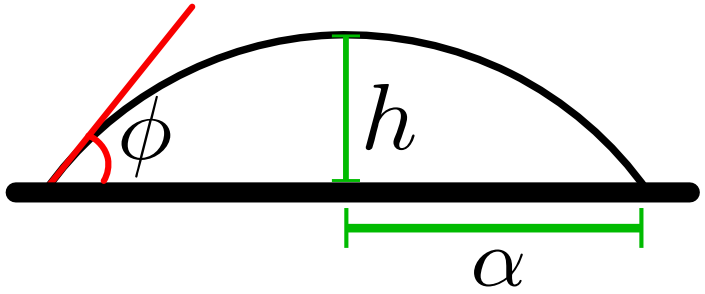
Higher visosity ⟹
worse efficiency of durotaxis

Larger droplets ⟹
larger the role of viscosity

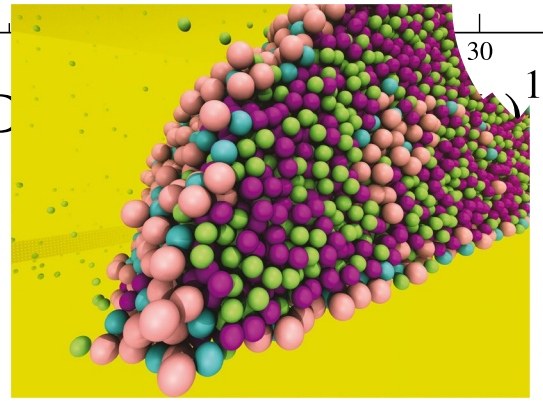
Effect of droplet size







$$\phi = \arcsin(1/\mu)$$
$$\mu = (1+\lambda^2)/2\lambda$$
$$\lambda = h/\alpha$$



Conclusions - Durotaxis

- Droplets move spontaneously from softer to stiffer parts of the substrate
- Durotaxis is enhanced with increasing stiffness gradient
- Durotaxis is enhanced for smaller droplets
- Durotaxis is enhanced for droplets of smaller viscosity
- Durotaxis is enhanced for higher wettability of the substrate

Acknowledgements

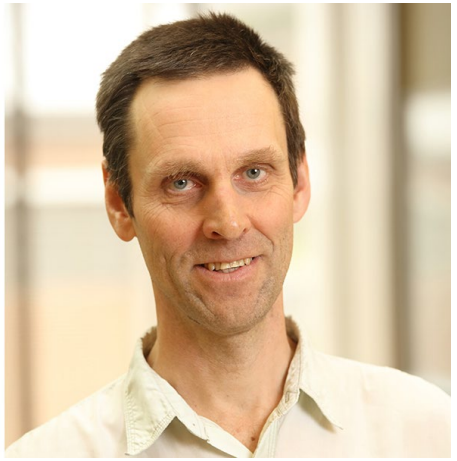
NATIONAL SCIENCE CENTRE
POLAND

THERMASMART

PL GRID

icm

Durotaxis Project



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Thanks to you

Thank you for your attention

Discussion