Title: Budding transition of a self-avoiding polymer confined by a soft membrane adhering onto a flat wall

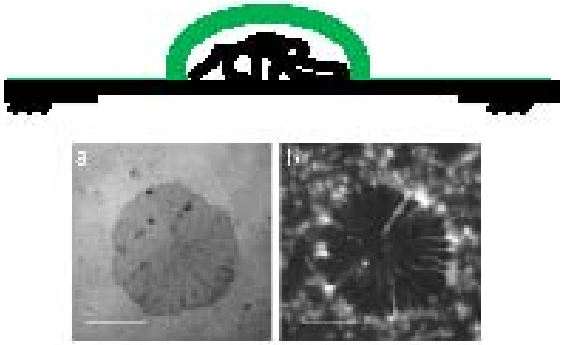
Date: Dec 05, 2013 05:50 PM

URL: http://pirsa.org/13120041

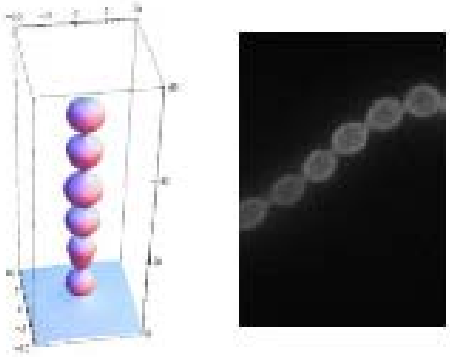
Abstract: Monte Carlo simulation is used to study the structural properties of the system consisting of a self-avoiding polymer chain confined between a fluid membrane and a flat hard surface. As the adhesion between the soft membrane and the hard-wall surface increases the polymer is subject to a strong confinement; a pancake-shaped polymer conformation state eventually yields to a bud state through an abrupt first-order phase transition. We explore the scaling behavior of the physical properties of the system as functions of the polymers size the membranes surface tension and the adhesion energy for both pancake and bud states in terms of Monte Carlo data and analytic scaling theories.

Theory and simulation of interactive membrane-macromolecule structures in biological systems

Polymer, membrane, and hard surface



Nanoparticles and membrane



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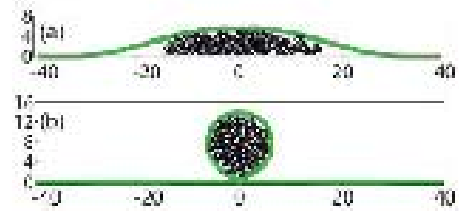
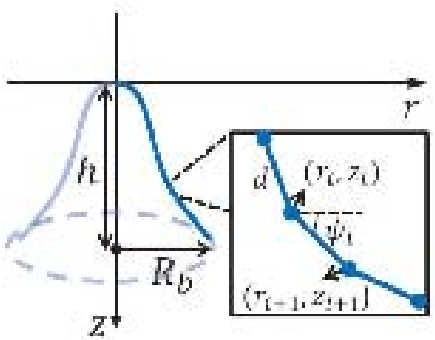
Methodology

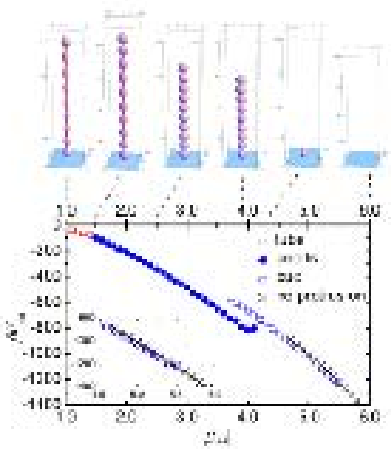
Theory

- Coarse-graining model
- Helfrich free energy



$$F_{\text{mem}} = \frac{\kappa}{2}\int \left[2M - c_0\phi(x)\right]^2 dA + \sigma\Delta A$$



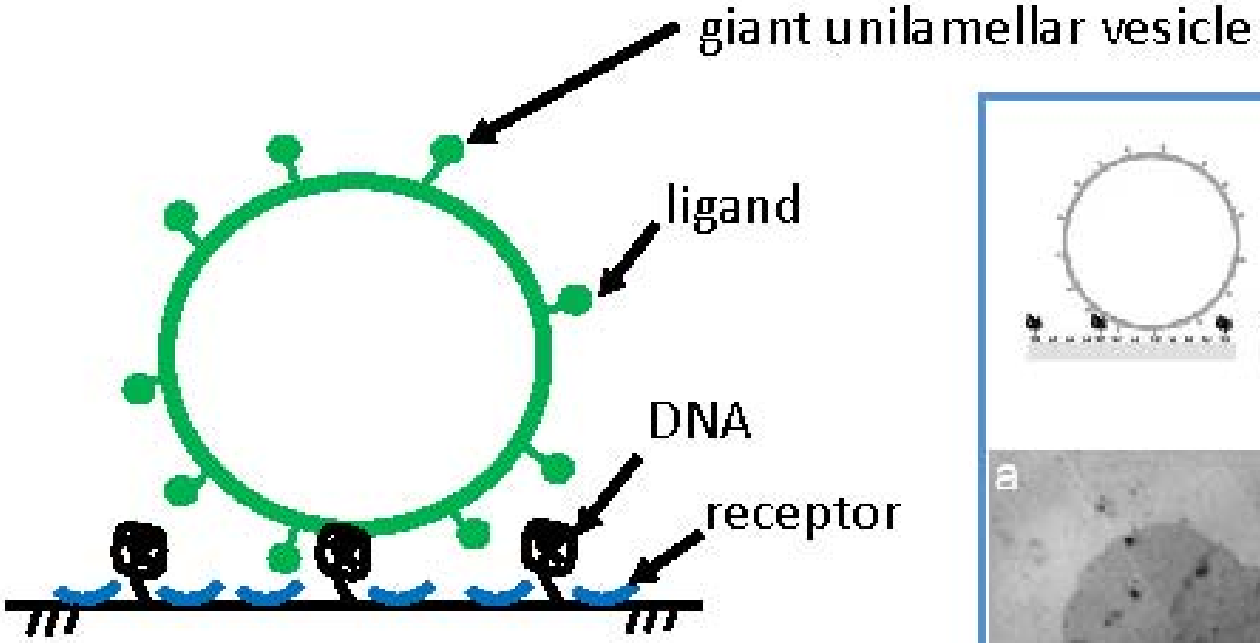


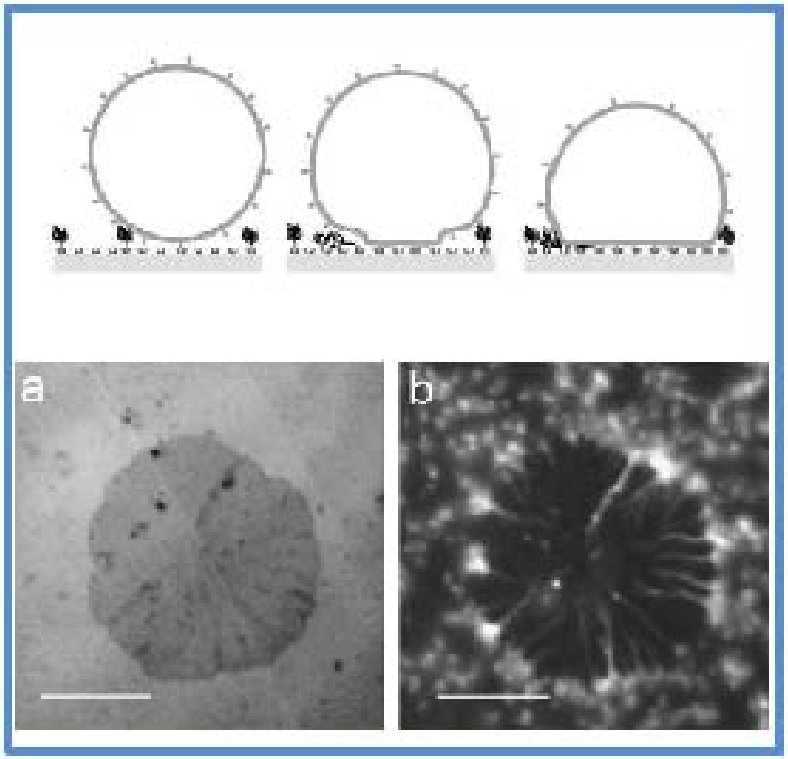
Tools

- Scaling theory
- Free energy analysis
- Monte Carlo method
- Simulated annealing

Motivation: recent experiments

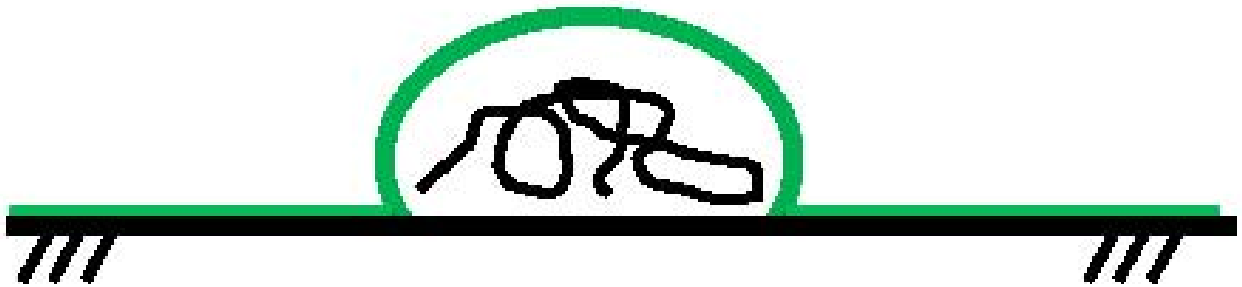
Vesicle adhered onto a DNA carpet



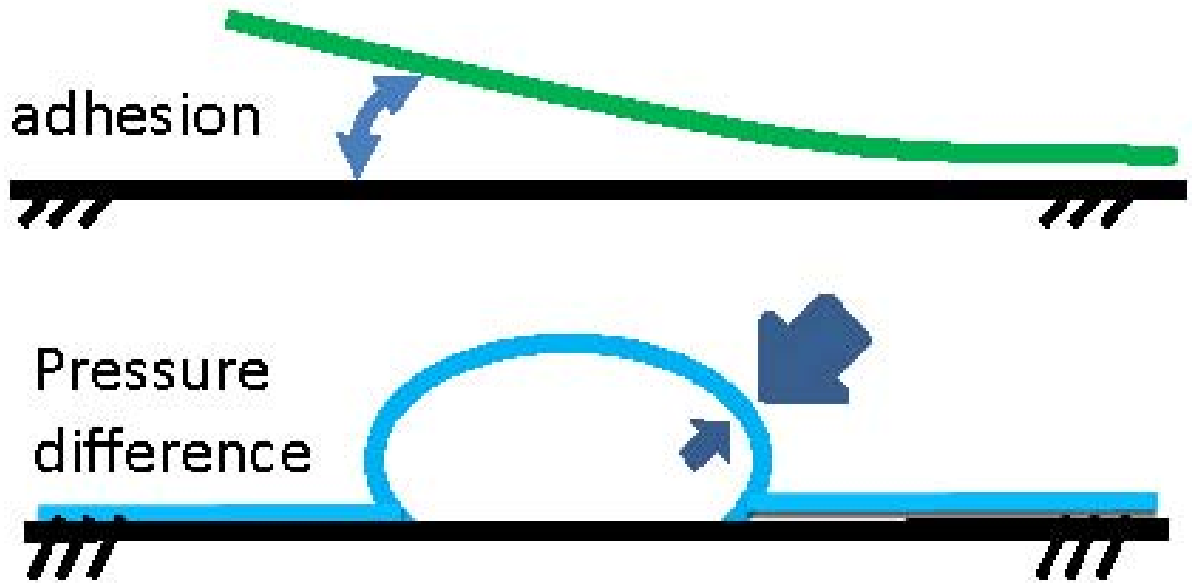


M.-L. Hisette, P. Haddad, T. Gisler, C. M. Marques and A. P. Schröder, *Soft Matter*, 2008, **4**, 828–832.

Polymer, membrane, and hard surface



Two possible scenarios:



Polymer, membrane, and hard surface

- **adhesion**

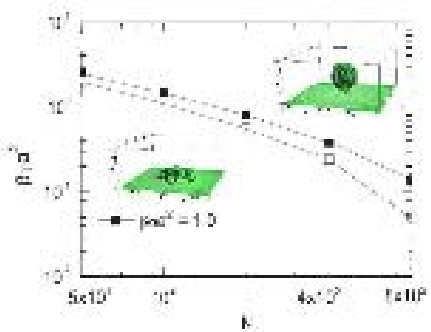
pancake

Excluded Volume Interaction

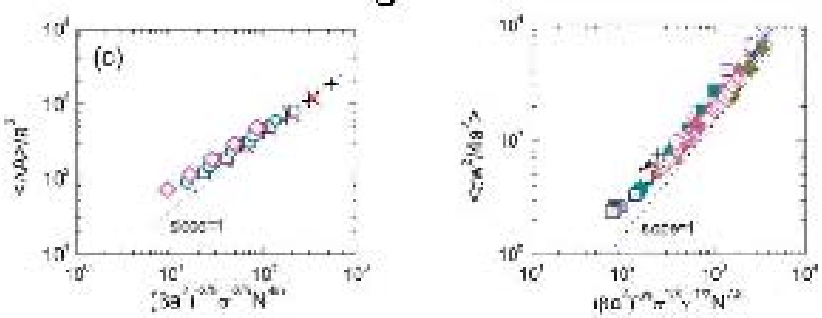
bud

Excluded Volume Interaction
Confinement entropy

Phase diagram



Scaling results



Y.-C. Su and J. Z. Y. Chen, *Soft Matter* **9**, 570 (2013)

Polymer, membrane, and hard surface

- **pressure difference**

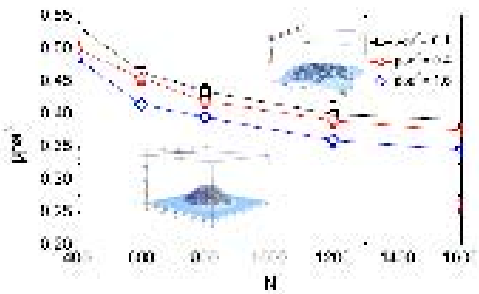
confined

Confinement entropy

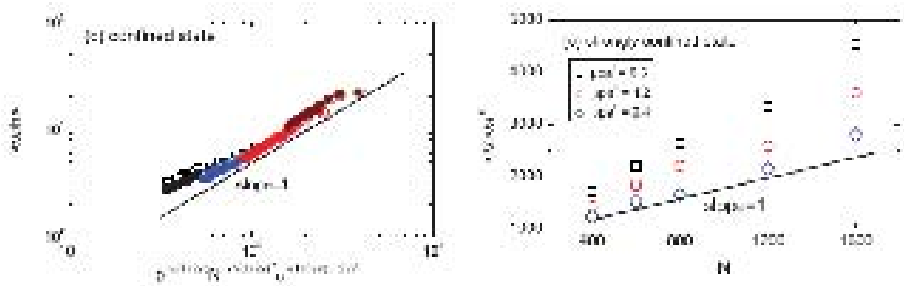
Strongly confined

No scaling!

Phase diagram



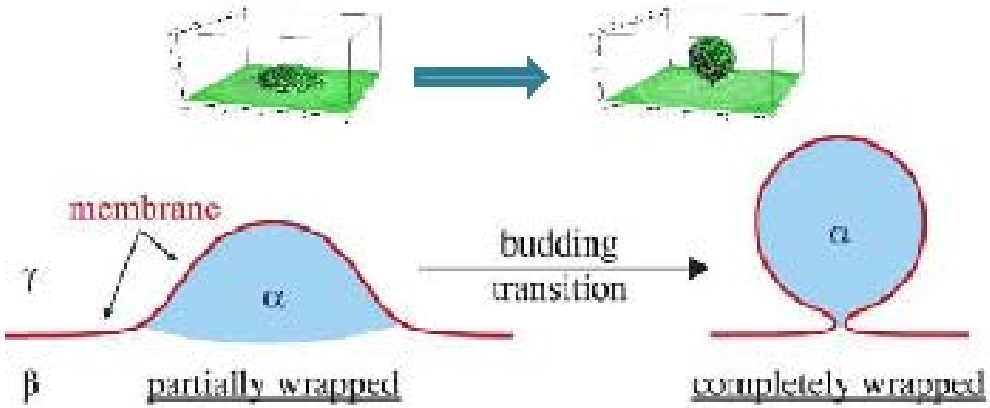
Scaling results



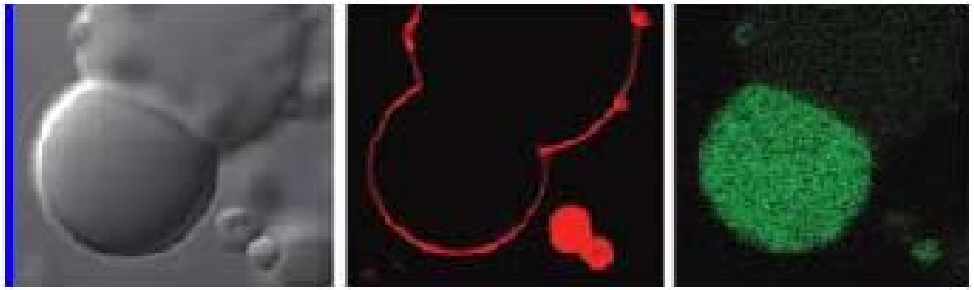
Y.-C. Su and J. Z. Y. Chen, *Phys. Rev. E* **87**, 052706 (2013)

Polymer, membrane, and hard surface

Related systems



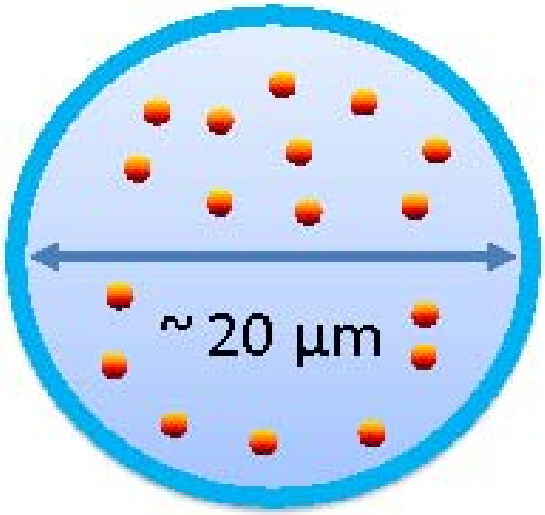
H. Kusumaatmaja and R. Lipowsky, *Soft Matter* 7, 6914 (2011)



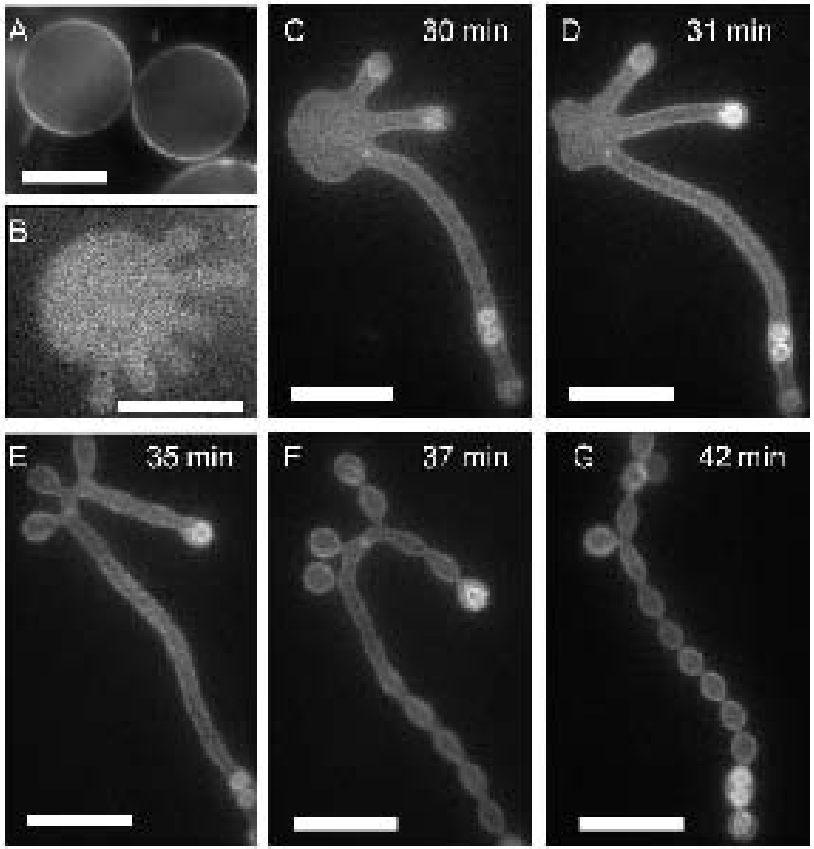
M. S. Long, A. S. Cans and C. D. Keating, *J. Am. Chem. Soc.* **130**, 756 (2008)

Motivation: recent experiments

Tubulation and pearling induced by nanoparticles adhesion



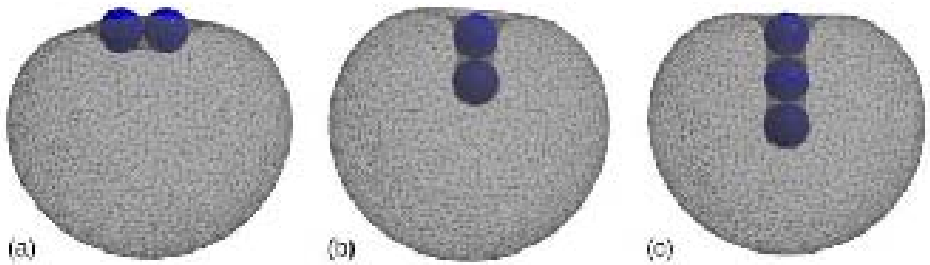
cationic nanoparticles
~ 100-200 nm



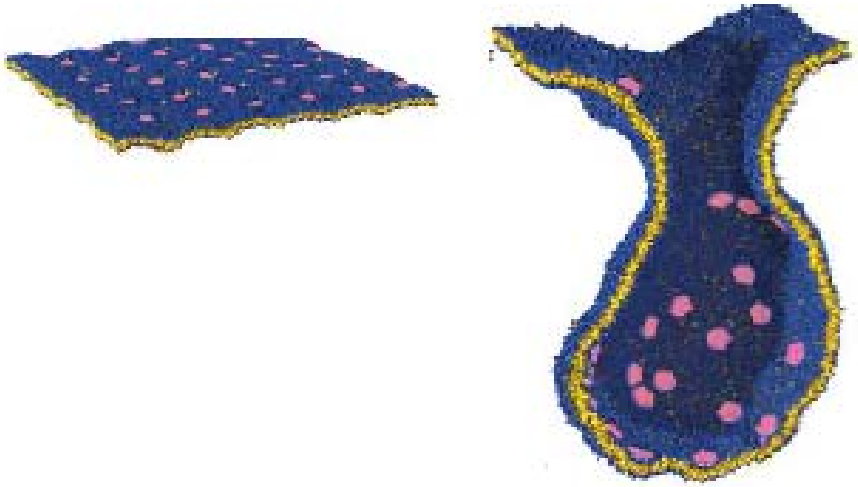
Yan Yu and Steve Granick, *J. Am. Chem. Soc.*, 2009, **131**, 14158-14159

Polymer, membrane, and hard surface

Previous works



A. H. Bahrami, R. Lipowsky, and T. R. Weikl, *Phys. Rev. Lett.* **109**, 188102 (2012)



B. J. Reynwar, G. Illya, V. A. Harmandaris, M. M. Müller, K. Kremer, and M. Deserno, *Nature* **447**, 461 (2007)

Nanoparticles and membrane

- **Phase diagram**

$$F = \frac{\kappa}{2}\int \left(2M - c_0(\varepsilon)\phi(r)\right)^2 dA + \sigma\Delta A + \frac{\mu}{A_p}\int \phi(r)\, dA$$

same adhesion strength
different deformation

Nanoparticles and membrane

- **Phase diagram**

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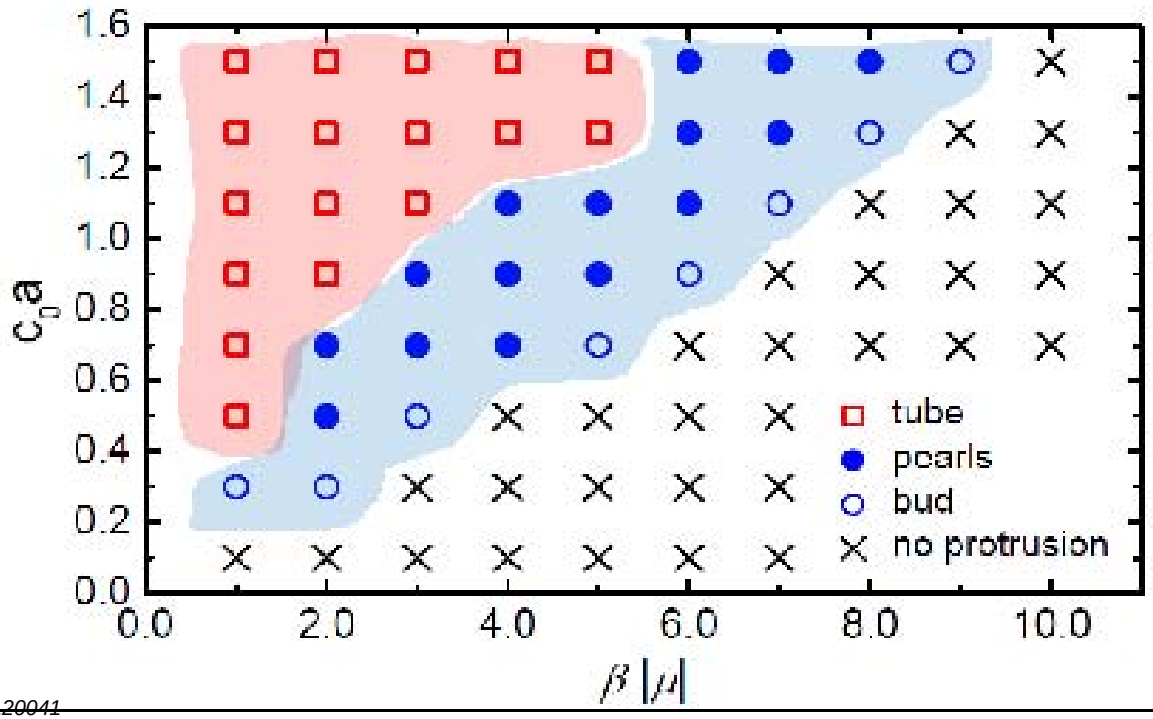
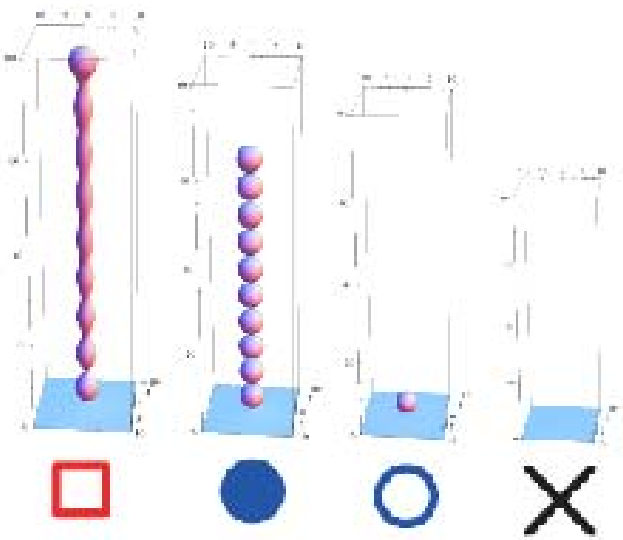
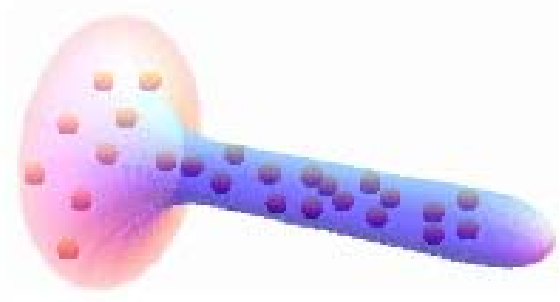




Questions?

Y.-C. Su and J. Z. Y. Chen, *Soft Matter* **9**, 570 (2013)
Y.-C. Su and J. Z. Y. Chen, *Phys. Rev. E* **87**, 052706 (2013)



Y.-C. Su and J. Z. Y. Chen (in preparation)