# Unidirectional Droplet Propulsion onto Gradient Brushes Without External Energy Supply


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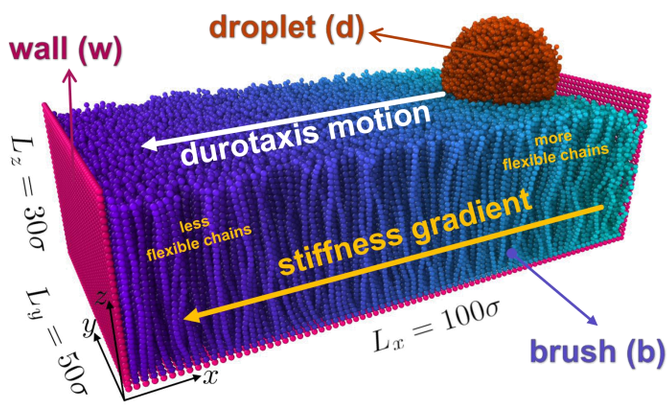
## Introduction

Using extensive molecular dynamics simulation of a coarse-grained model, we demonstrate the possibility of sustained unidirectional motion (durotaxis) of droplets without external energy supply when placed on a polymer brush substrate with stiffness gradient in a certain direction.

It is shown that this durotaxial motion is driven by the steady increase of the interfacial energy between droplet and brush as the droplet moves from softer to stiffer parts of the substrate whereby the mean driving force gradually declines with decreasing roughness of the brush surface.

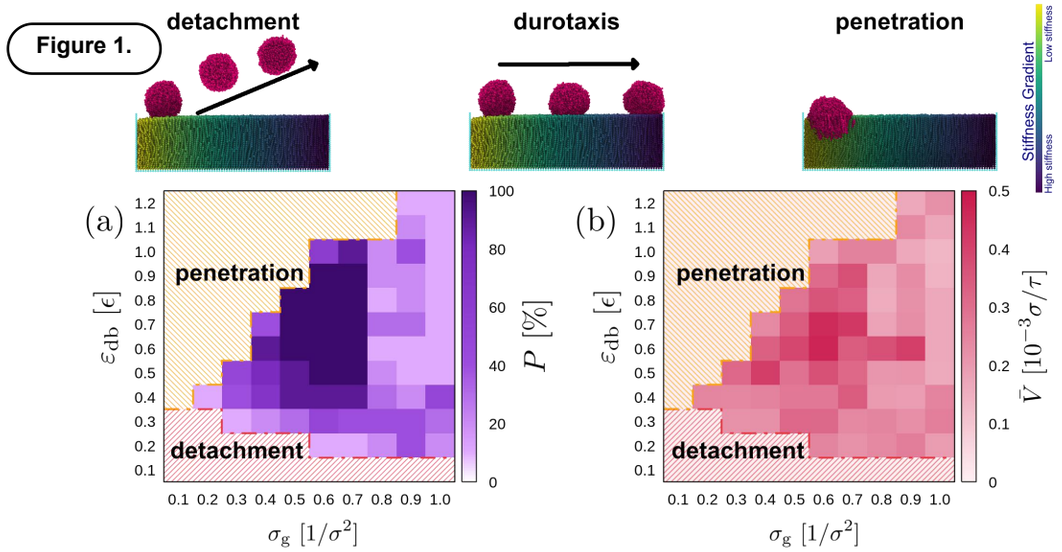
## Simulation Setup




- Durotaxis occurs by increasing stiffness on the brush substrate

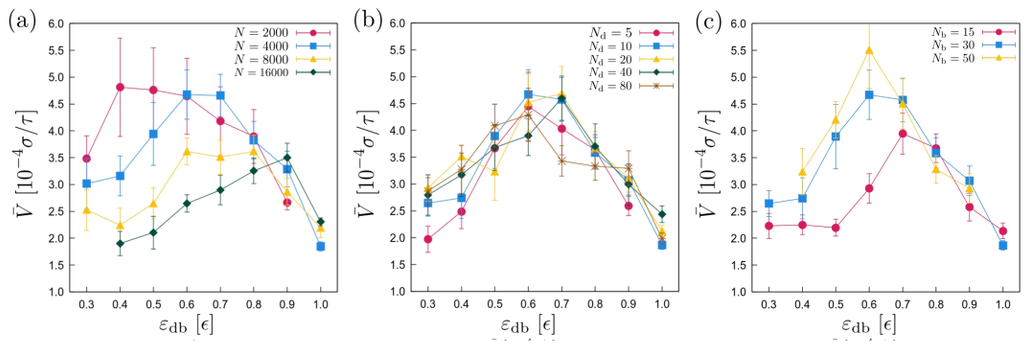
## Results

Figure 1.




- Moderate-range grafting densities and affinities favour durotaxis.
- Moderate-range grafting densities and affinities have the highest durotaxis possibility.
- Highest velocity belongs to the moderate-range of grafting density.

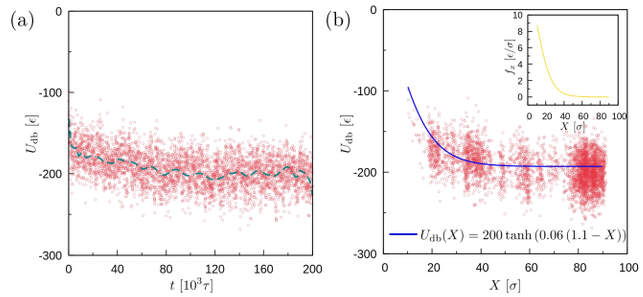
Figure 2.



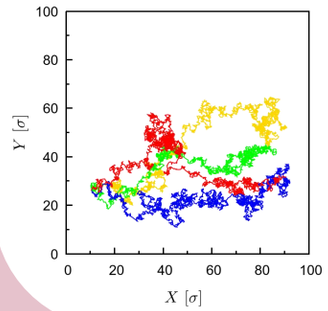

- Bigger droplets have slower velocity(a).
- Optimum affinity is increased by enhancing droplet size (Total number of beads)(a).
- Altering viscosity of the system does not play crucial role on durotaxis motion (b).
- Longer brush chains enhance the droplet velocity (c).

## Results

Figure 3.




- Interfacial energy is minimised as function of time and x component of the droplet's centre of mass.




- Typical trajectories at the X-Y plane.

## Conclusions

We have proposed a new design of brush polymer substrates that is capable of leading to the durotaxis motion of nanodroplets. The knowledge gained here may lead to new experimental brush-based substrate designs and provide a further understanding of relevant biological processes, such as the motion of cells on tissues, or the mucus flow around lung cilia.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This research has been supported by the National Science Centre, Poland, under grant No. 2019/35/B/ST3/03426.



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