Modelling polymer brush coatings in contact with gasses

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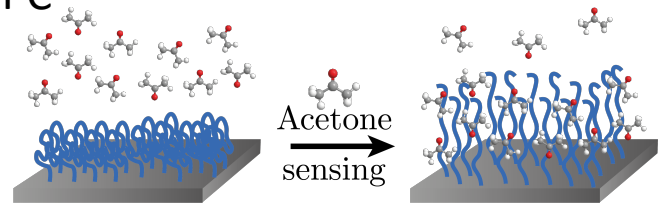
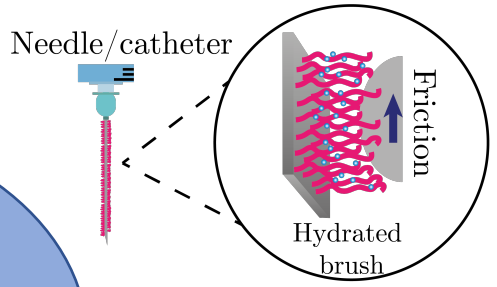
since nov 2016



Sensing Applications

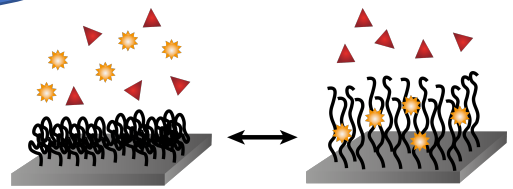
Low friction coating

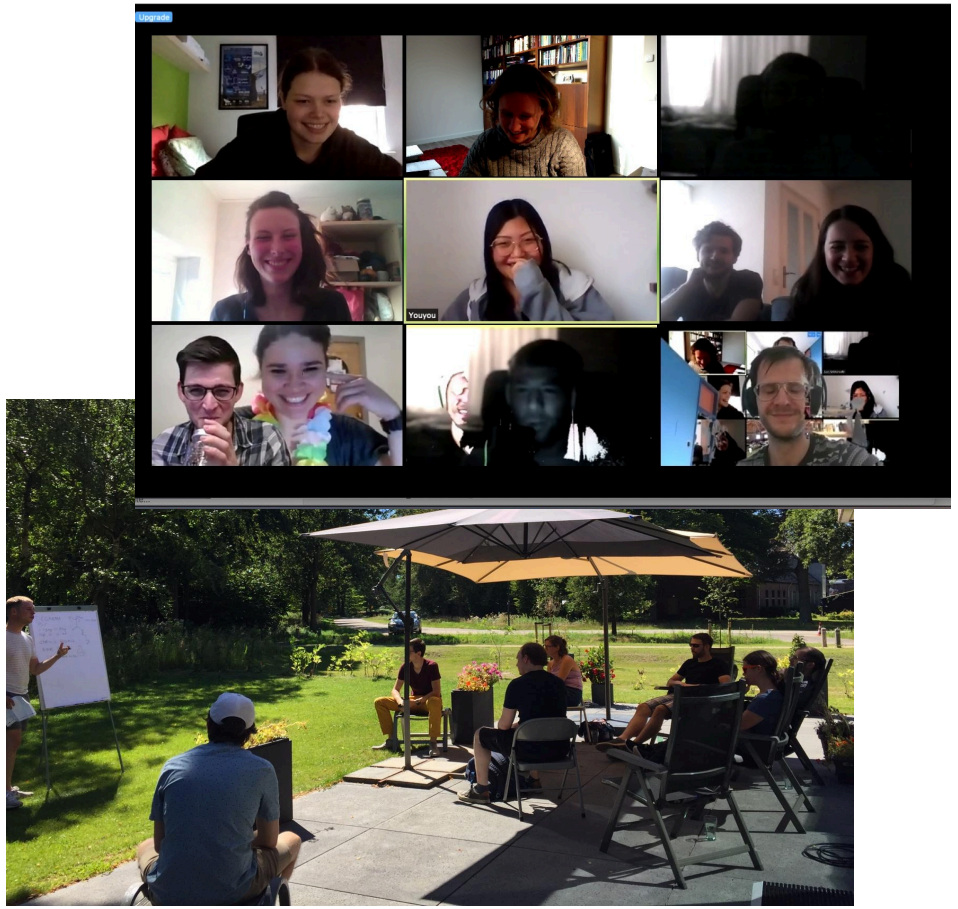


Functional Coatings

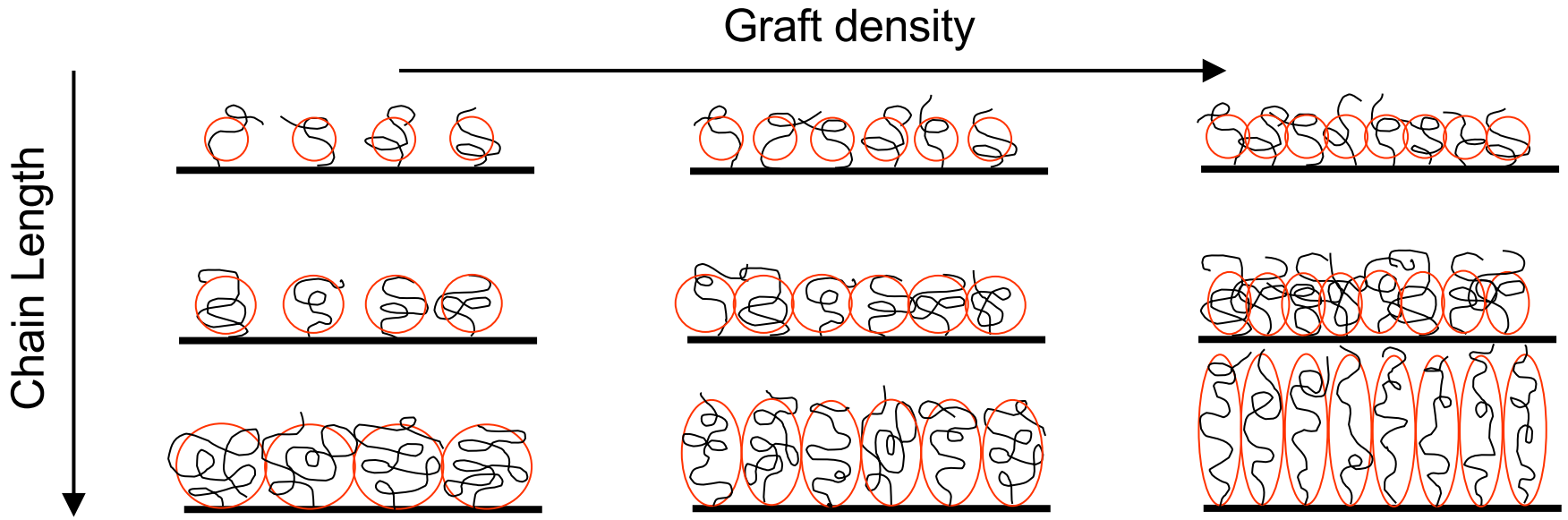
Friction Control

Separations for Circularity

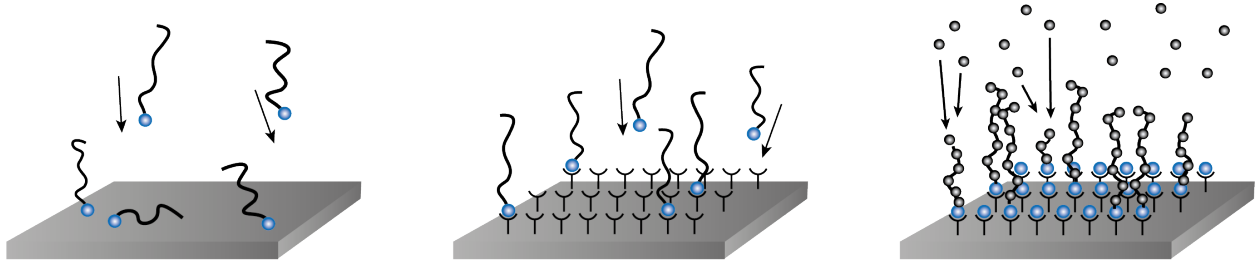




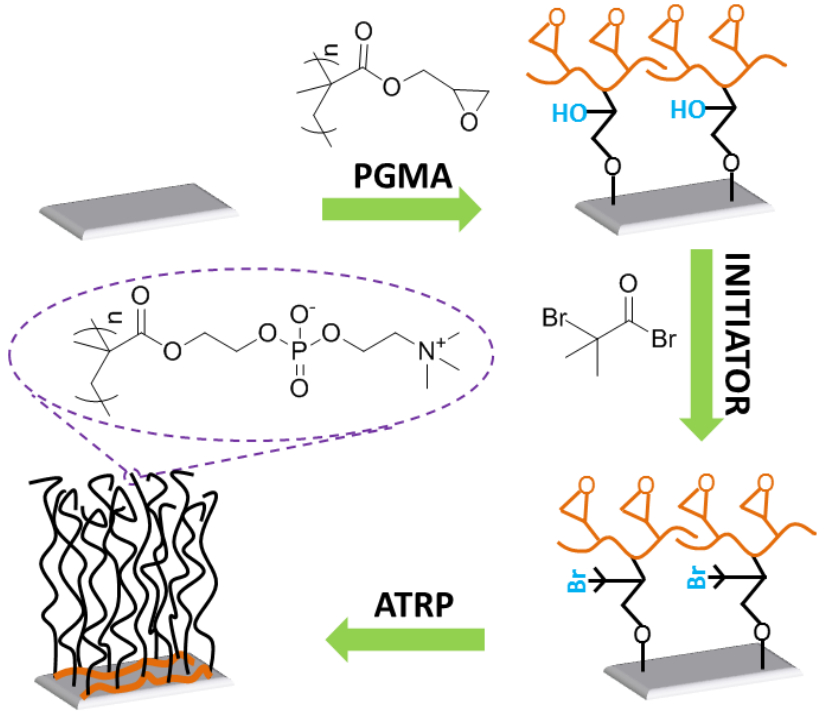
What is a polymer brush?



How to prepare such brushes?

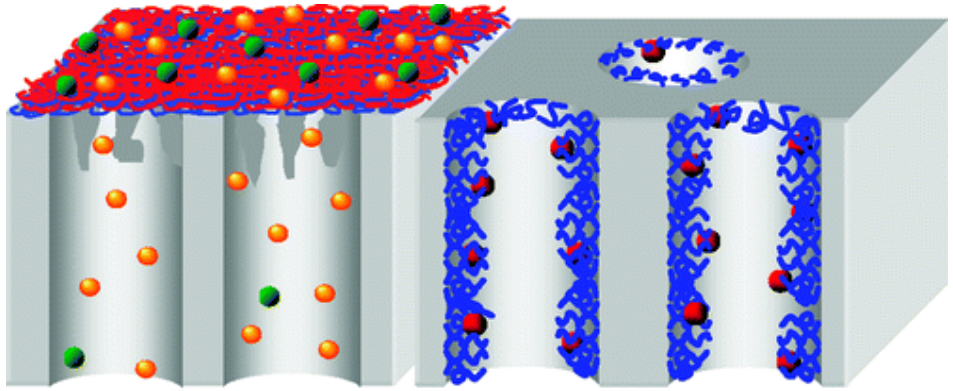


a) Physisorption b) Grafting to- c) Grafting from-

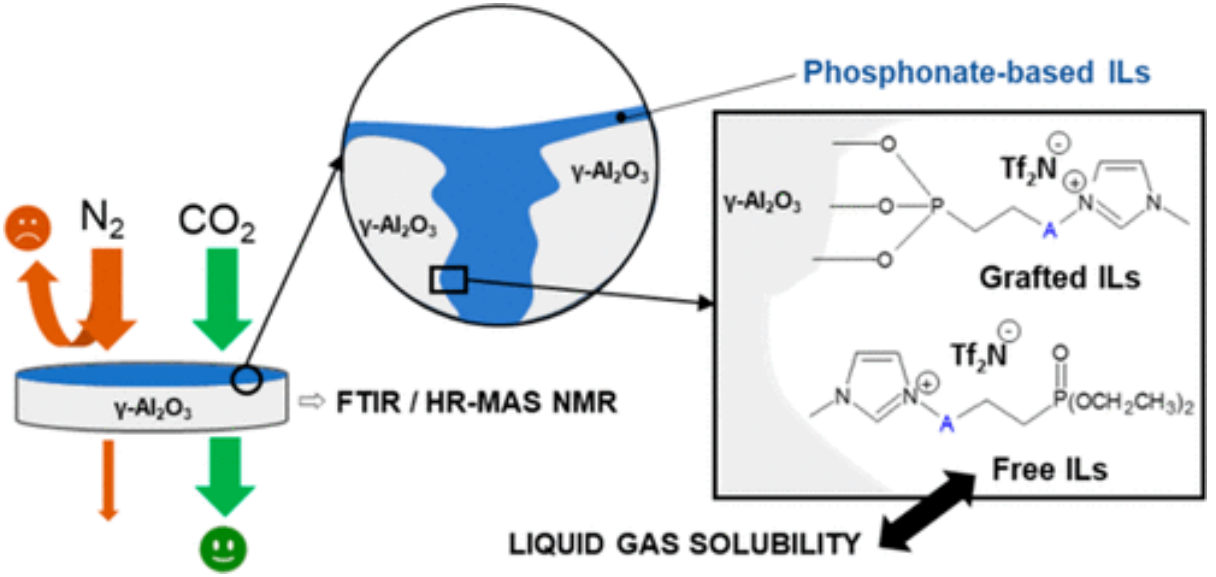


Yu, Y.; Vancso, G. J.; de Beer, S. Eur. Polym. J. 2017, 89, 221–229

Polymer brushes for gas separations

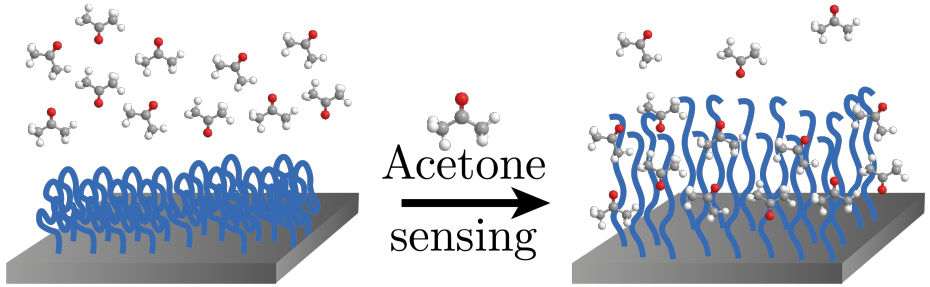


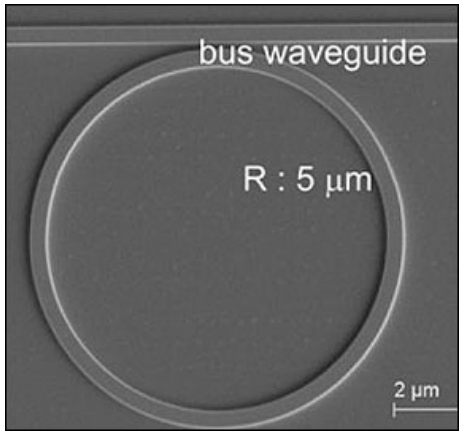
Bruening et al. Langmuir 2008, 24, 7663–767

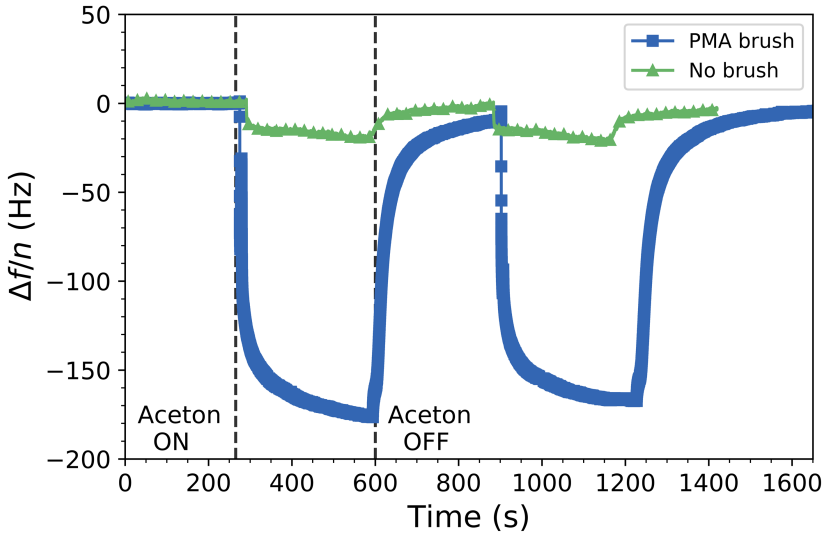


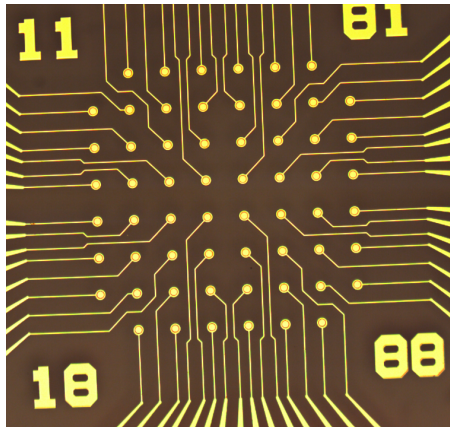
Pizzoccaro-Zilamy et al., Industrial & Engineering Chemistry Research 2018, 57, 16027–1604

Polymer brushes for sensing









R. J. Horst, M. Brió Pérez, et al., Langmuir 36 12053–12060 (2020)

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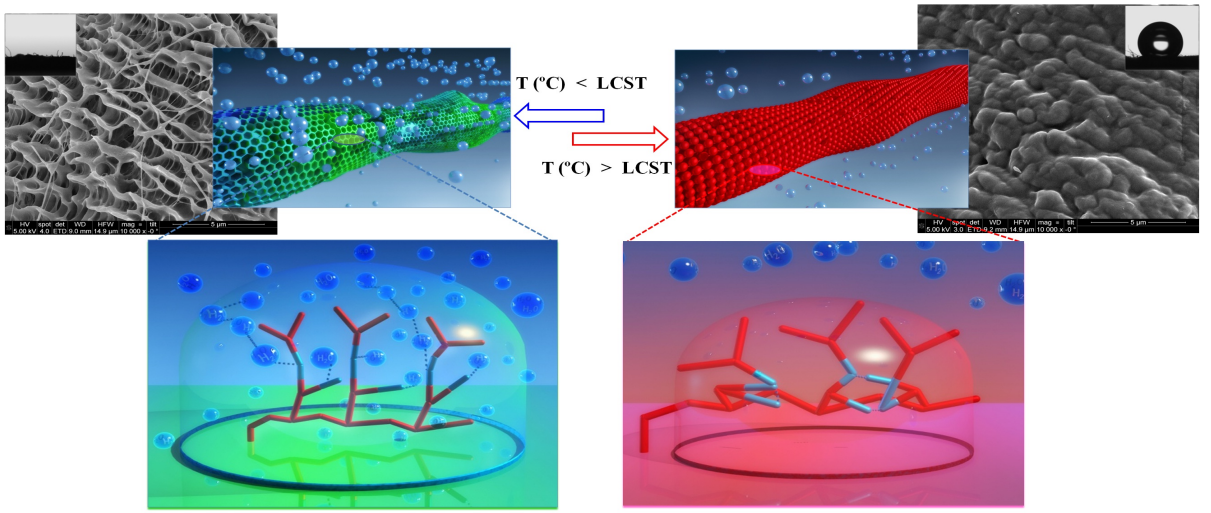
By Catarina Esteves



Yang et al. Advanced Materials 25, 1150 (2013)

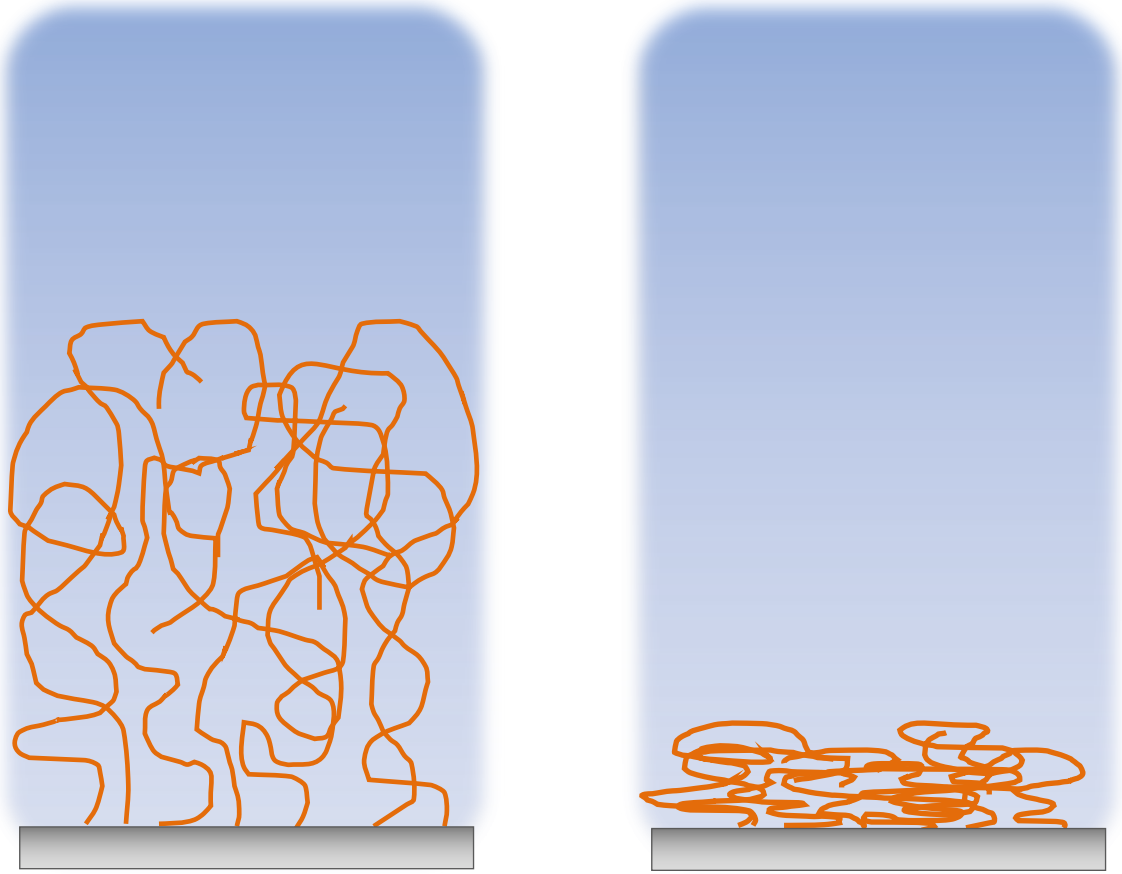
Polymer Brushes in Contact with Air / Vapors

Guido Ritsema van Eck
Lars Veldscholte

Leon Smook

Rick Cohen, Maria Brio Perez and Rens Horst

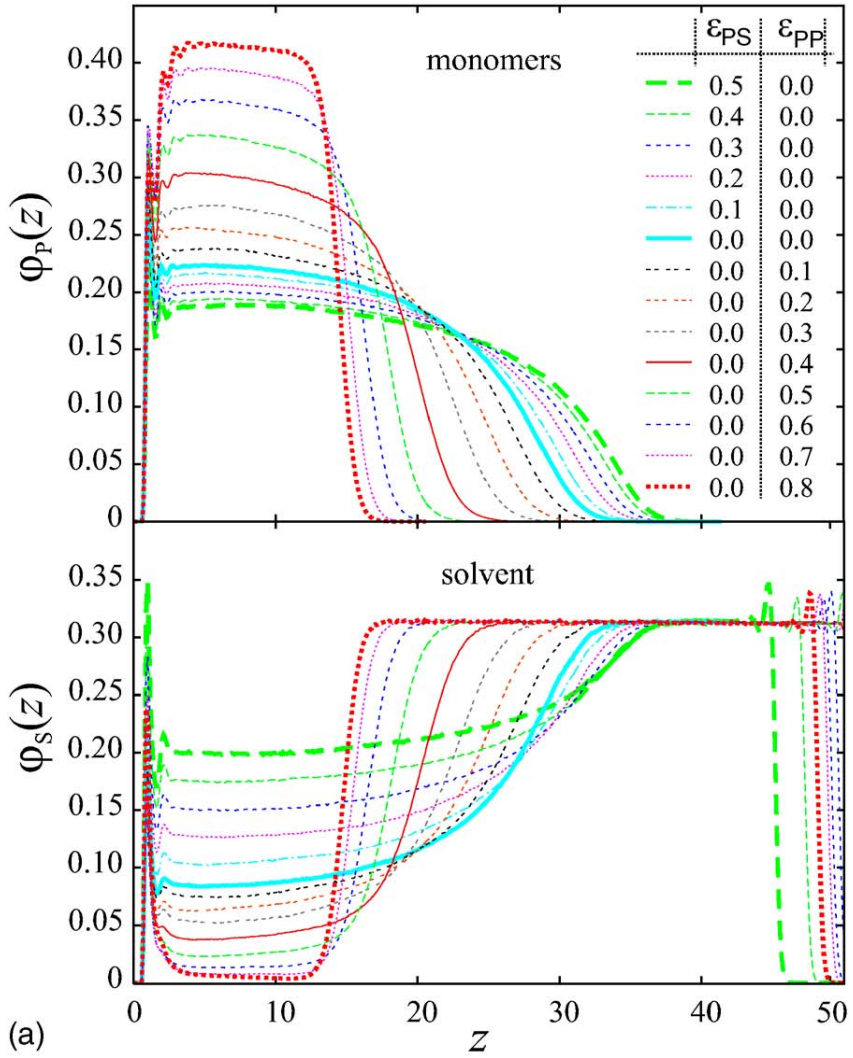
Summary Brushes in Liquid



good solvent

poor solvent

Summary Brushes in Liquid

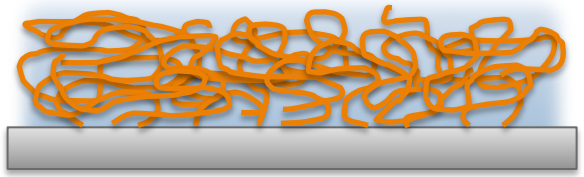


D. I. Dimitrov, A. Milchev and K. Binder, *J. Chem. Phys.*, 2007, **127**, 084905

Brushes in Air are Different

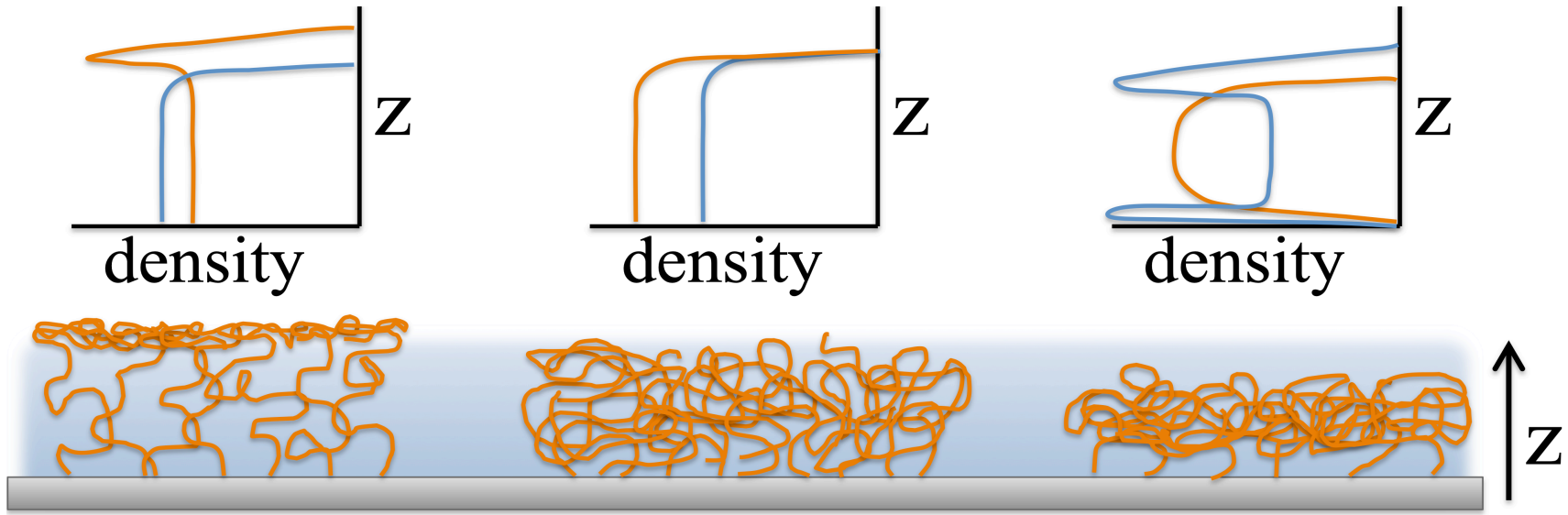
liquid

At 100% relative humidity
there is only 2 wt. % water in the air

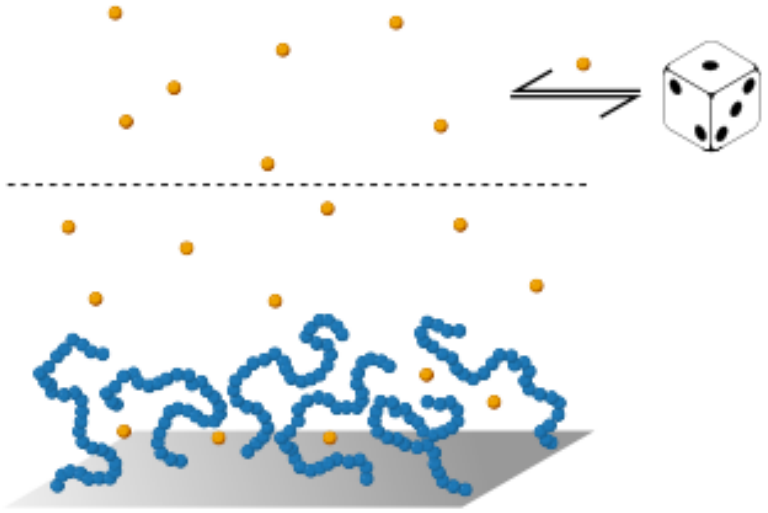


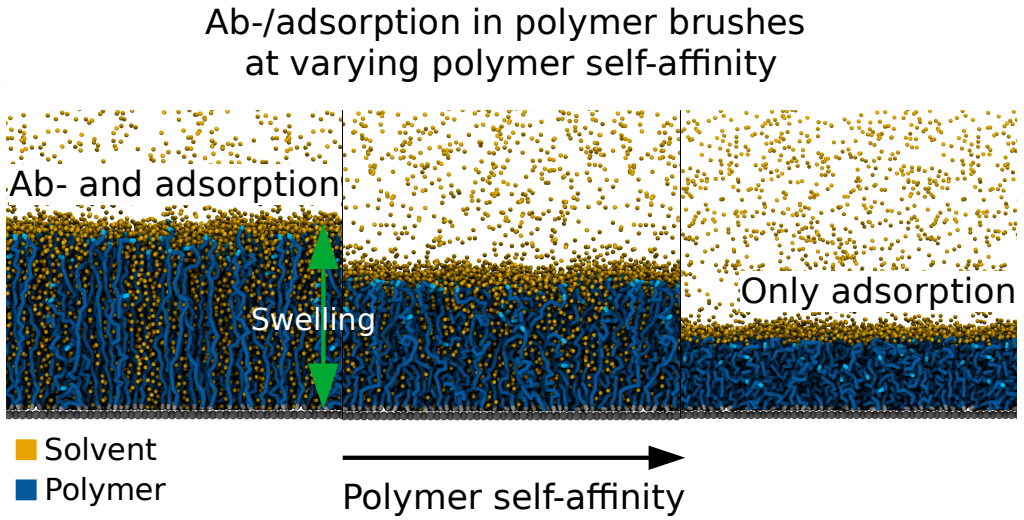
air

Three component system

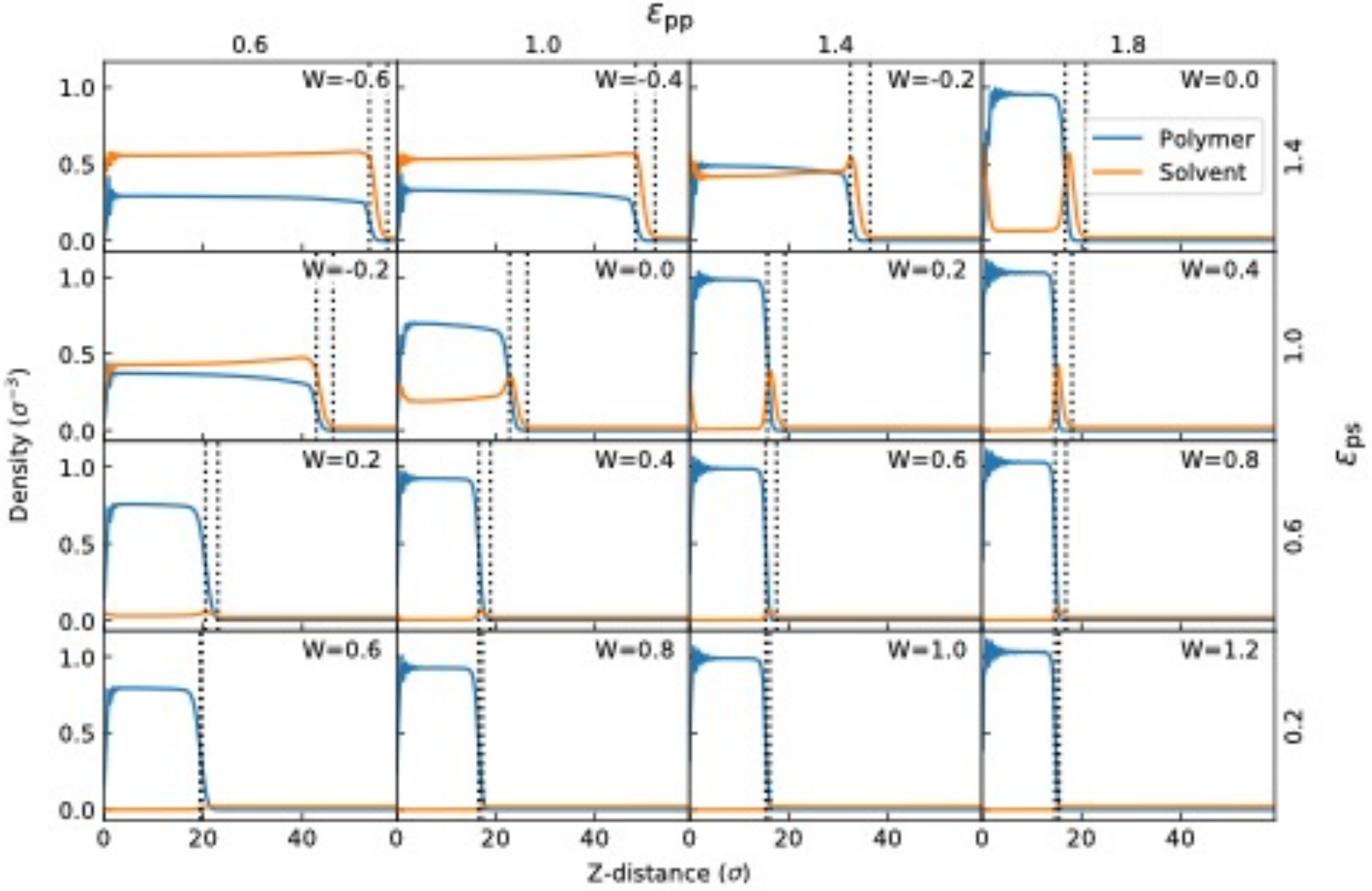


Brushes in Contact with Vapors





Brushes in Contact with Vapors

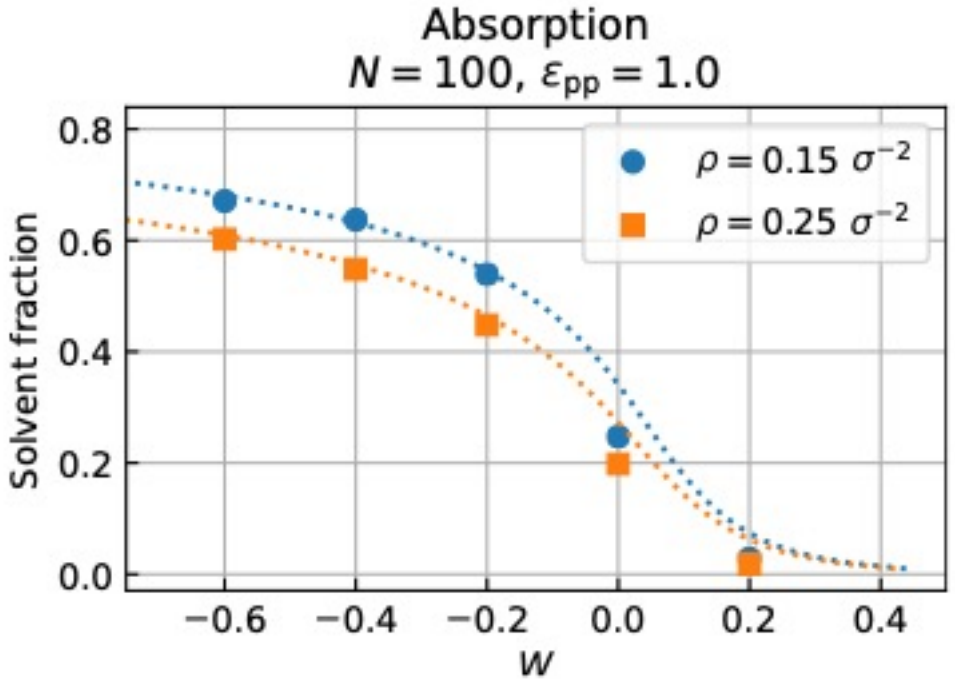


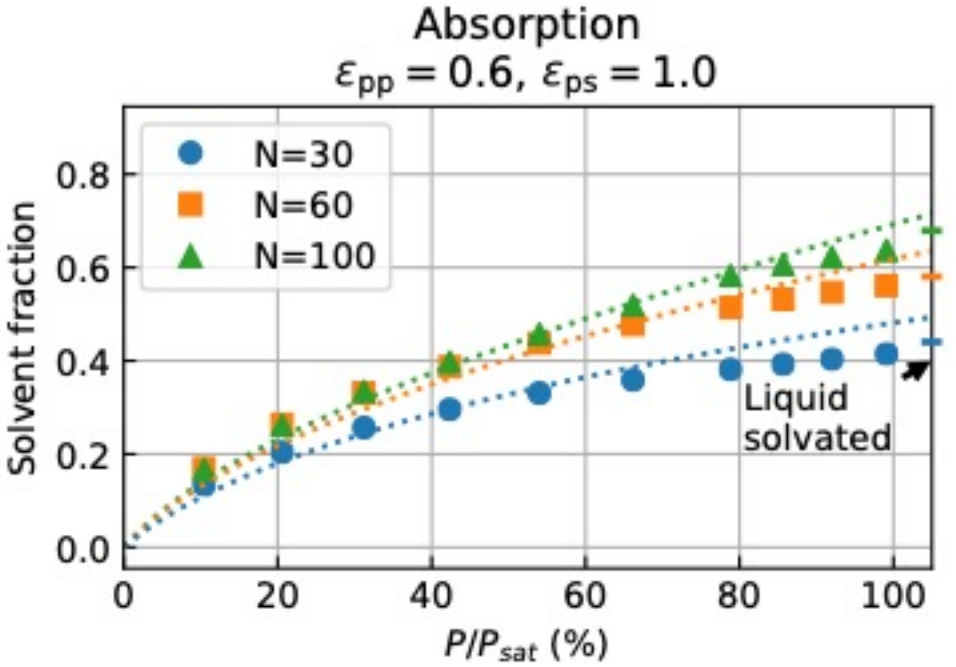
$$W = -\epsilon_{ps} + \frac{1}{2}(\epsilon_{ss} + \epsilon_{pp})$$

$$\chi = \frac{zW}{k_B T}$$

Comparison to Theory

$$\ln\left(\frac{P}{P_{\mathrm{sat}}}\right) = \ln(1-\phi_{\mathrm{p}}) + \phi_{\mathrm{p}} + \chi\phi_{\mathrm{p}}^2 + \frac{3\rho_{\mathrm{g}}^2}{\phi_{\mathrm{p}}}$$





G. C. Ritsema van Eck, L. B. Veldscholte, et al., Macromolecules 53 8428–8437 (2020)

Summary

- Polymer brush coatings behave different in air then in liquid
- The Flory Huggins theory can be employed to describe vapor aborption in brushes
- The correct brush-design can lead to collaborative effects and enhanced gas-sorption

Thank you!