Liquid Crystals defects

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Liquid Crystal Physics

Observed two melting points when heating up Cholesteryl Benzoate.

Friedrich Reinitzer (1888)

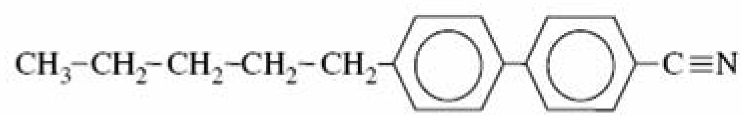
Lehmann (1900)

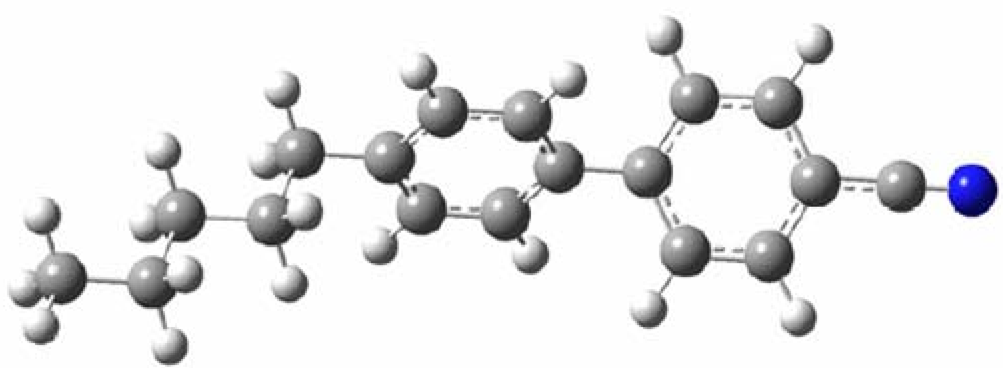
Established the term ***liquid crystal***

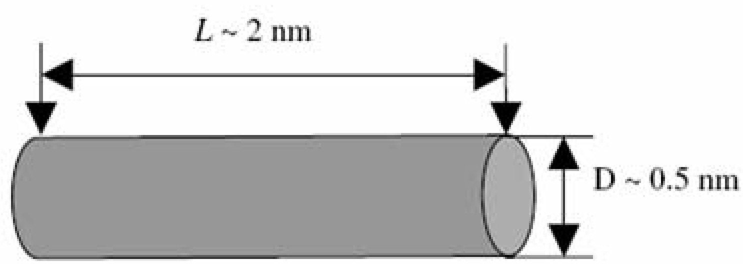
Liquid Crystals (rod like)

Liquid crystal materials generally have several common characteristics. Among these are a rod-like molecular structure, rigidness of the long axis, and strong dipoles and/or easily polarizable substituents.

4’-n-pentyl-4-cyano-biphenyl

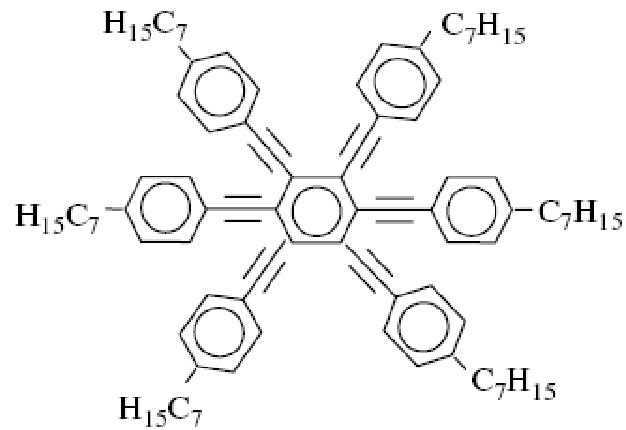


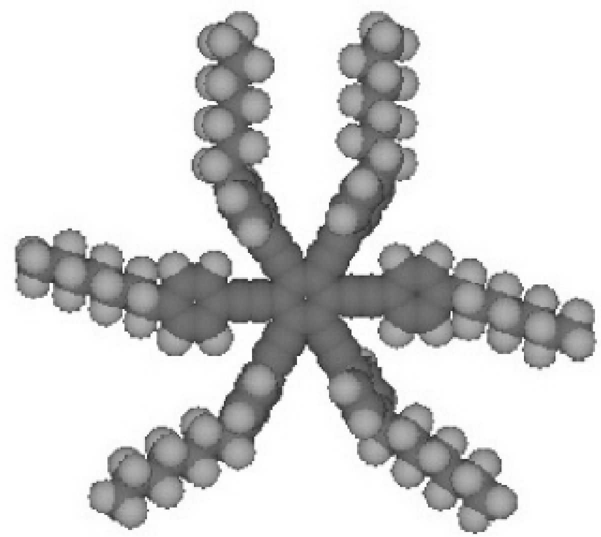


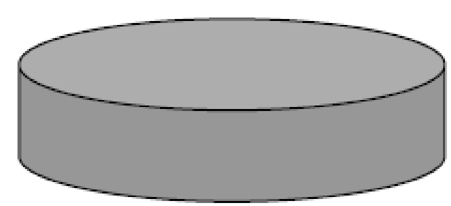


Liquid Crystals (disk like)

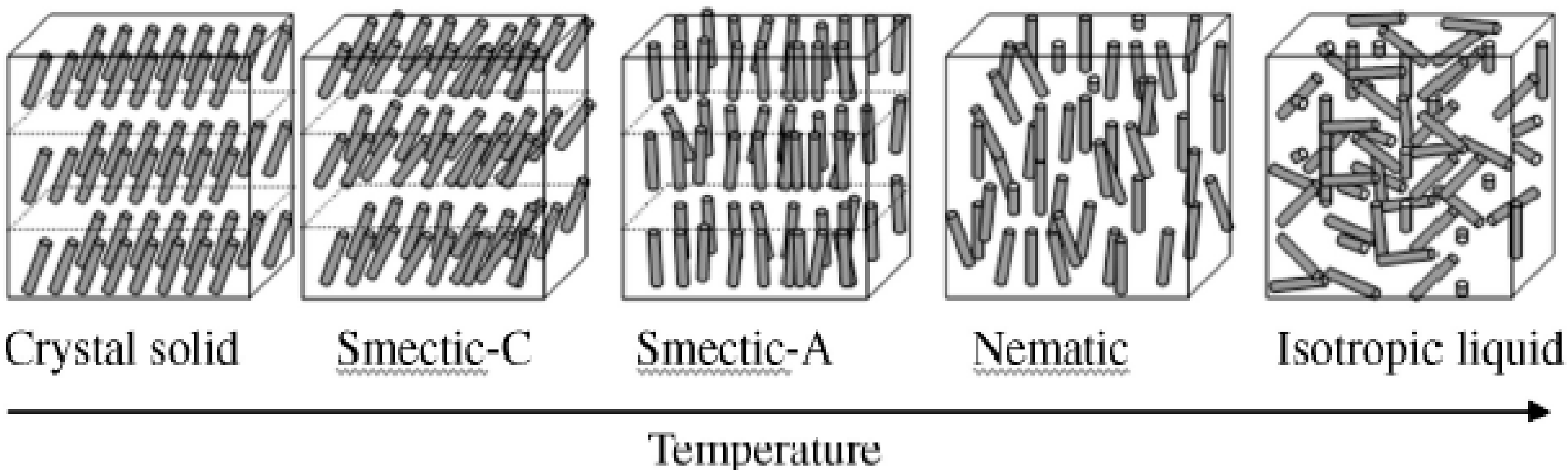
- Rigid core and flexible tails.
- The branches are approximately on one plane.
- There is no permanent dipole moment perpendicular to the plane of the molecule

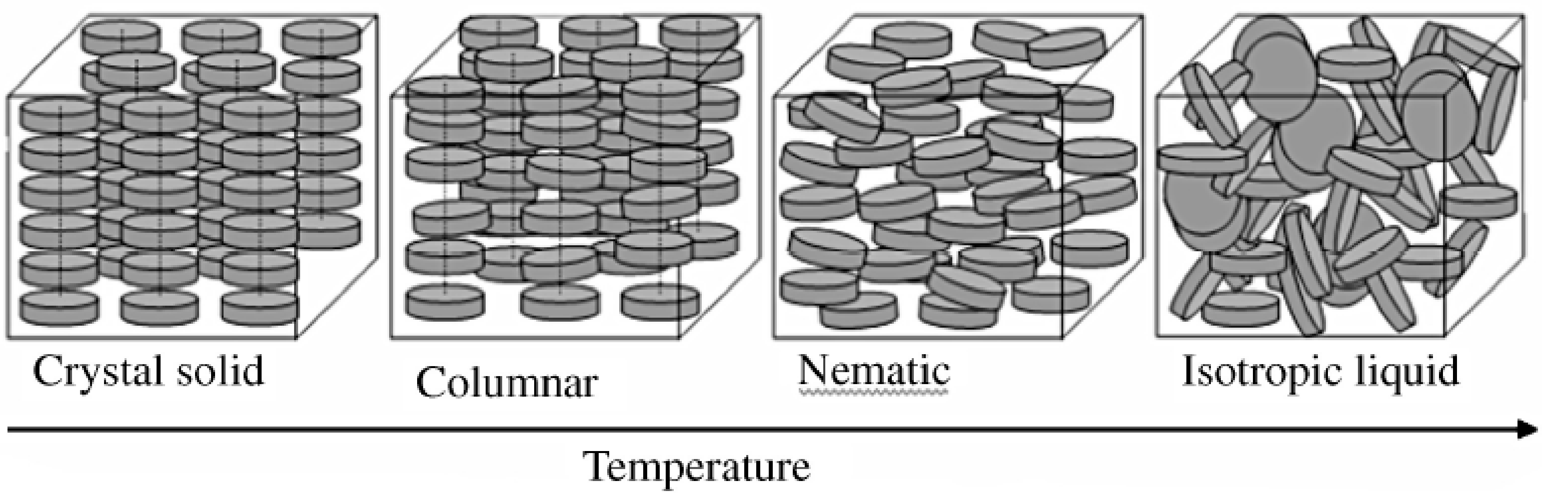






Liquid Crystal Physics

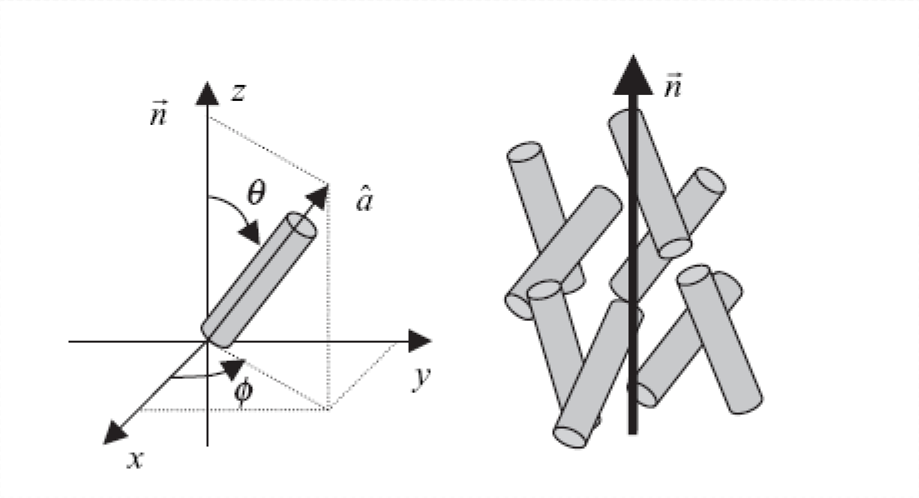




Orientational Order

The average directions of the molecular axes are along a common direction: namely, the liquid crystal ***director*** , $\hat{n}$.
The orientation of individual molecules, $\hat{a}$, is specified by the polar angle ϕ and the azimuthal angle θ where the z axis is chosen parallel to $\hat{n}$.
In general the orientational order of $\hat{a}$ is specified by an orientational distribution function: $g(\theta,\phi)$

$g(\theta,\phi)d\Omega$ probability that $\hat{a}$ is oriented along the direction specified by θ and ϕ within the solid angle $d\Omega$.



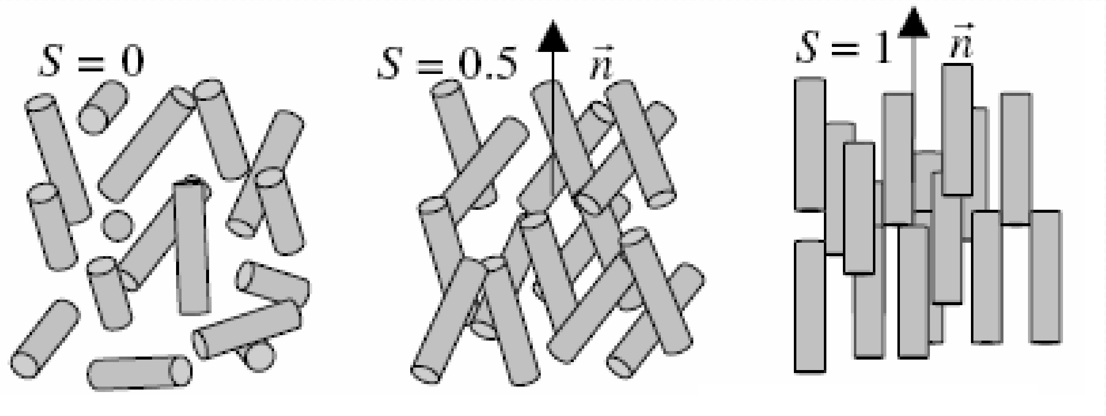
Liquid Crystals

Order Parameter

- Definition of the order parameter: $S = \langle P_2(\cos\theta)\rangle = \left\langle \frac{3\cos^2\theta - 1}{2} \right\rangle$

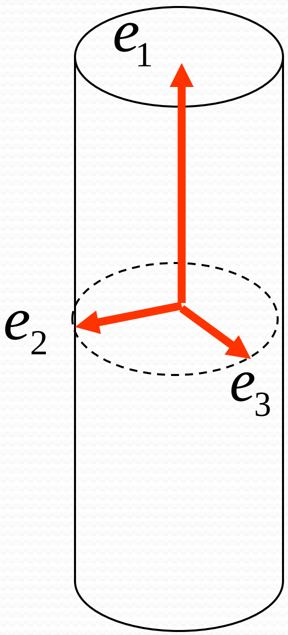
- Order parameter tensor is defined as follows: $Q_{ij} = \left\langle \frac{3n_i n_j - \delta_{ij}}{2} \right\rangle$

  The largest eigenvalue of ***Q*** gives ***S*** and the corresponding eigenvector determines the director.



Orientational Order

Uniaxial ordering

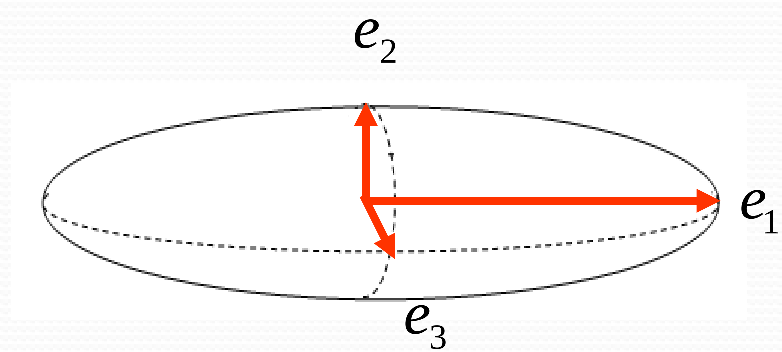


$$\lambda_1 = \frac{2}{3}S \quad , \quad \lambda_2 = -\frac{1}{3}S \quad , \quad \lambda_3 = -\frac{1}{3}S$$

Nematics are uniaxial in the bulk.
The wetting layer may exhibit *biaxiality* due to the lower symmetry near the surface.

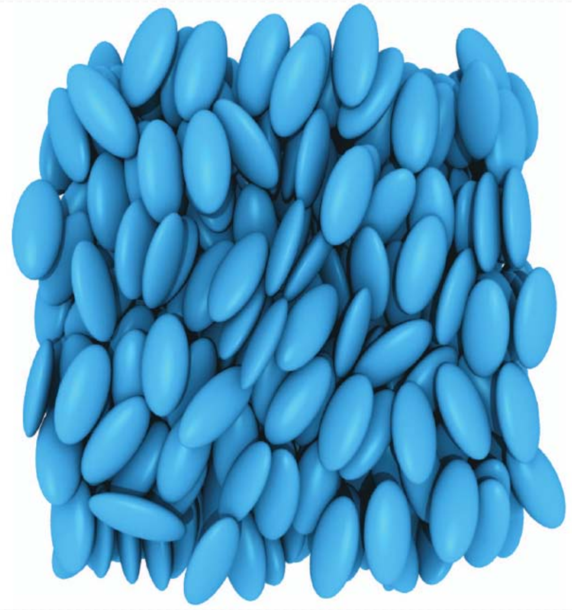
T. J. Sluckin and A. Poniewierski, *Phys. Rev. Lett.*, **55 2907**(1985).

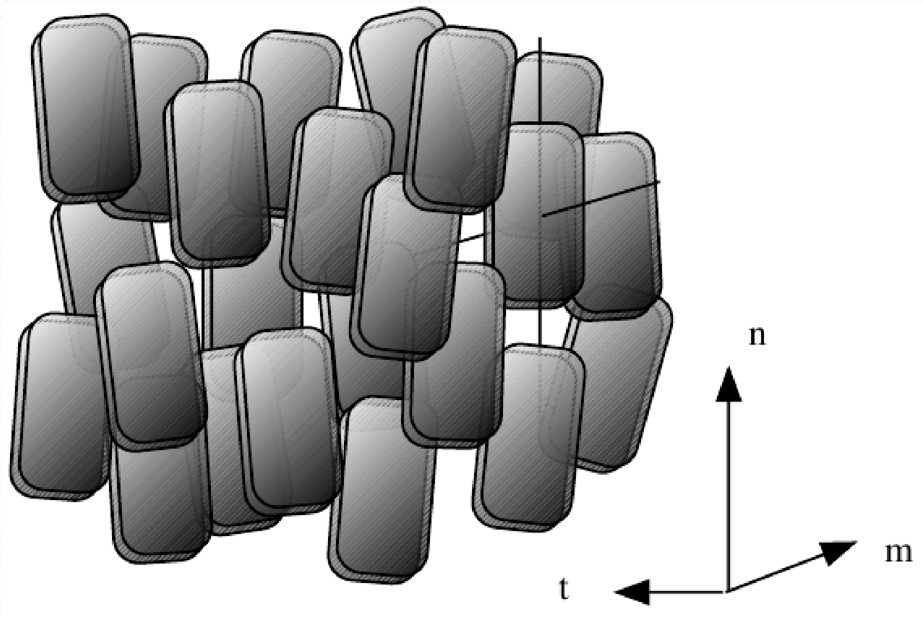
Biaxial ordering



$$\lambda_1 = \frac{2}{3}S \quad , \quad \lambda_2 = -\frac{1}{3}S(1+B) \quad , \quad \lambda_3 = -\frac{1}{3}S(1-B) \quad , \quad 0 \le B \le 1$$

Biaxial nematic phase

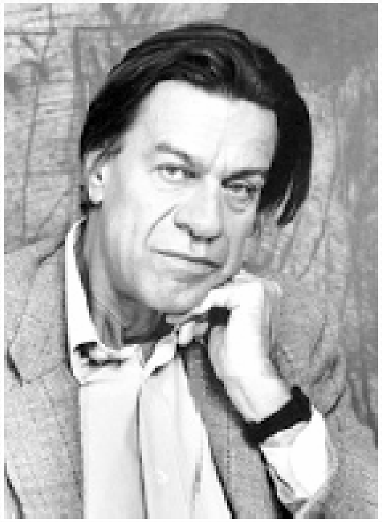




R. Berardi, J. S. Linturuori, M. R. Wilson, C. Zannoni, J. Chem. Phys. (2011)
M. Kleman, O. Lavrentovich, Soft Matter Physics An Introduction (2003)

Isotropic – Nematic transition

Landau-de Gennes theory



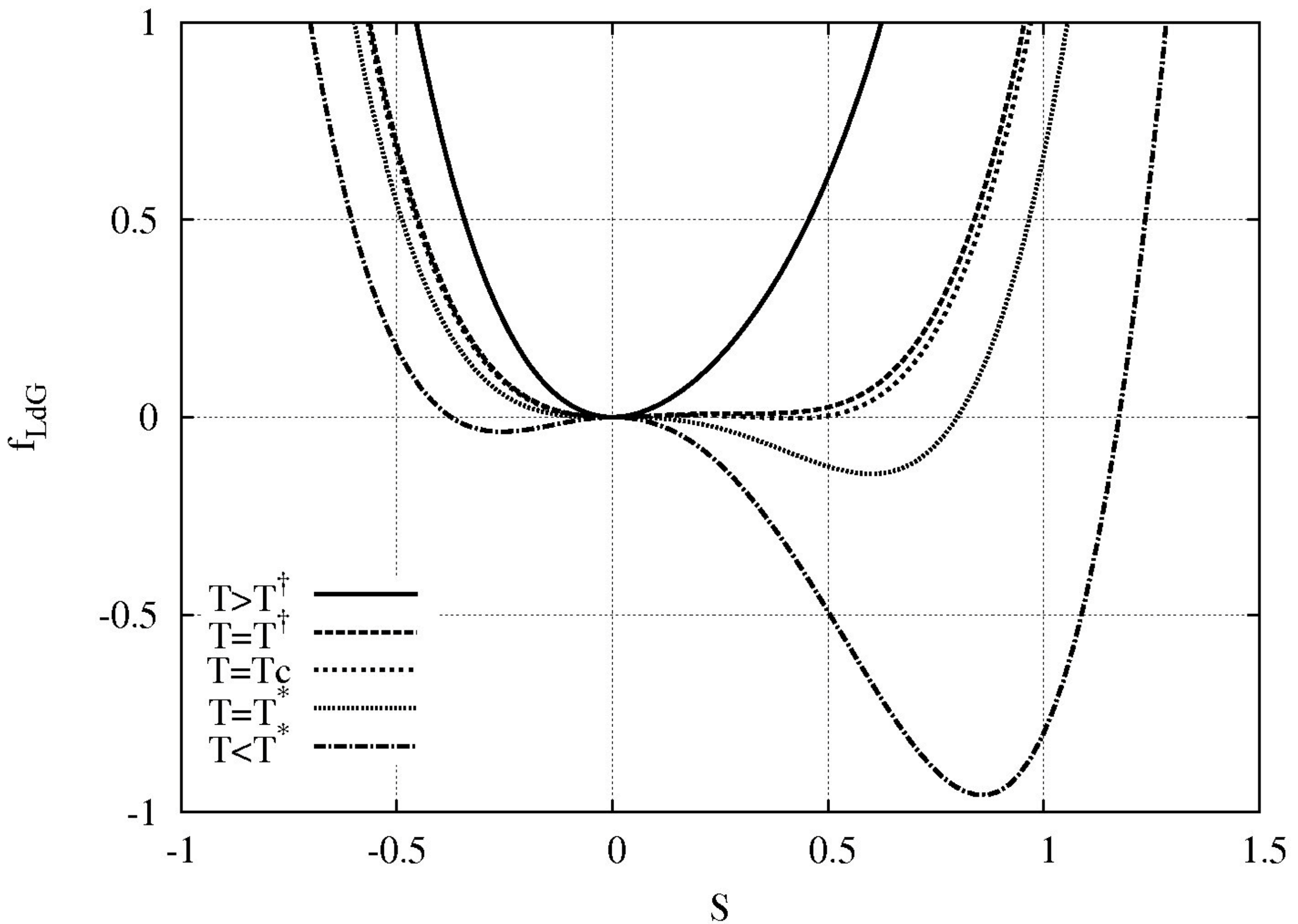
De Gennes

- De Gennes extended Landau's theory to the isotropic–nematic transition because it is a weak first-order transition.
- The free energy density *f* of the material can be expressed in terms of the order parameter *S* as

$$f = \frac{1}{2}a(T - T^*)S^2 - \frac{1}{3}bS^3 + \frac{1}{4}cS^4$$

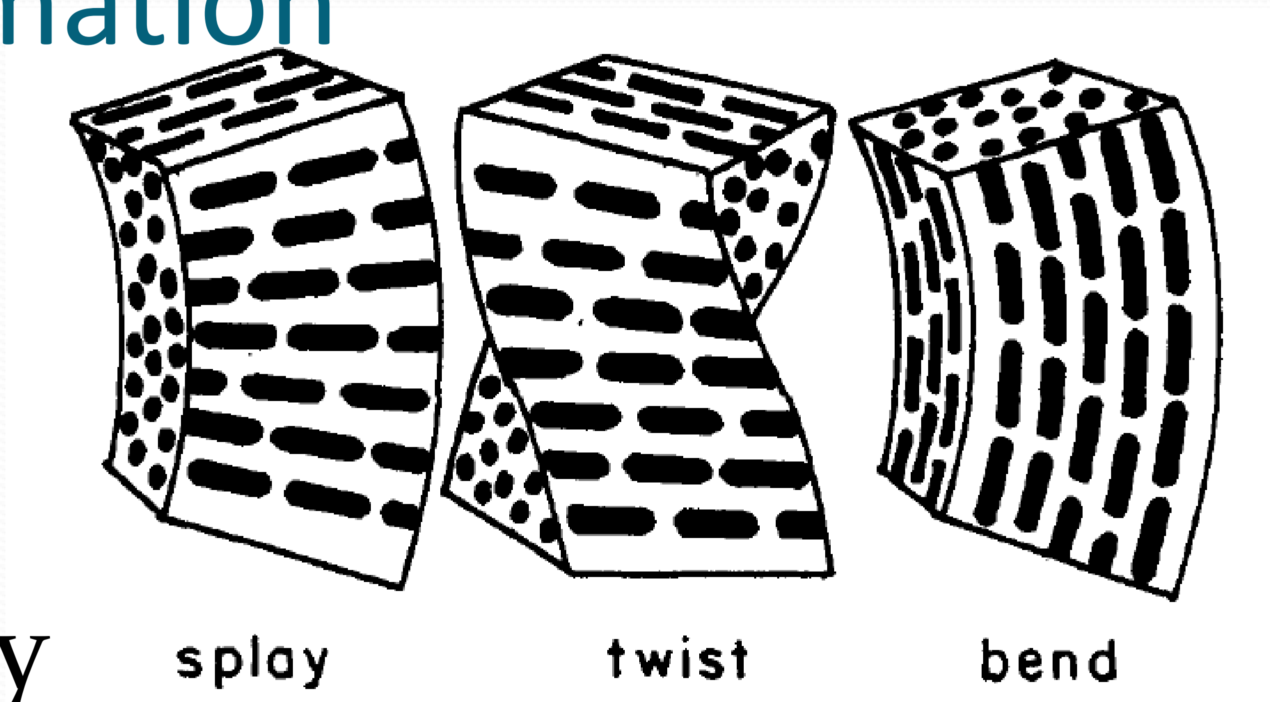
$$F_{LdG}[Q] = \int_{\Omega} \left\{ \frac{1}{2}a(T - T^*)Tr[Q.Q] - \frac{1}{3}BTr[Q.Q.Q] + \frac{1}{4}C(Tr[Q.Q])^2 \right\} dV$$

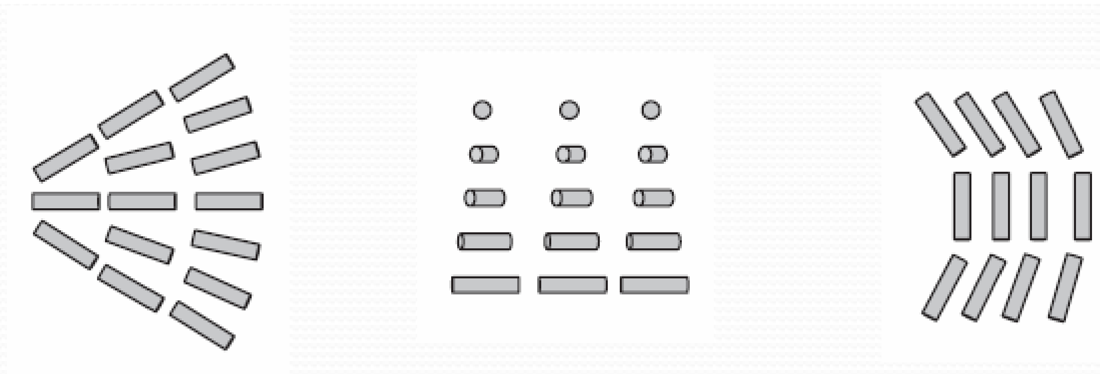
Landau- de Gennes theory



Deformation

Elasticity





Straley Stephen, Reviews of Modern Physics, 46, 4, (1974)

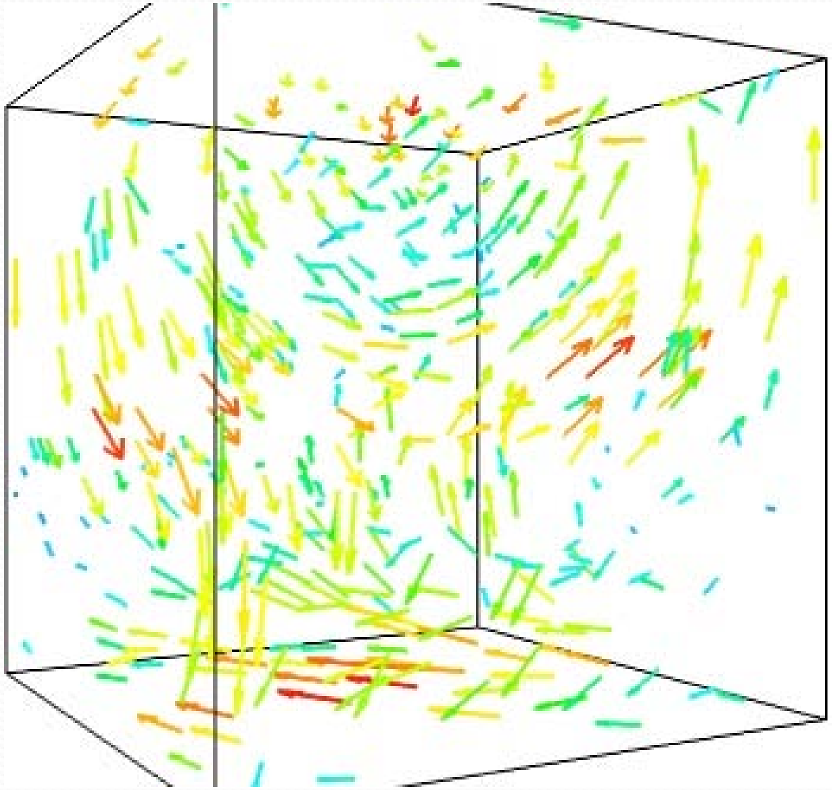
Elastic Energy

$$f_{Elastic} = \frac{1}{2} K_{splay} \left(\vec{\nabla} \cdot \hat{n} \right)^2 + \frac{1}{2} K_{twist} \left(\hat{n} \cdot \vec{\nabla} \times \hat{n} \right)^2 + \frac{1}{2} K_{bend} \left(\hat{n} \times \vec{\nabla} \times \hat{n} \right)^2$$

P.G. de Gennes and J. Prost, *The Physics of Liquid Crystals*,
2nd ed. (Oxford University Press, Oxford, 1993).

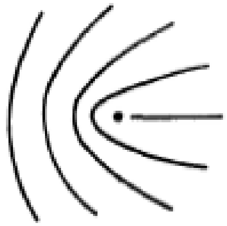
Boundary condition effect

Defects

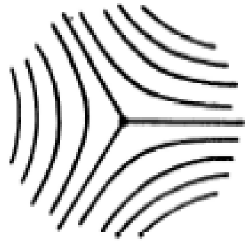


Defects

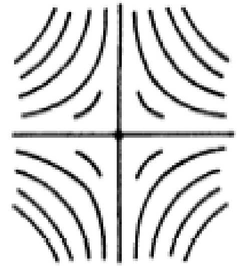
$$\theta(x,y) = s\tan^{-1}\left(\tfrac{y}{x}\right) + c$$



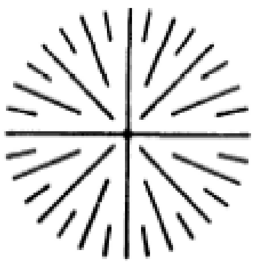
$s=\frac{1}{2}$



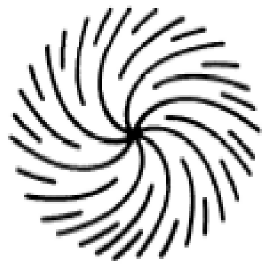
$s=-\frac{1}{2}$



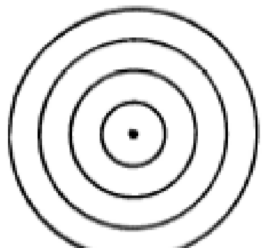
$s=-1$



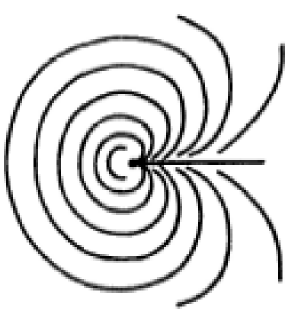
$s=1,\ c=0$



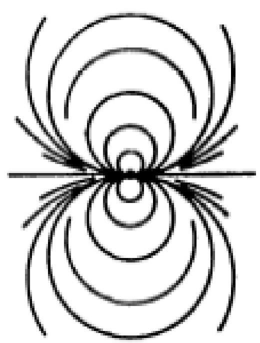
$s=1,\ c=\pi/4$



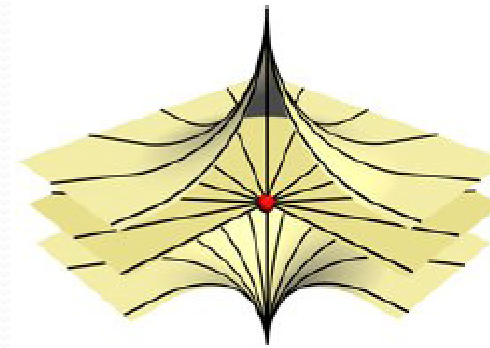
$s=1,\ c=\pi/2$

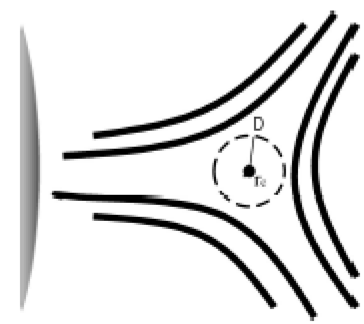


$s=3/2$



$s=2$





$$\theta_1(x,y) = s_1\tan^{-1}\left(\tfrac{y}{x}\right) + c_1$$

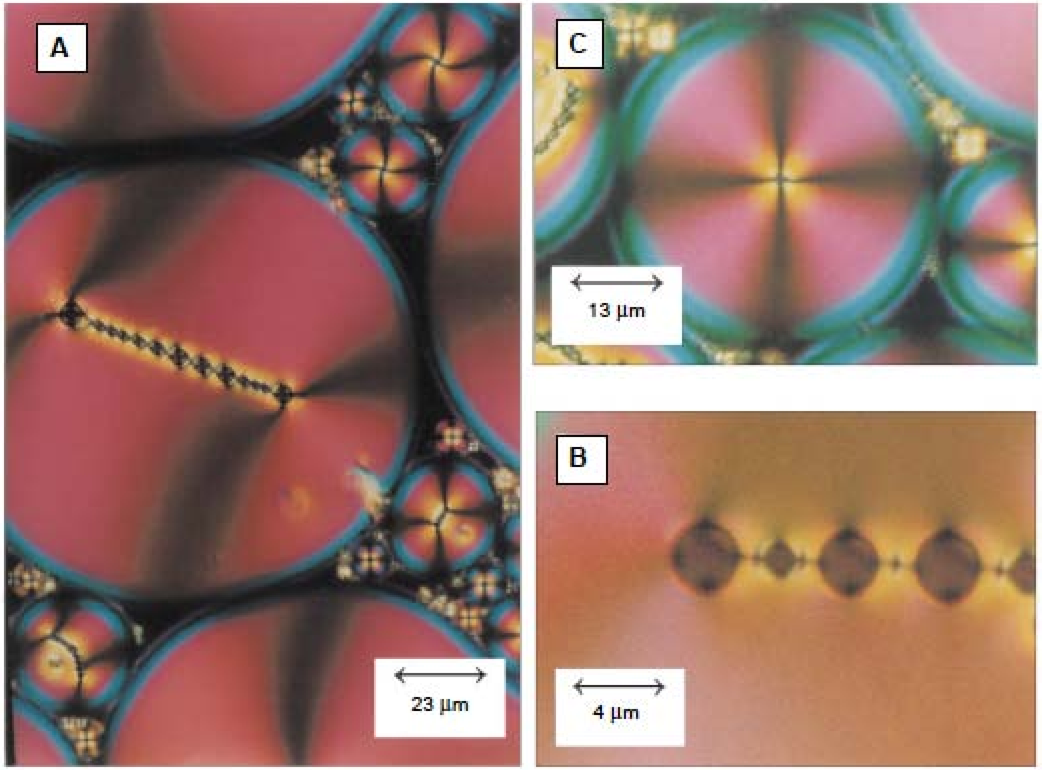
$$\theta_2(x,y) = s_2\tan^{-1}\left(\tfrac{y}{x}\right) + c_2$$

$$\theta = \theta_1 + \theta_2$$

Defects

The control of the anchoring is achieved experimentally by using various amphiphilic compounds which are adsorbed at the water–liquid-crystal interface. Molecular **surfactants** are used to induce strong normal anchoring, while a **polymer** is used to induce strong planar anchoring.

P. Poulin, and D. A. Weitz, Phys. Rev. E 57, 626 (1998).



Philippe Poulin, Holger Stark, T. C. Lubensky, D. A. Weitz, *Science* 75, 1770 (1997)

Colloidal droplets in nematic medium

The alignment of a nematic liquid crystal by a ***bounding interface*** is of considerable interest both for fundamental and technological reasons.

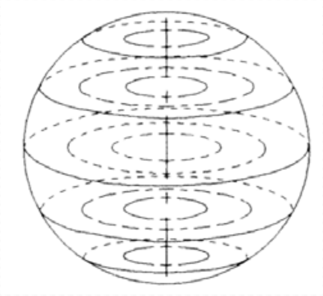
- ***homeotropic*** anchoring, where the preferred, or "easy", average orientation corresponds to ***n*** normal to the interface.

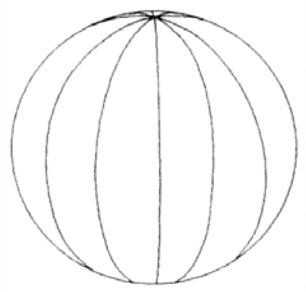
- ***planar*** anchoring, where the preferred average orientation corresponds to ***n*** lying in one particular direction parallel to the interface

- ***planar degenerate*** anchoring, where all the planar orientations for ***n*** are equivalent easy directions.

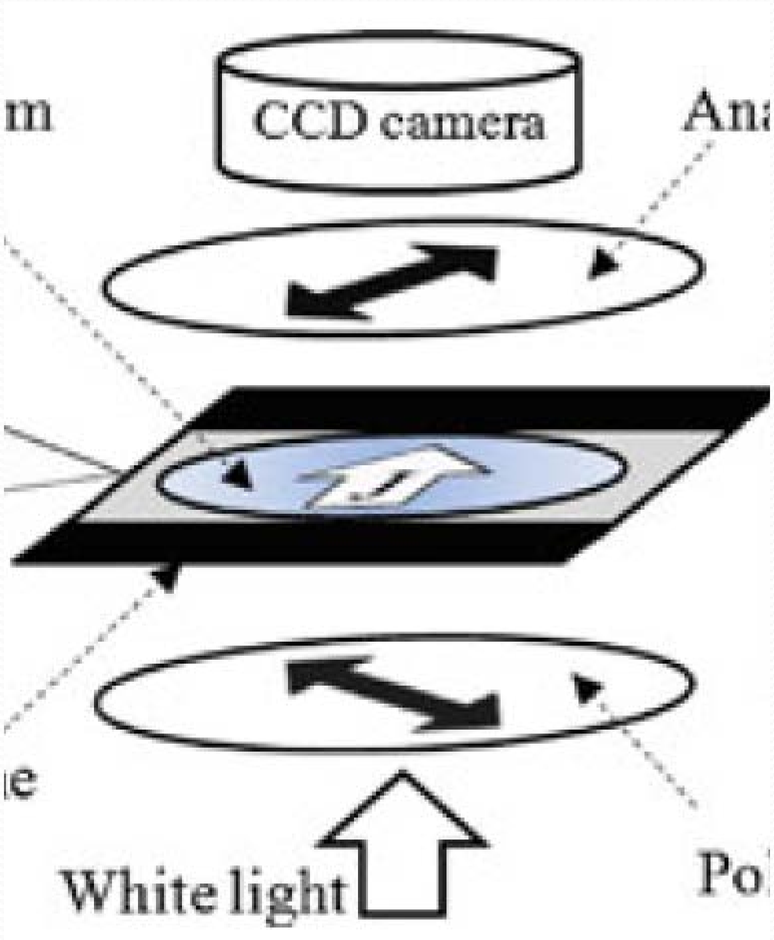
J.-B. Fournier and P. Galatola, *Europhys. Lett.*, **72** (3), pp. 403–409 (2005).

Planar anchoring on sphere

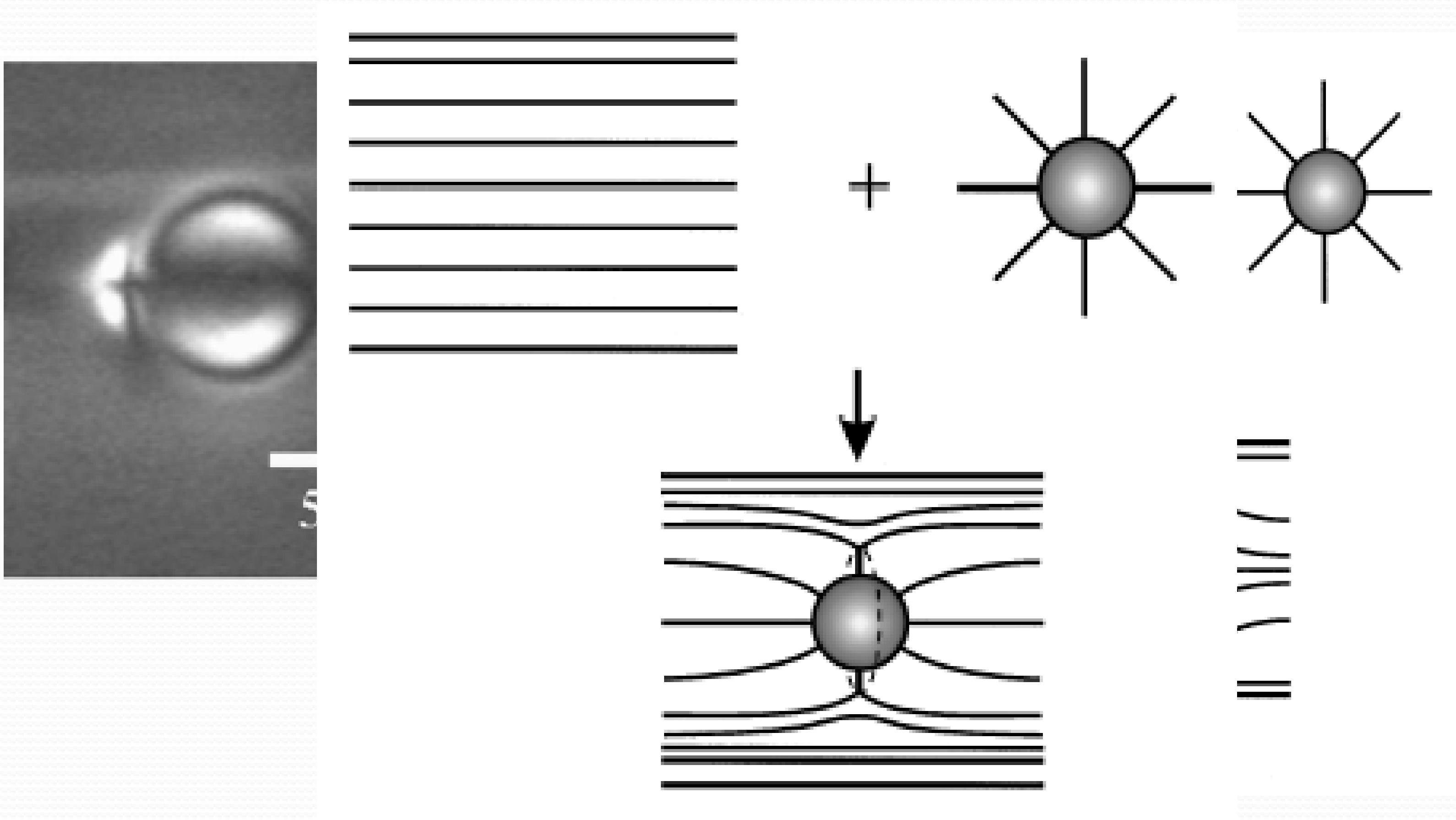




How to observe

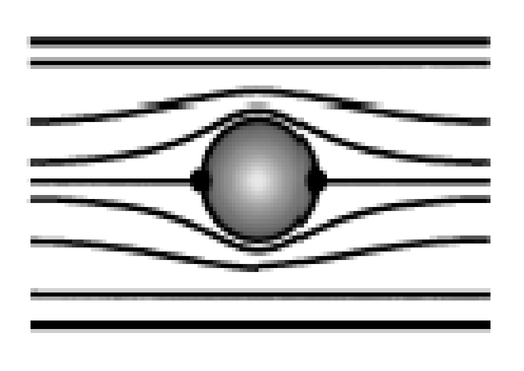


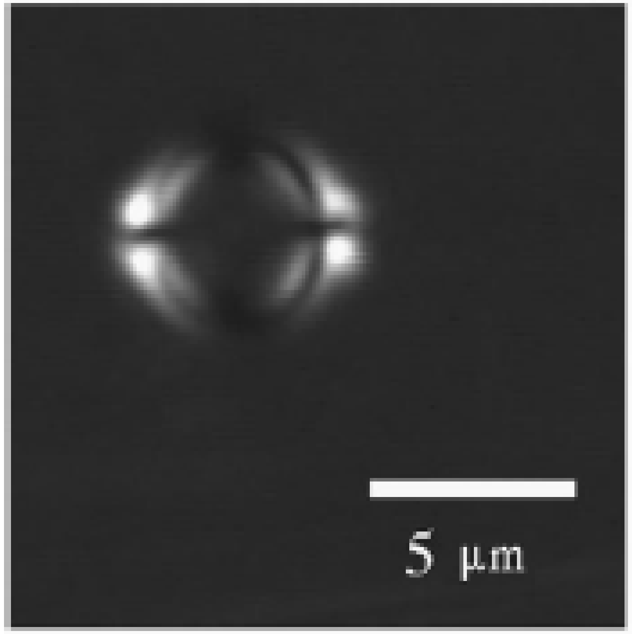
Colloids in Nematic



Poulin & Weitz, PRE 1998

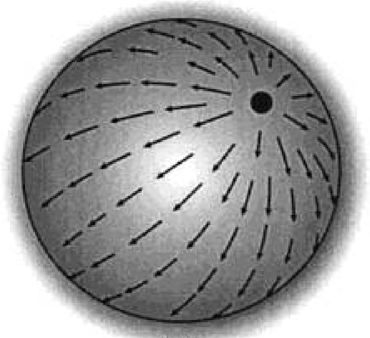
Colloids in Nematic



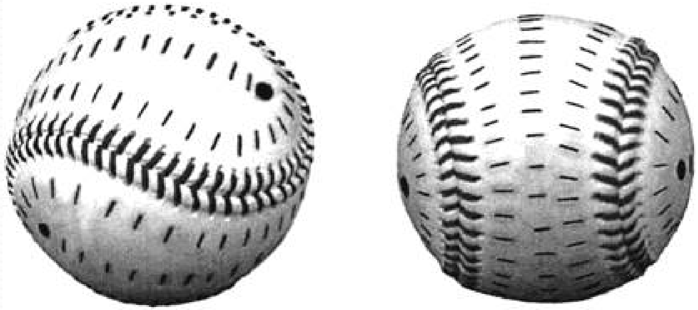


Poulin & Weitz, PRE 1998

Quadrapolar configurations



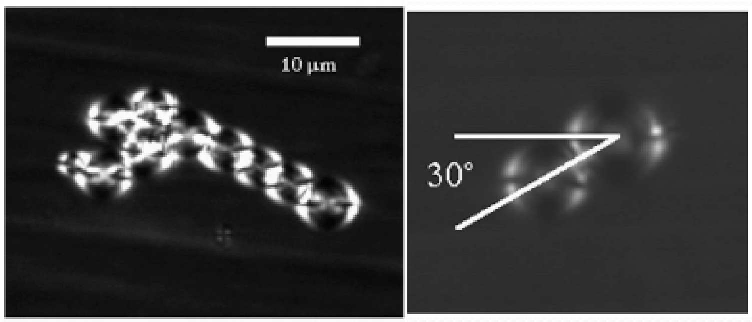
(a)

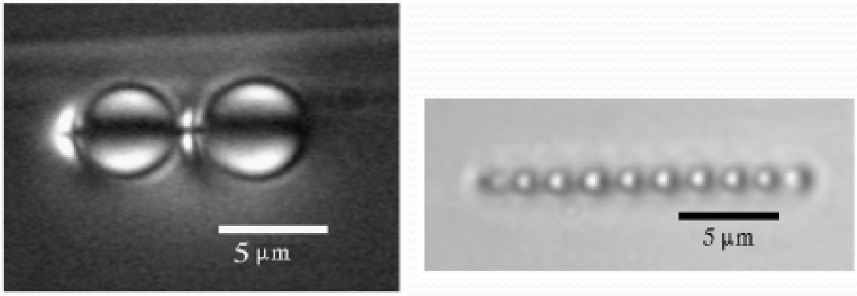


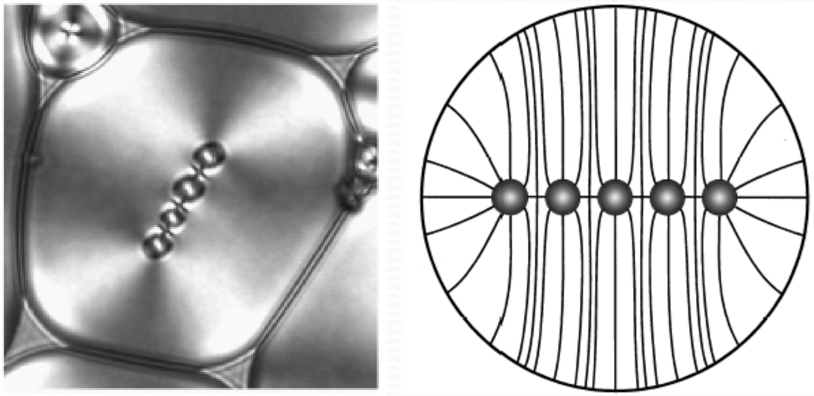
(b)

Nano Letters, Vol.2, No.10 ,1125-1129 (2002)

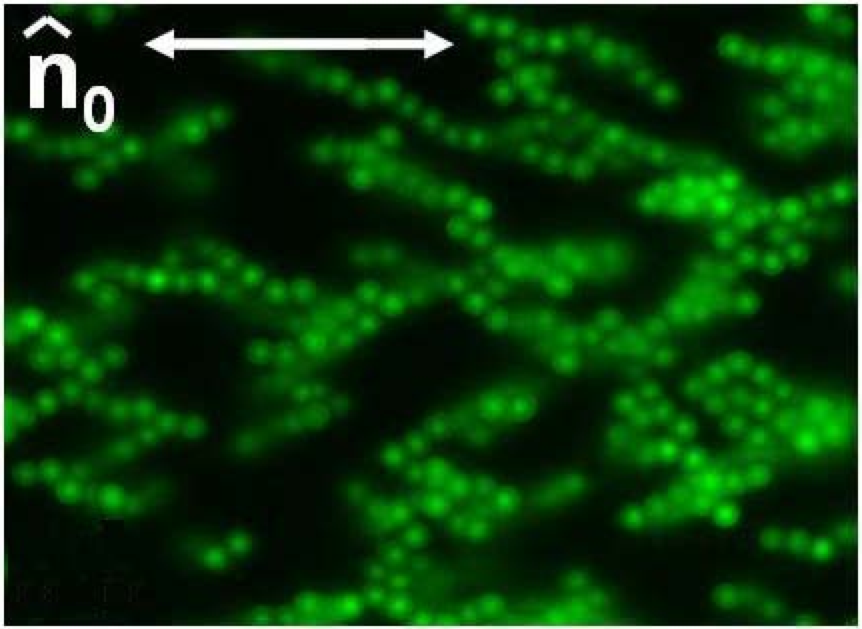
Aggregations

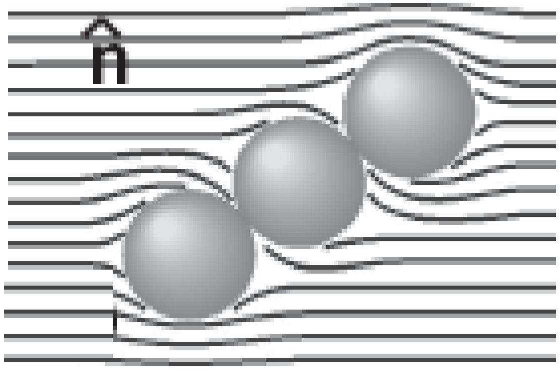


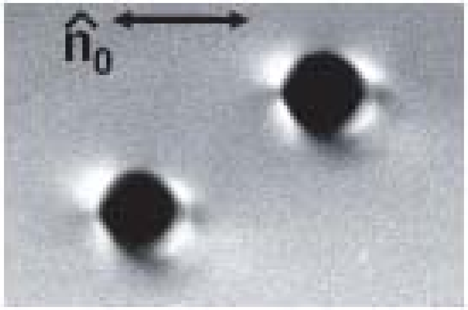


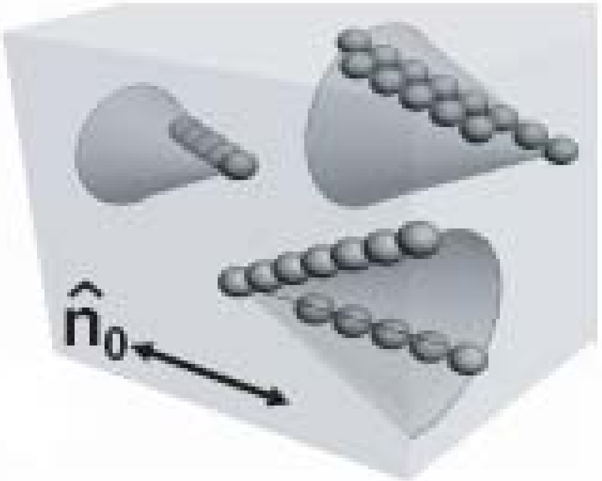


Poulin & Weitz, PRE 1998





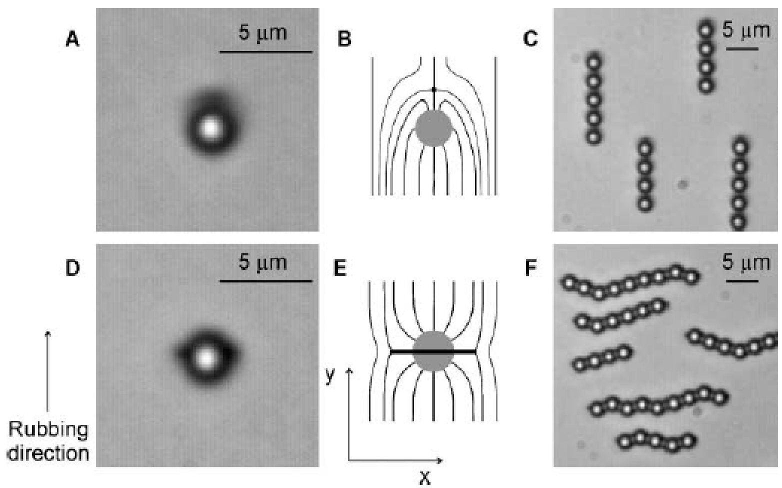


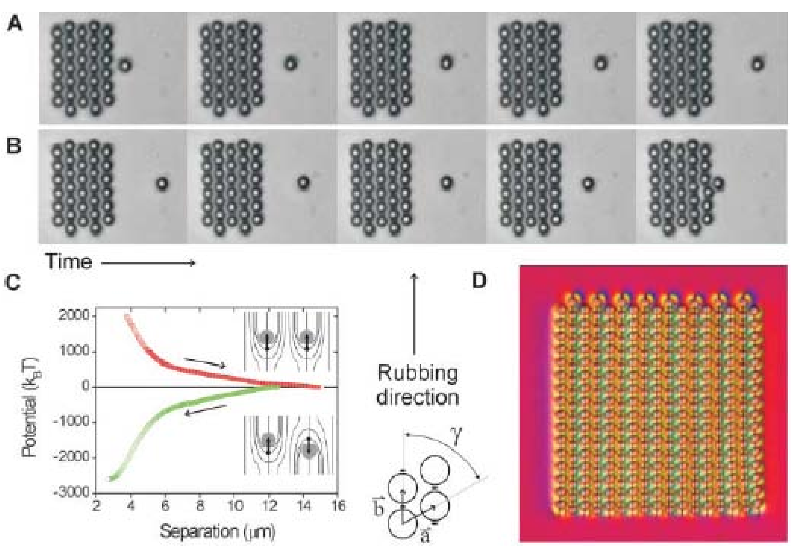


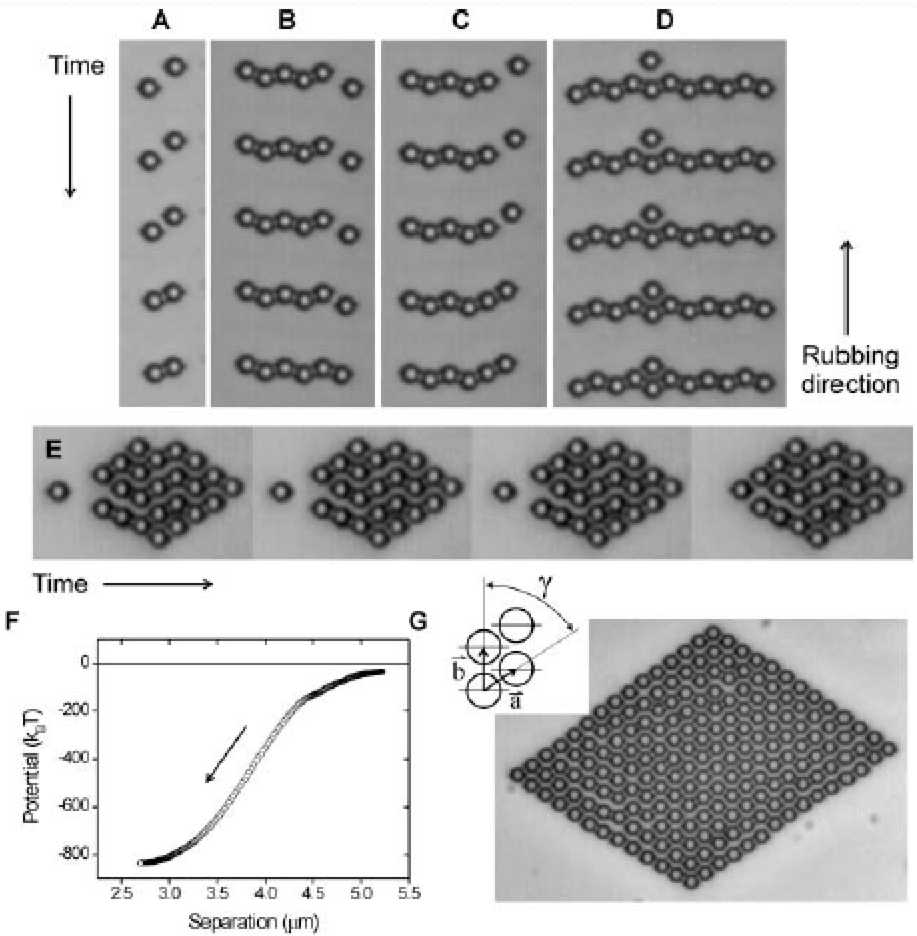
fluorescence confocal polarizing microscopy (FCPM) to characterize the director distortions around the particles and ***optical trapping with laser tweezers*** to measure the pair interaction force

I. I. Smalyukh, *et al.*, PRL **95**, 157801 (2005)

Two-Dimensional Nematic Colloidal Crystals Self-Assembled by Topological Defects
Igor Musevic, *et al.*
Science **313**, 954 (2006);
DOI: 10.1126/science.1129660







PRL 100, 217803 (2008) PHYSICAL REVIEW LETTERS week ending 30 MAY 2008

2D Interactions and Binary Crystals of Dipolar and Quadrupolar Nematic Colloids

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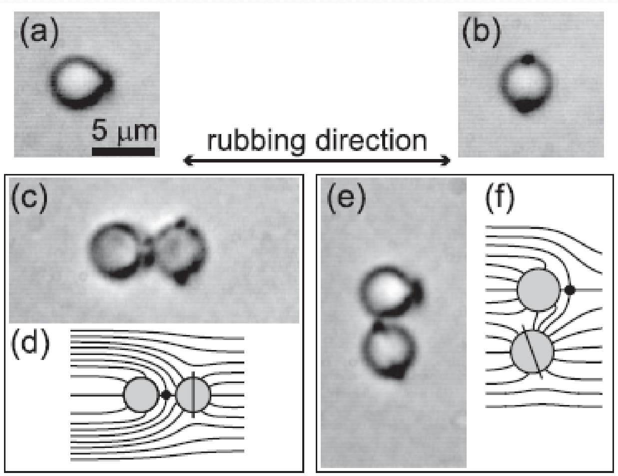
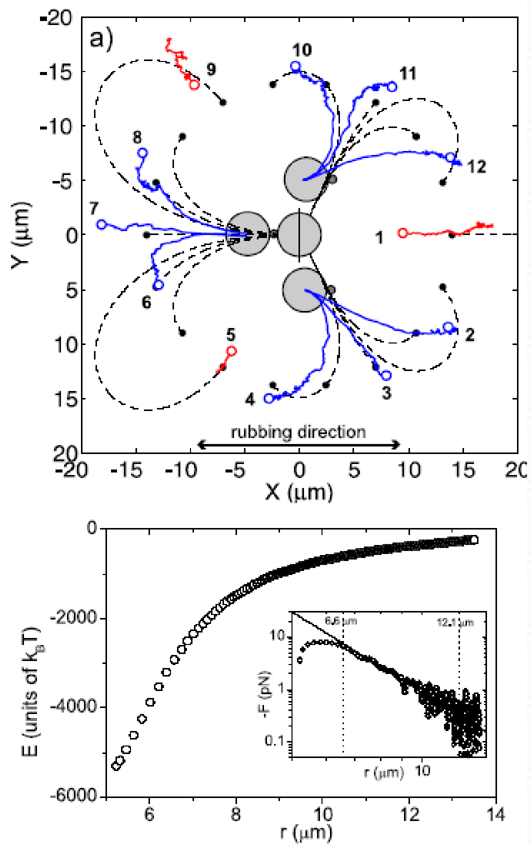
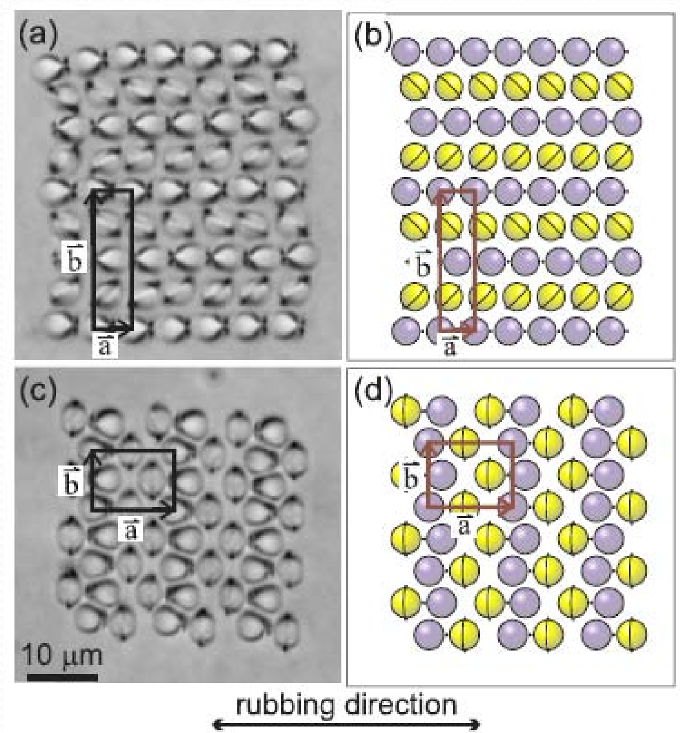
(Received 15 February 2008; published 30 May 2008)







VOLUME 92, NUMBER 18 PHYSICAL REVIEW LETTERS week ending 7 MAY 2004

Direct Observation of Anisotropic Interparticle Forces in Nematic Colloids with Optical Tweezers

Makoto Yada,[1,*] Jun Yamamoto,[1] and Hiroshi Yokoyama[1,2]
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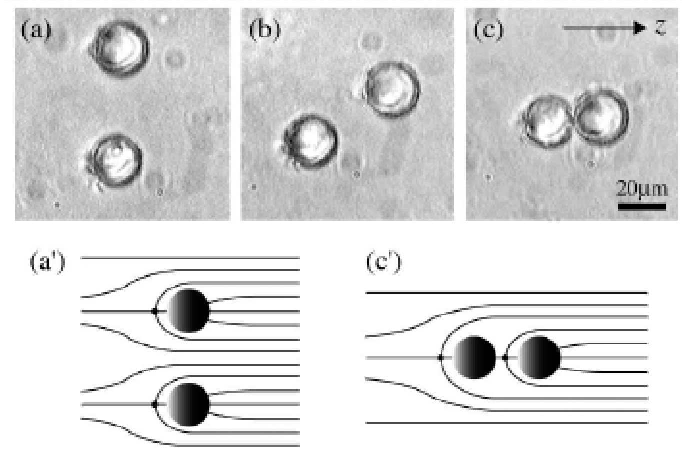
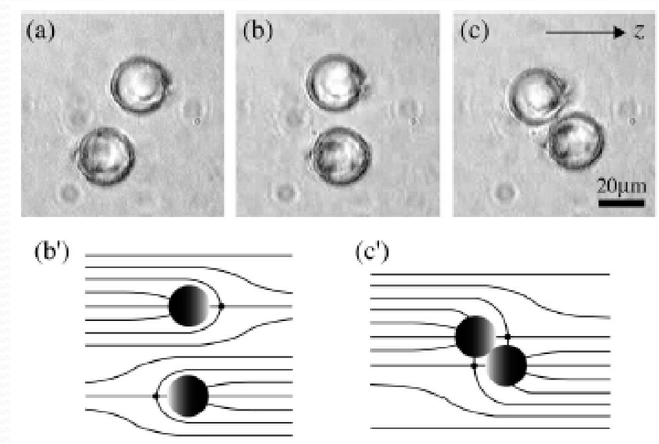
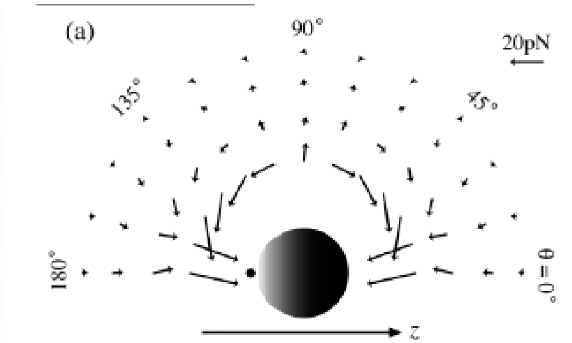
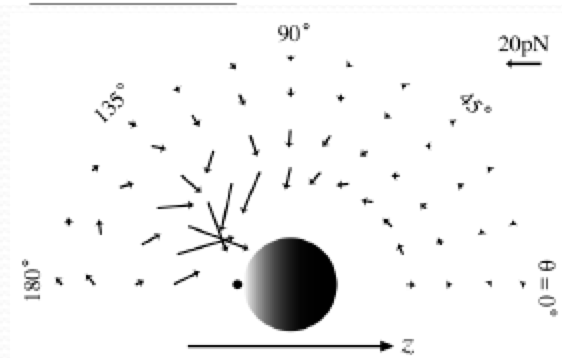
(Received 23 November 2003; published 3 May 2004)

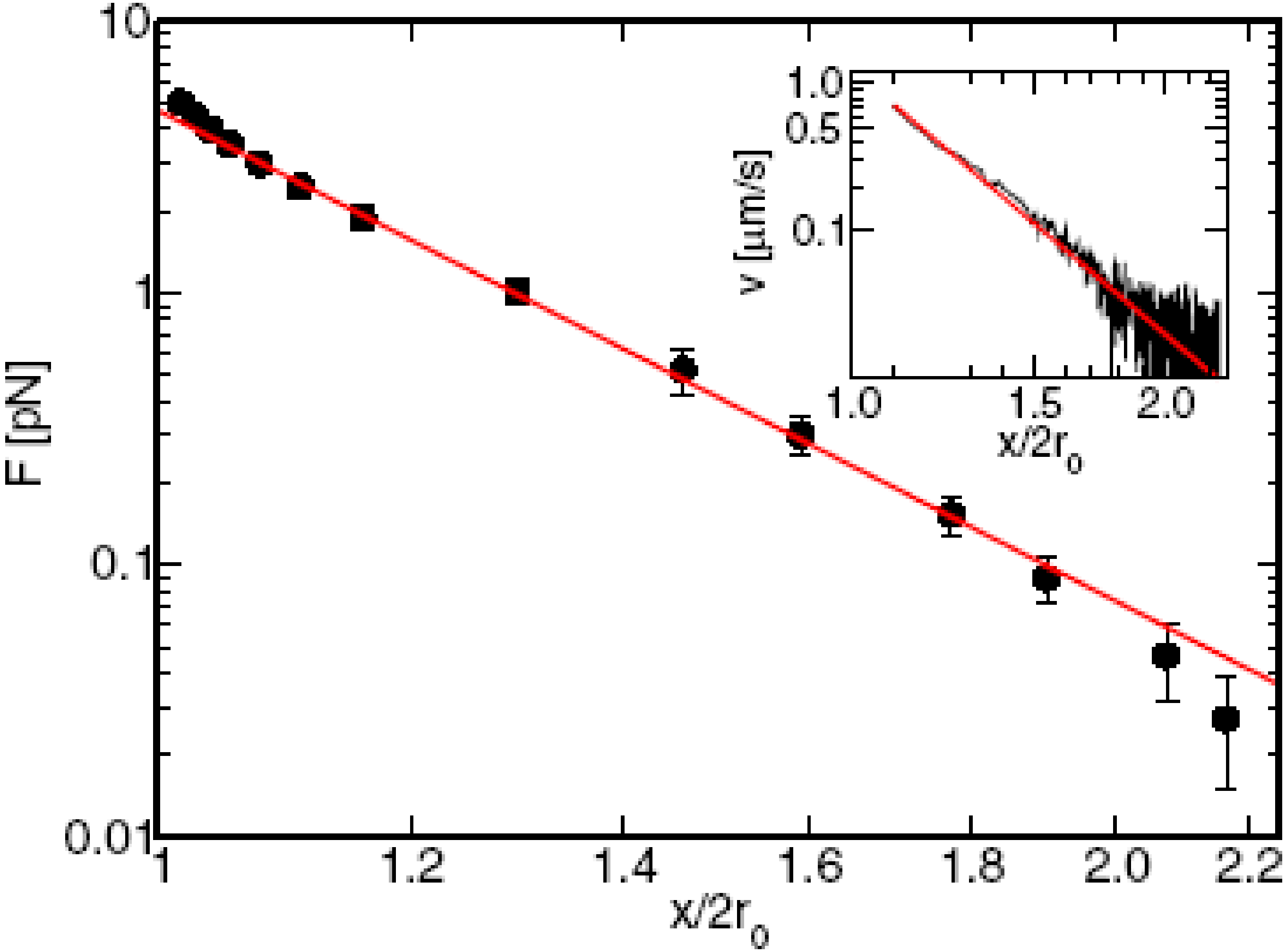


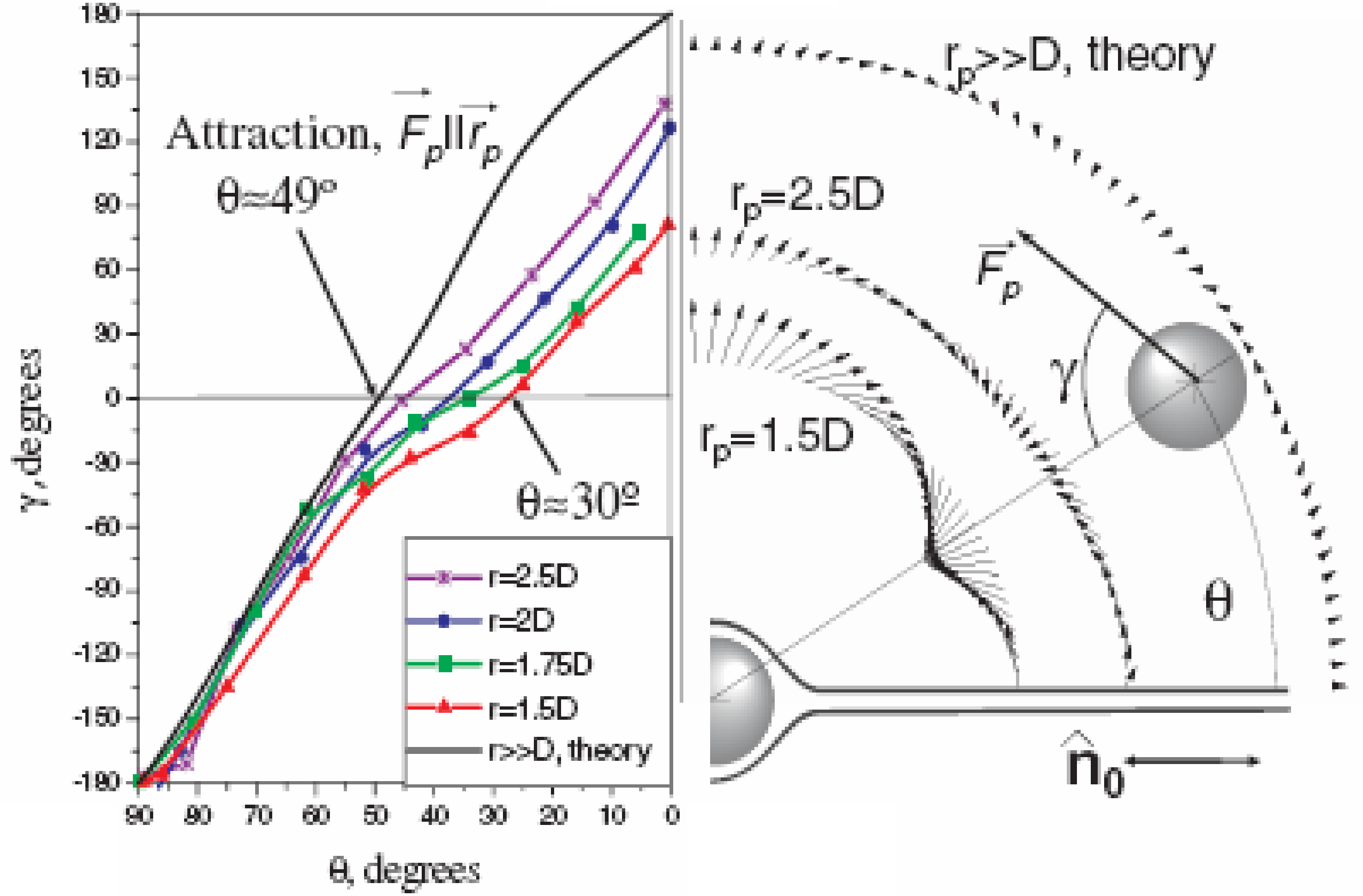






Interparticle Potential and Drag Coefficient in Nematic Colloids



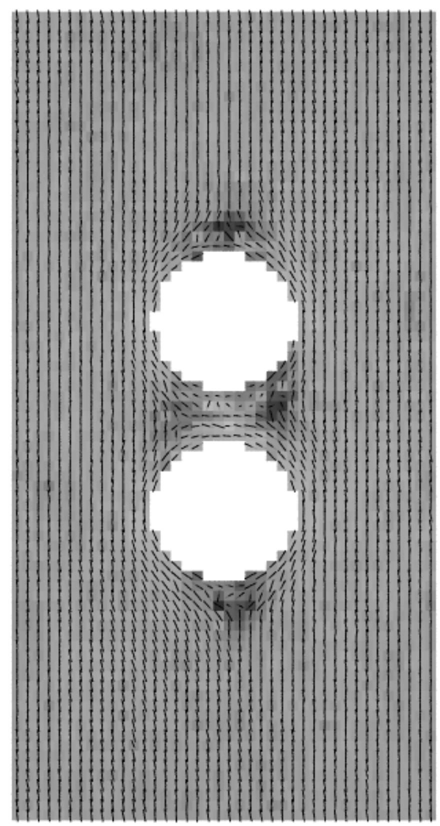


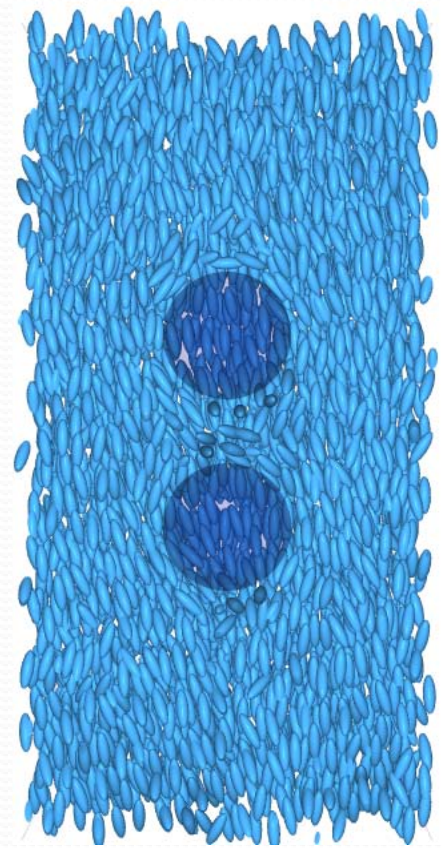
I. I. Smalyukh, *et al.*,
PRL **95**, 157801 (2005)

Two colloidal droplets in nematic medium (Parallel)

Rigid Body MD

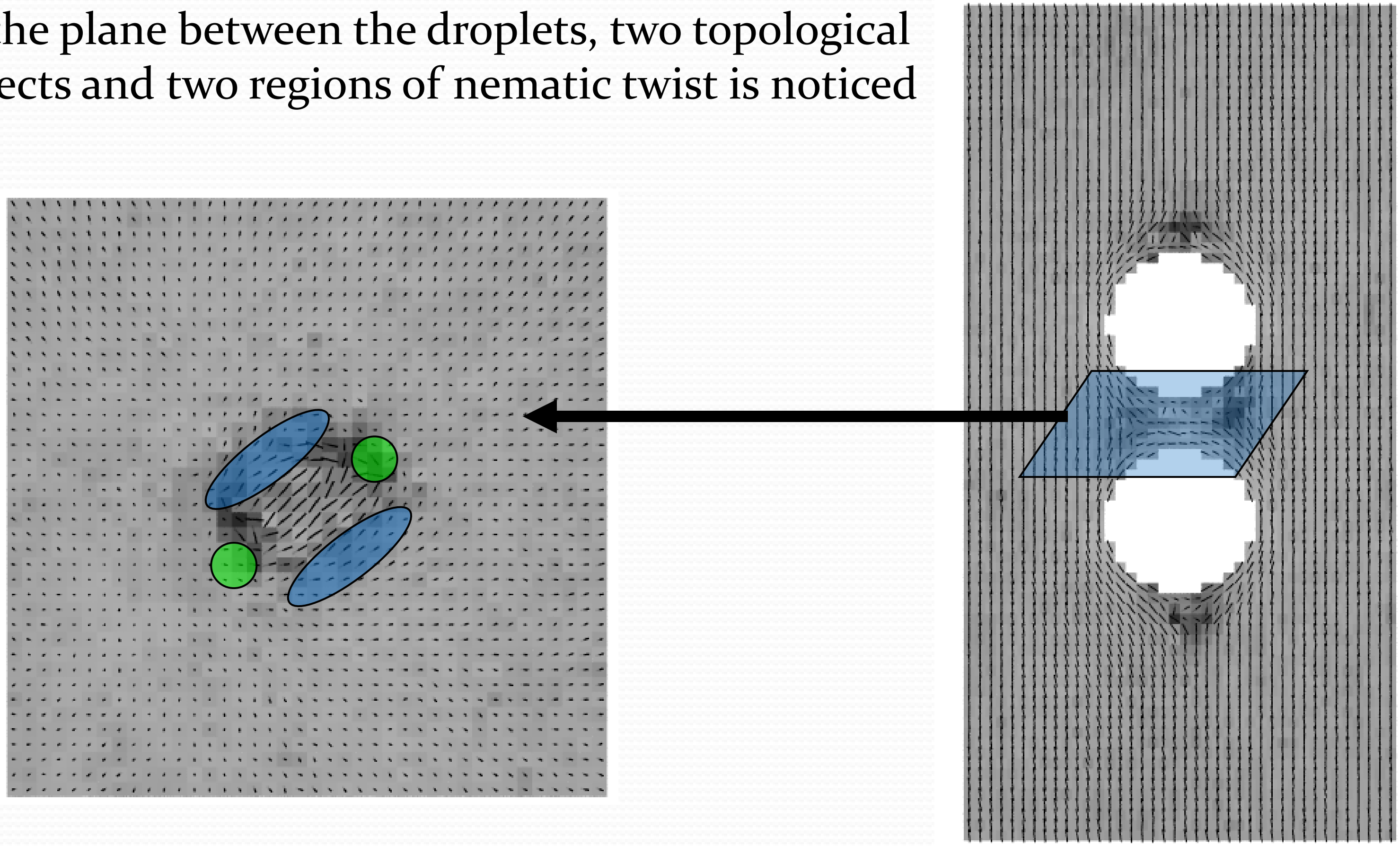
- Mean force exerted to the droplets along their connecting line is $1.9 \pm 0.3\ [\varepsilon/\sigma]$
- A spontaneous symmetry breaking mechanism positions the mesogens between the droplets in an orthogonal configuration
- Two boojums appear on the northern pole of the upper and southern pole of the lower droplet
- The nematic director tends to tilt





Two colloidal droplets in nematic medium (Parallel)

- In the plane between the droplets, two topological defects and two regions of nematic twist is noticed

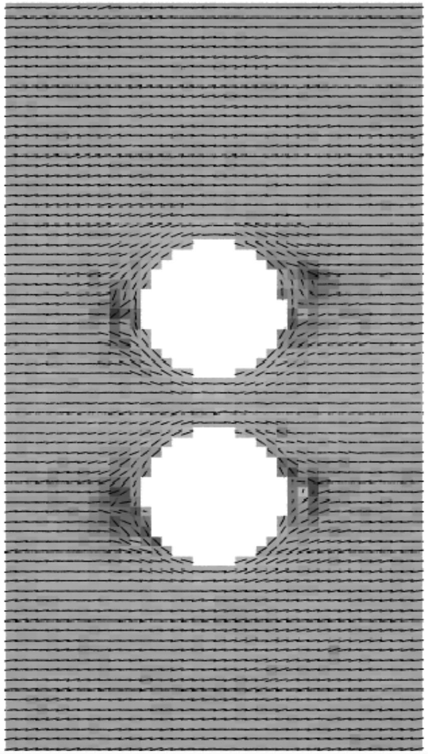


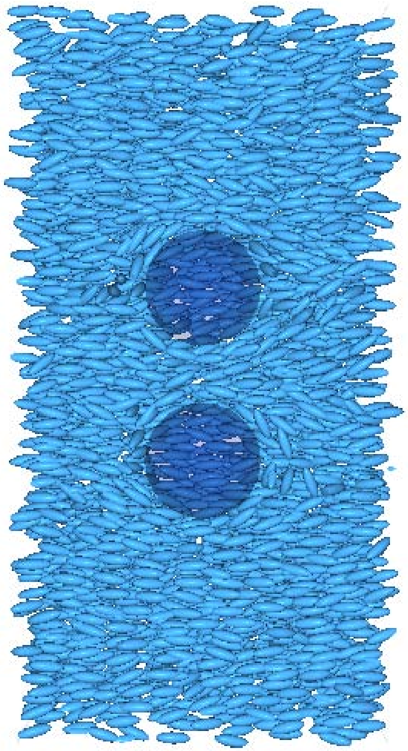
Two colloidal droplets in nematic medium (Perp.)

- Mean force exerted to the droplets along their connecting line was in the order of measurement error

- A boojum appears on each pole of the droplets along the nematic director

- The nematic director tends to tilt





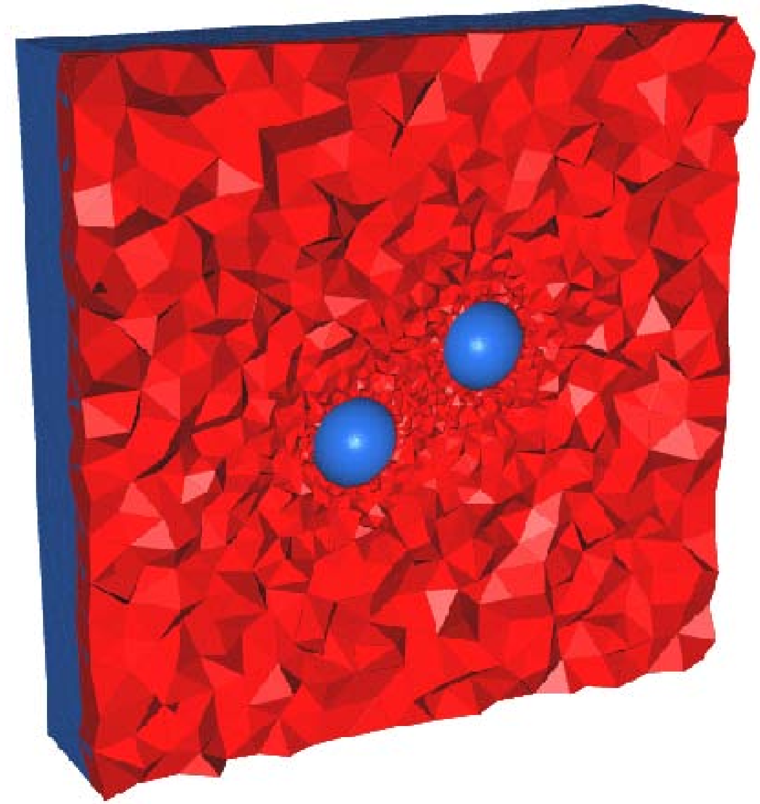
Finite element method

$$\hat{F} = (\hat{F}_{LdG} - f_o V) + \hat{F}_{Elastic} + \hat{F}_{Surface}$$

$$\hat{F}[q] = \int_{\Omega} \left\{ \frac{\tau}{2} Tr[q.q] - \frac{\sqrt{6}}{4} Tr[q.q.q] + \frac{1}{4} (Tr[q.q])^2 - f_o \right\} d\hat{V}$$

$$+ \frac{1}{2} \left(\frac{\xi}{R} \right)^2 \int_{\Omega} (\hat{\partial}_k q_{ij} \hat{\partial}_k q_{ij}) d\hat{V}$$

$$+ \left(\frac{\hat{W}}{R} \right) \int_{\partial\Omega} (\tilde{q}_{ij} - \tilde{q}_{ij}^{\perp})(\tilde{q}_{ij} - \tilde{q}_{ij}^{\perp}) d\hat{S}$$

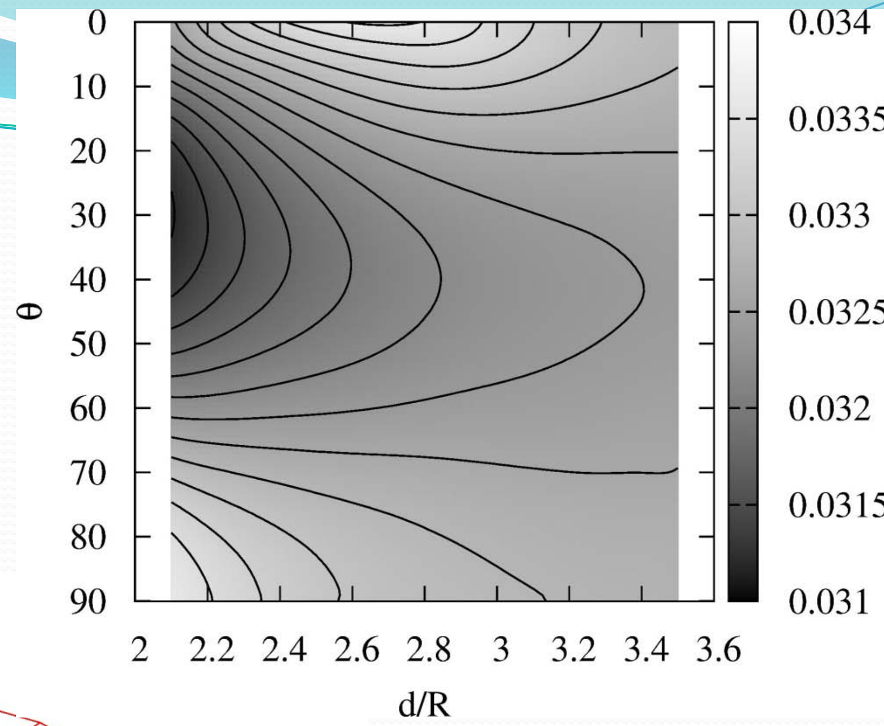


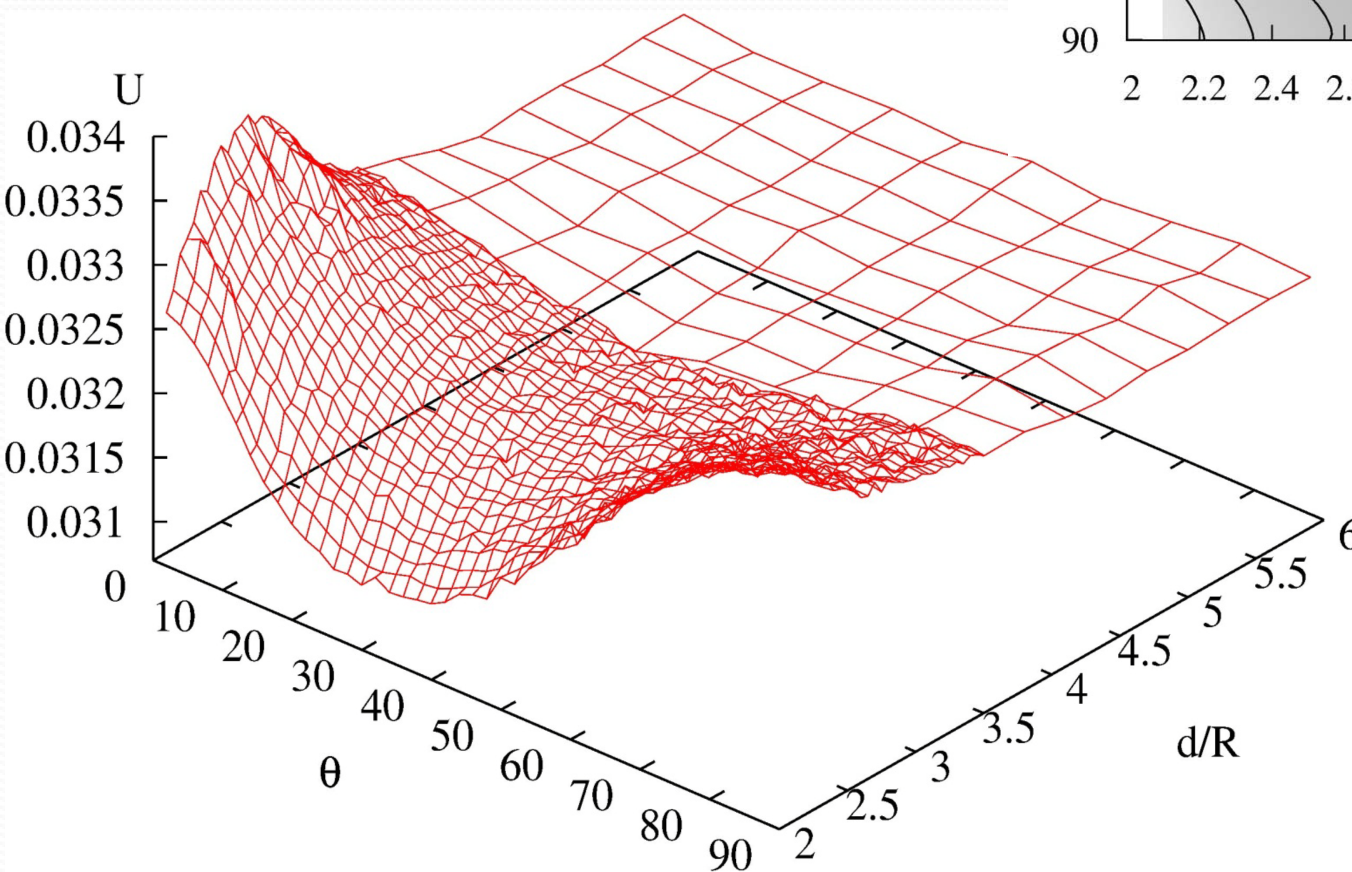
Gmsh mesh generator

Conjugate Gradient minimizing method

3D calculations

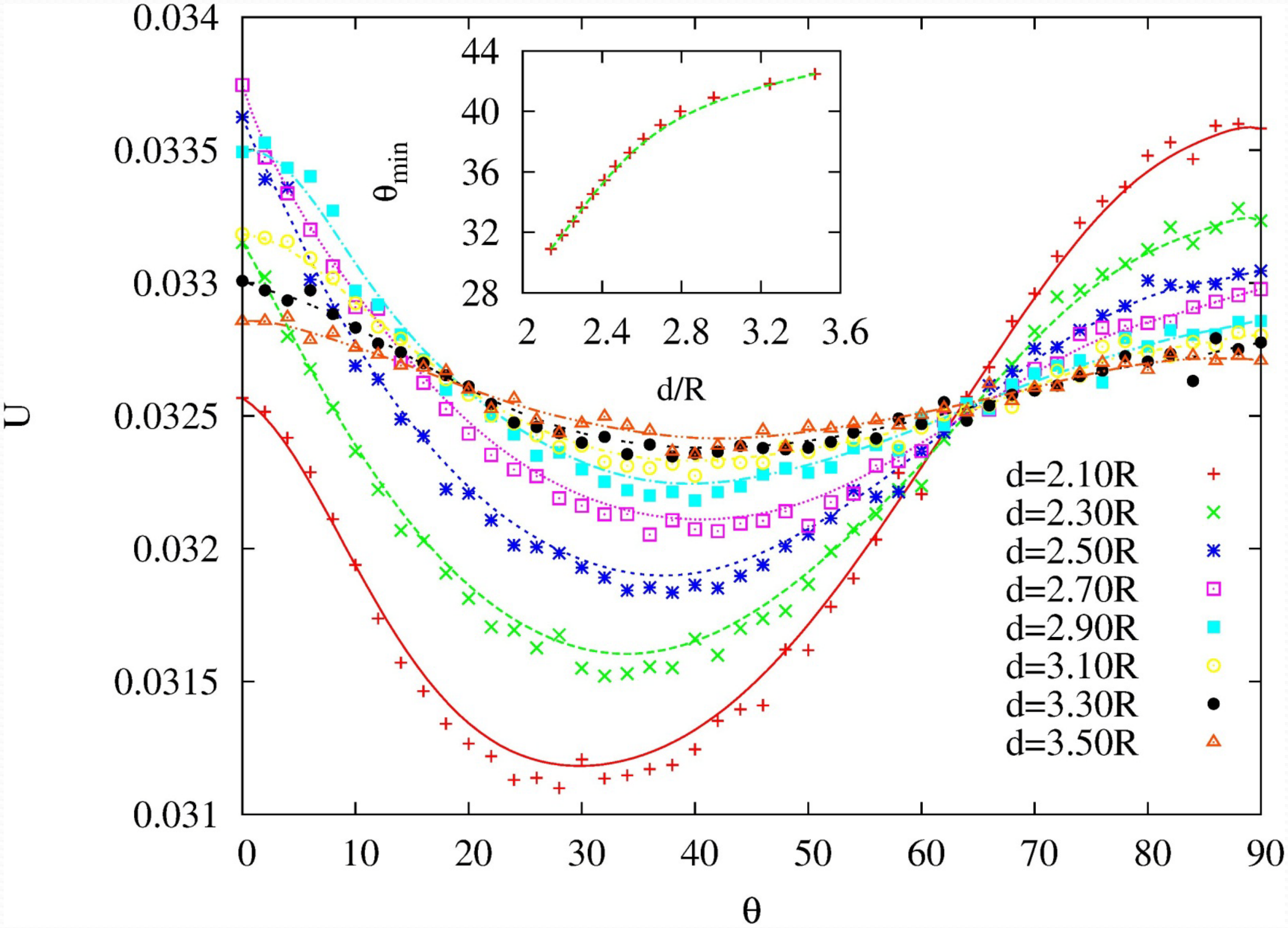
Planar anchoring





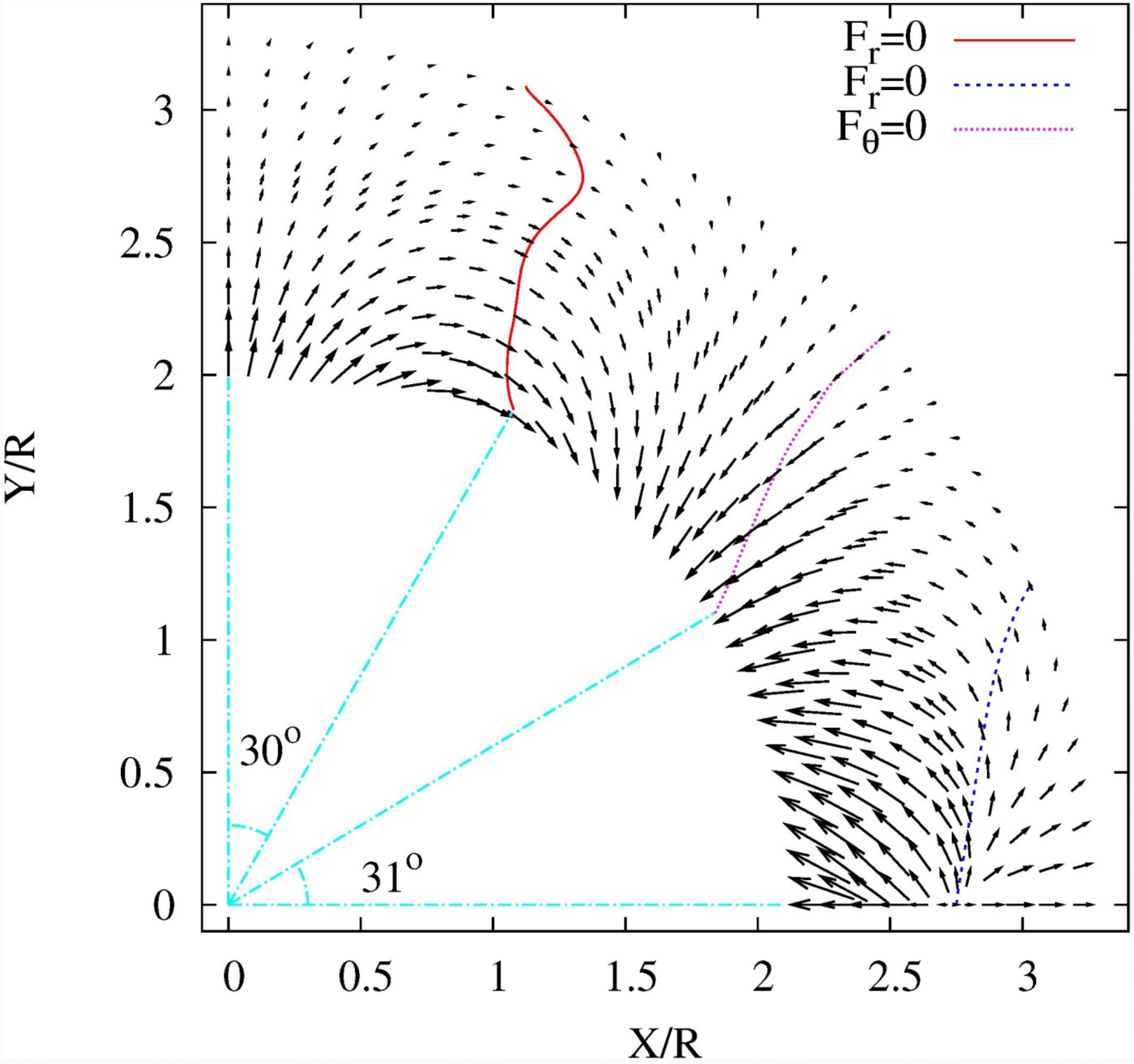
3D calculations

Planar anchoring



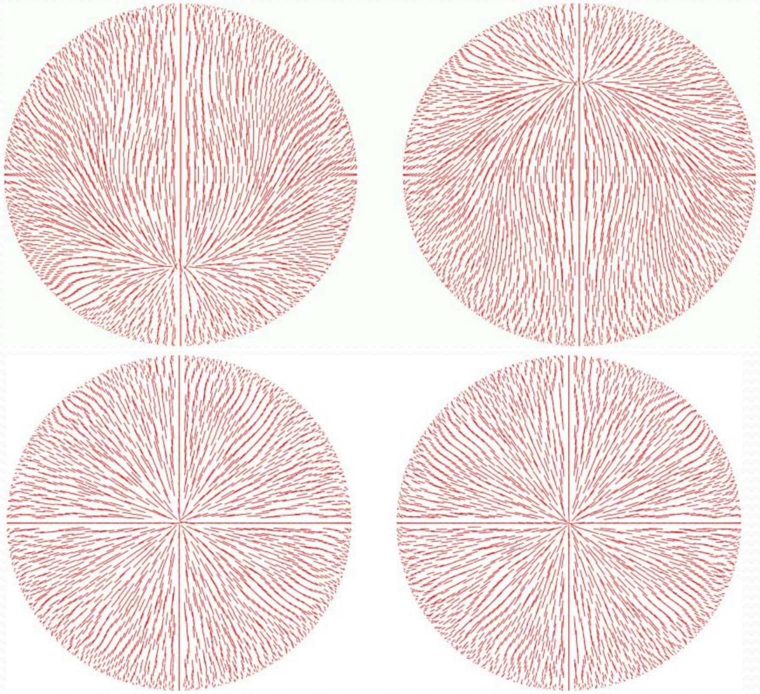
3D calculations

Planar anchoring

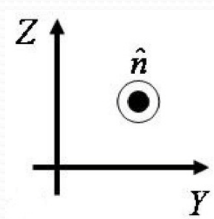


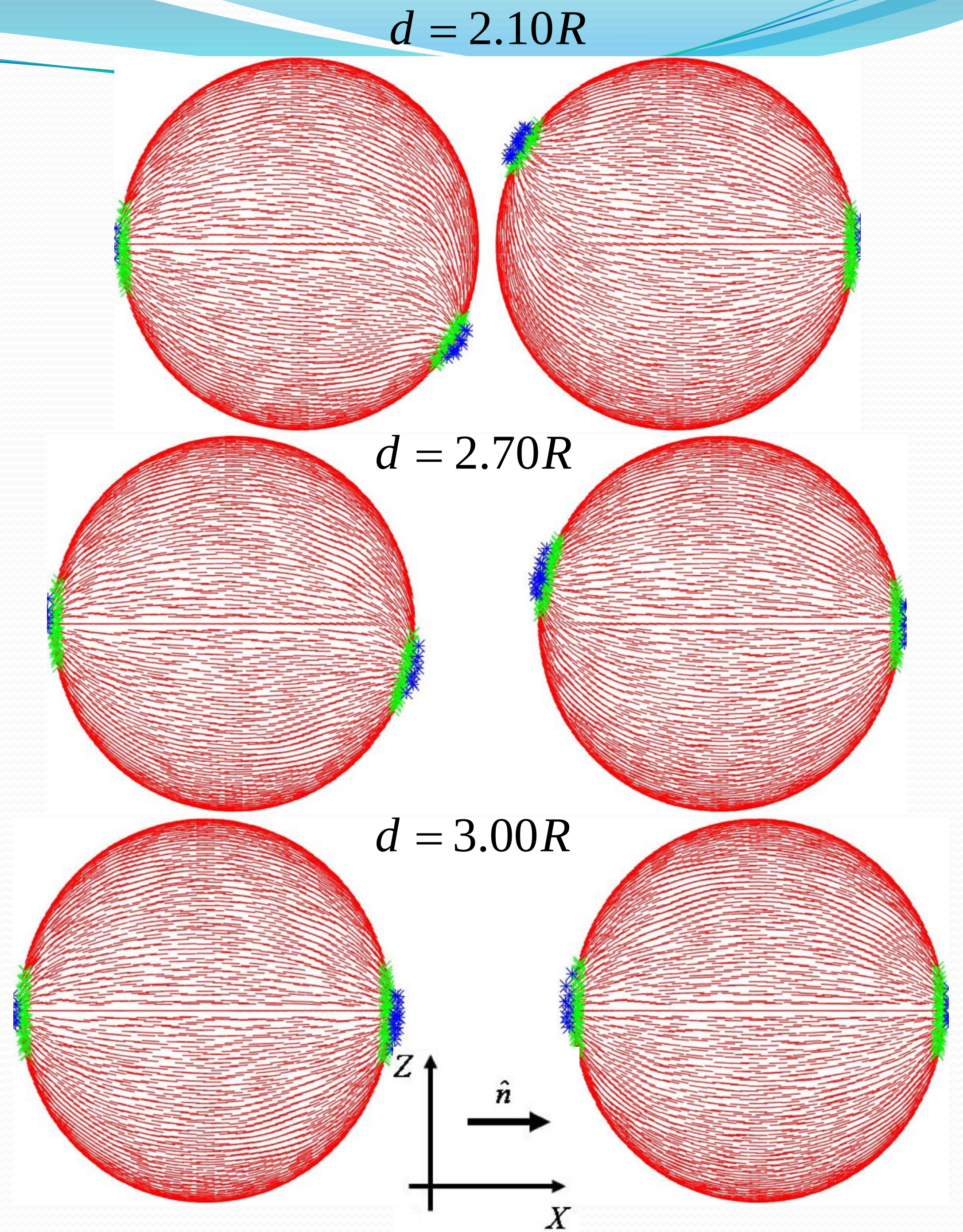
3D calculations

Planar anchoring



$d = 2.10R, \quad \theta = 0^\circ$

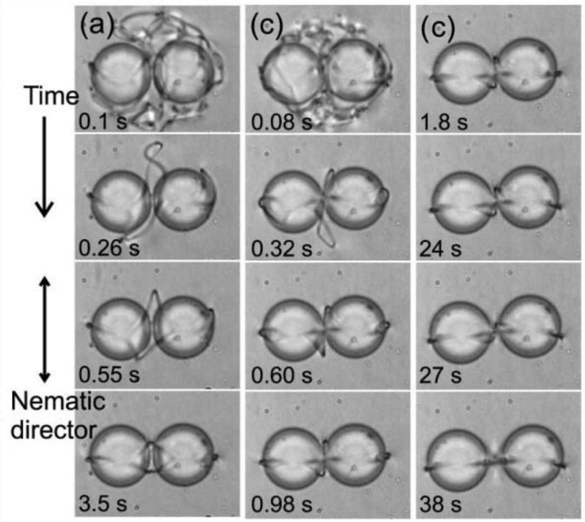


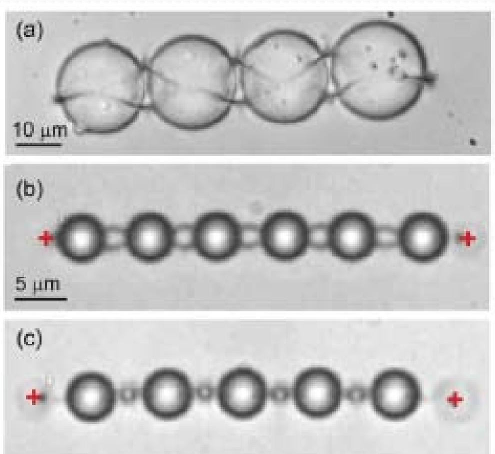


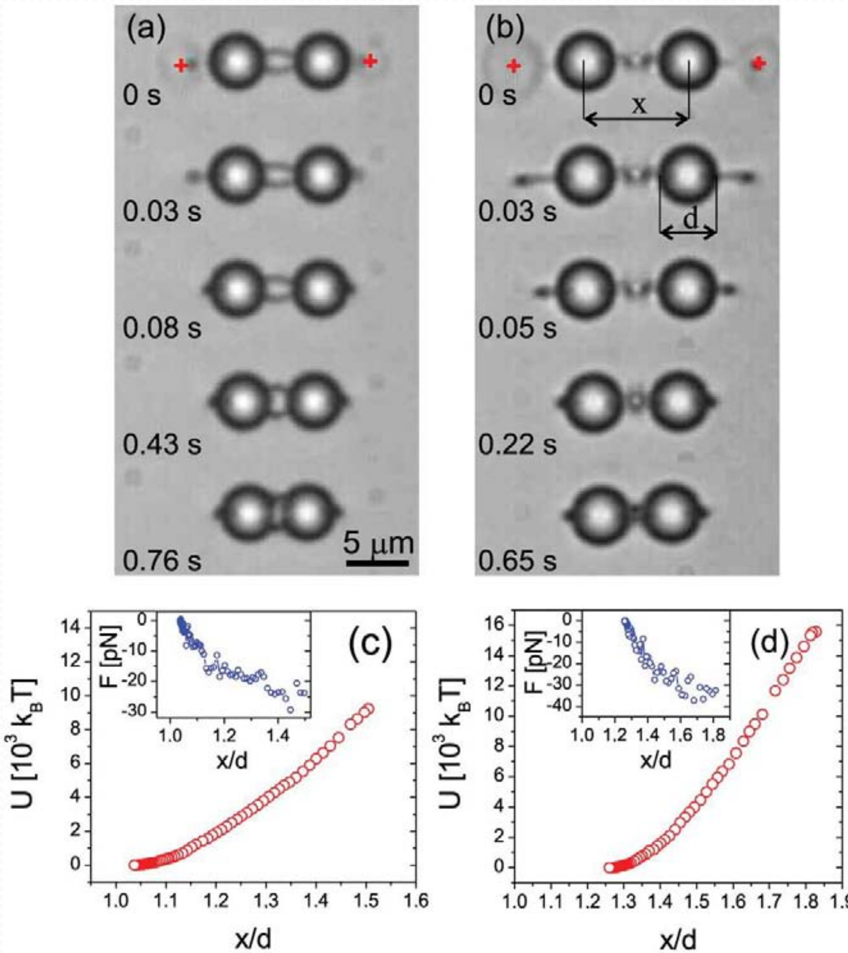
PRL 99, 247801 (2007) PHYSICAL REVIEW LETTERS week ending 14 DECEMBER 2007

Entangled Nematic Colloidal Dimers and Wires

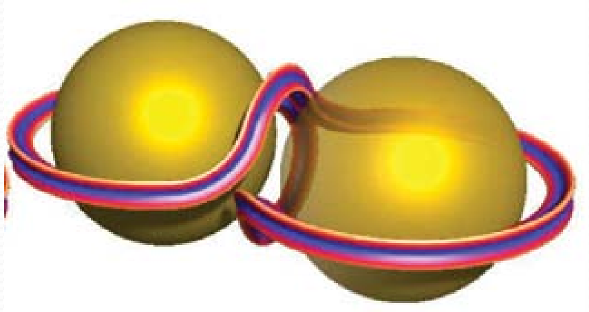
M. Ravnik,[1] M. Škarabot,[2] S. Žumer,[1,2] U. Tkalec,[2] I. Poberaj,[1] D. Babič,[1] N. Osterman,[1] and I. Muševič[1,2,*]

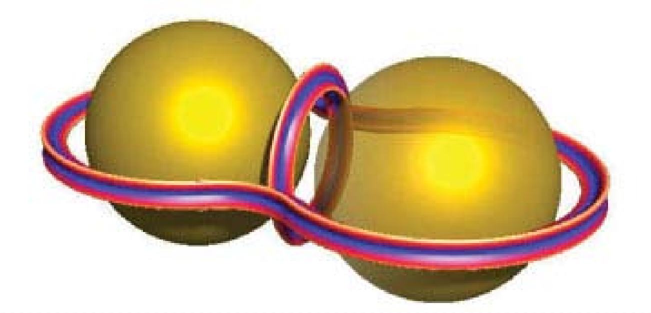




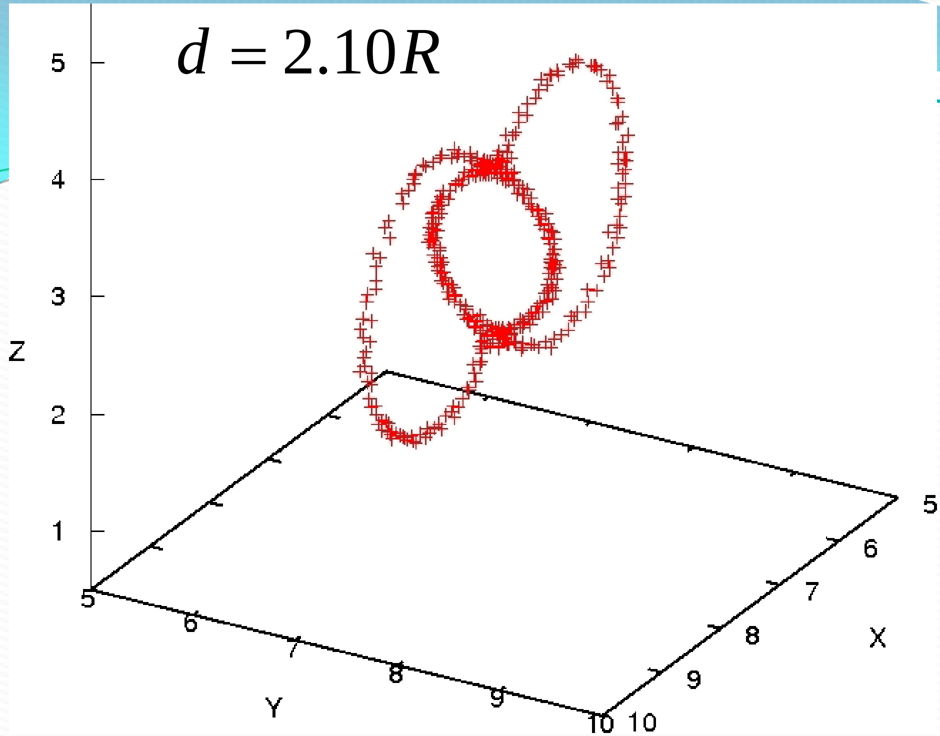


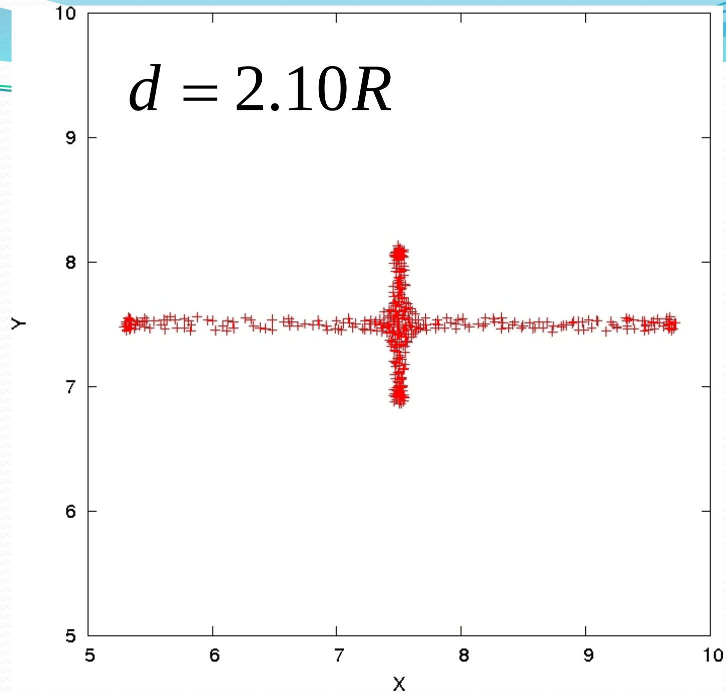
More Complicated geometries of defects

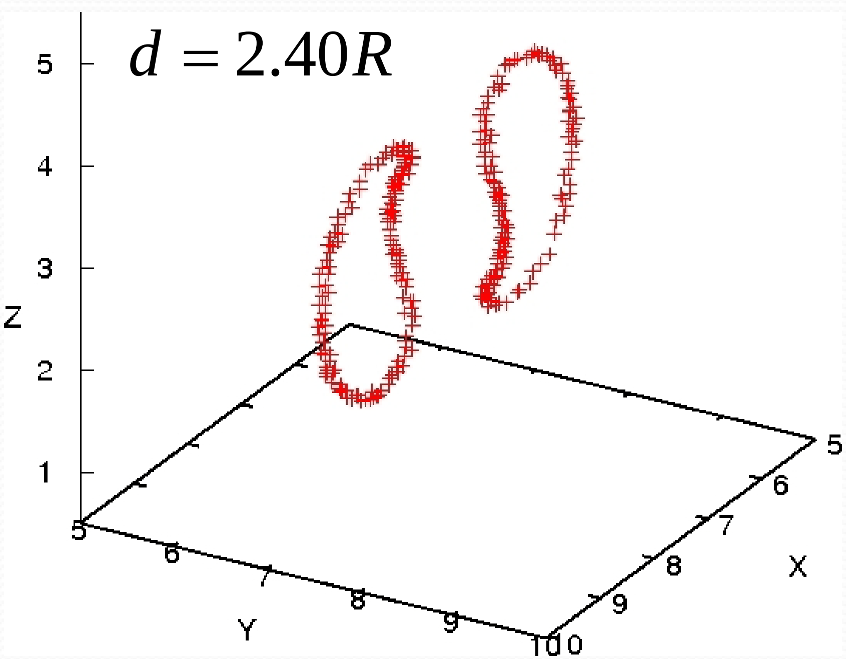


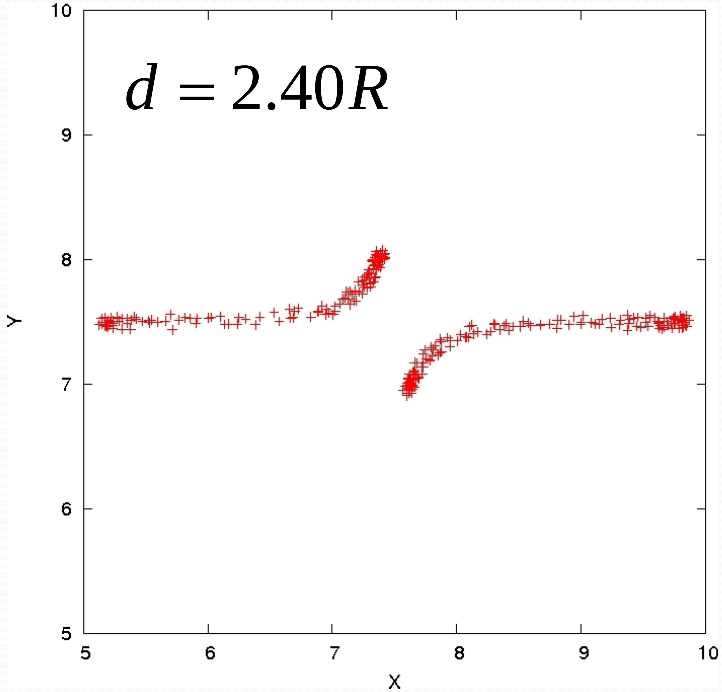


PRL 106, 177801 (2011)

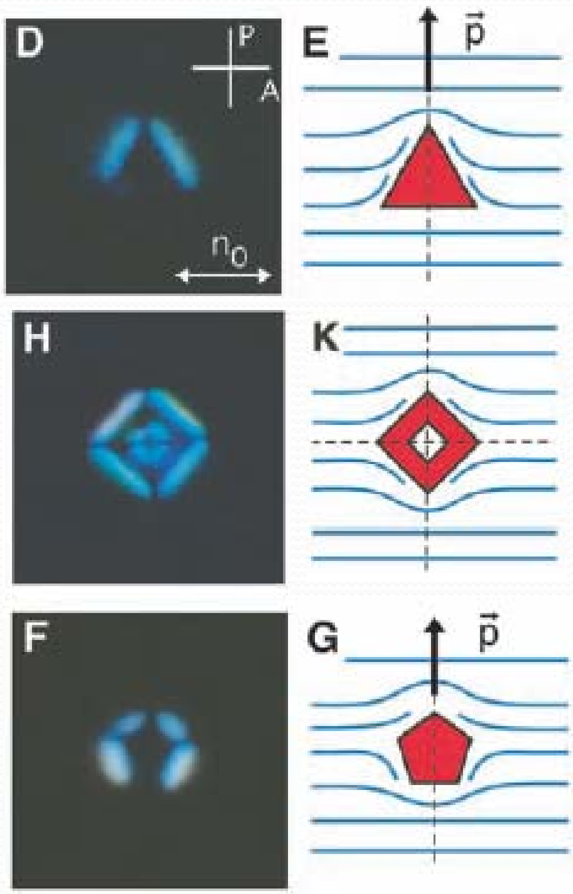

$d = 2.10R$
Z
Y
X

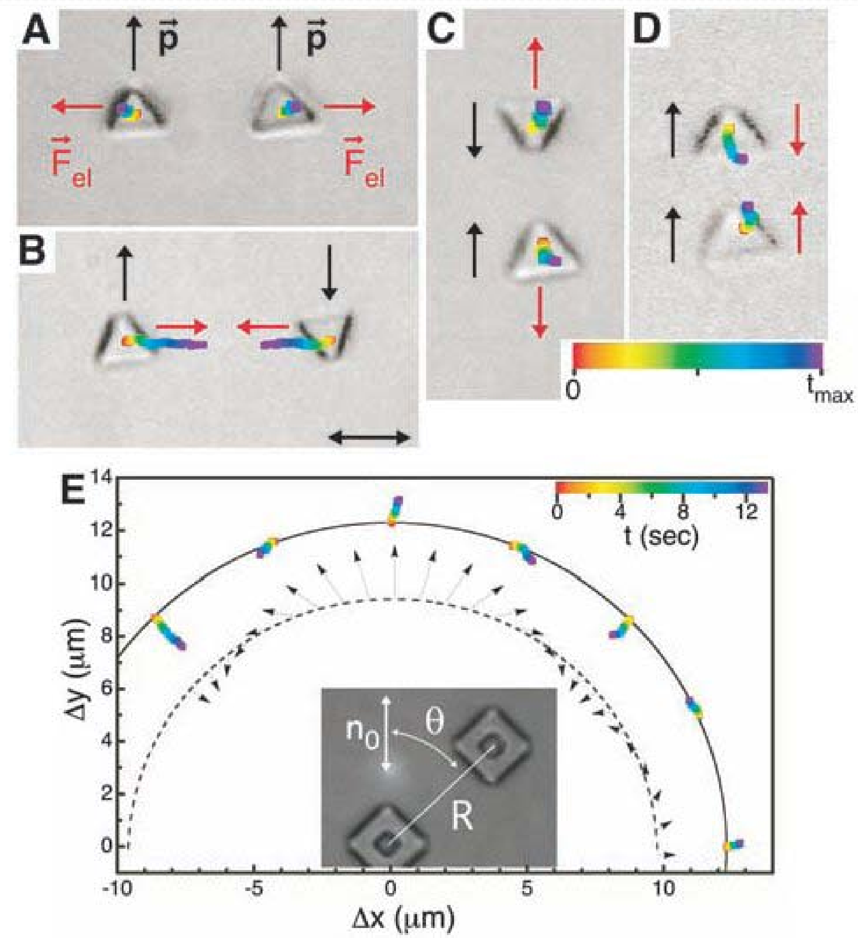

$d = 2.10R$
Y
X


$d = 2.40R$
Z
Y
X


$d = 2.40R$
Y
X

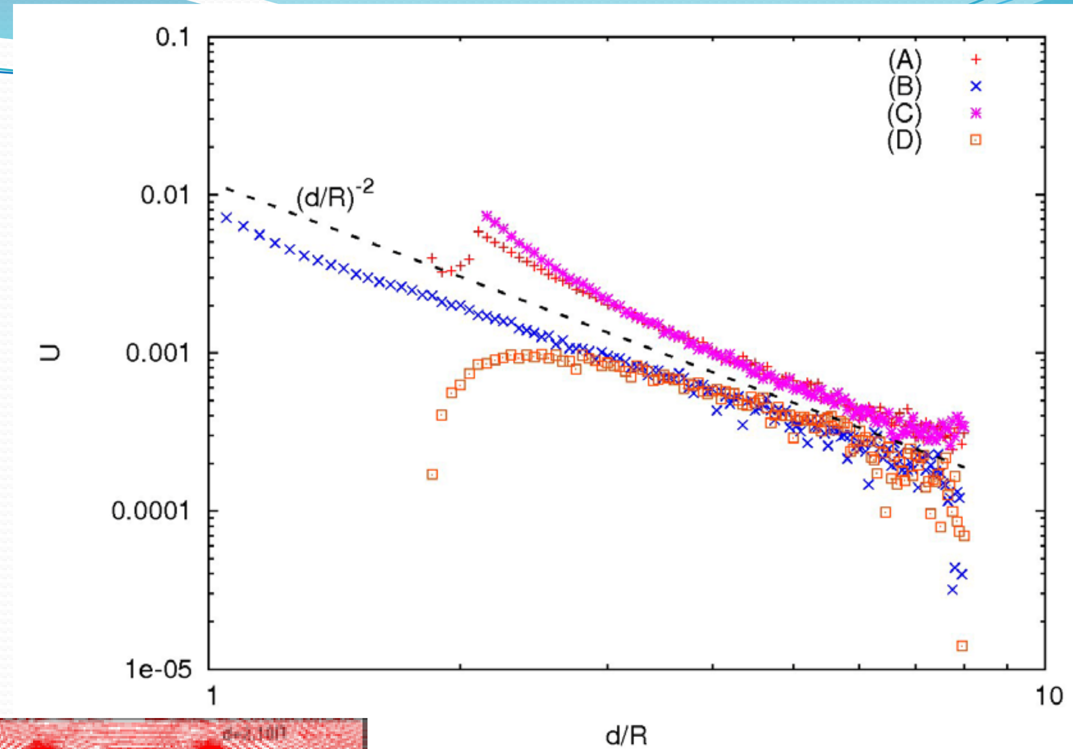
Shape-Controlled Colloidal Interactions in Nematic Liquid Crystals
Clayton P. Lapointe, *et al.*
Science **326**, 1083 (2009);
DOI: 10.1126/science.1176587

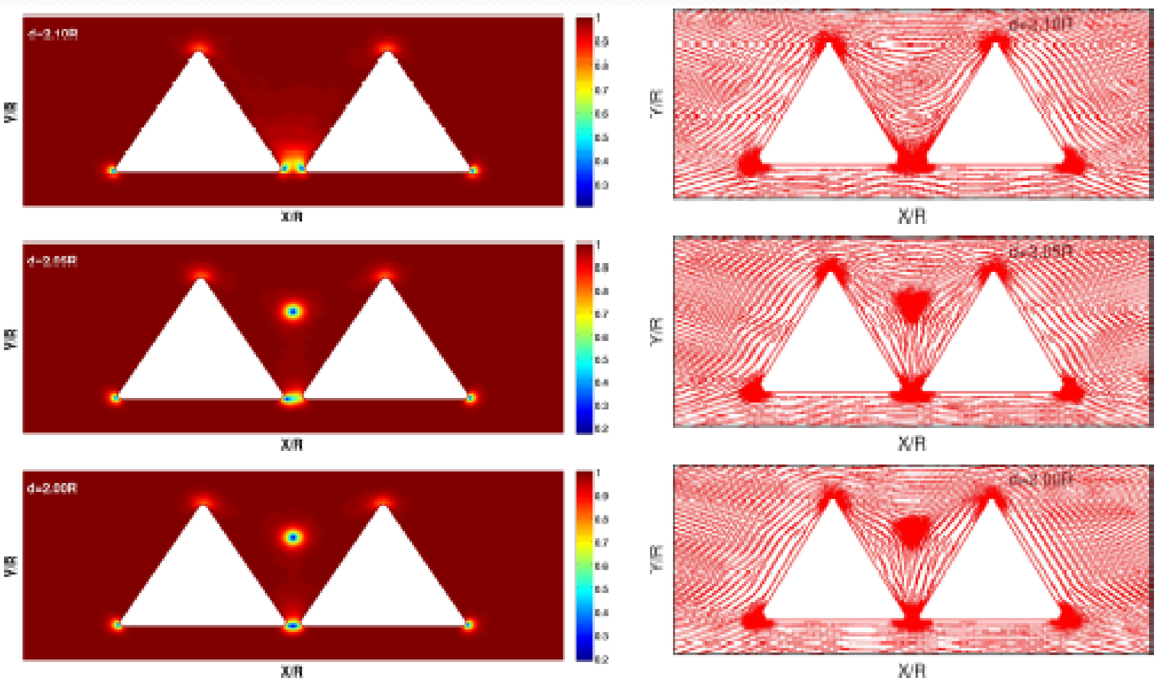




2D calculations

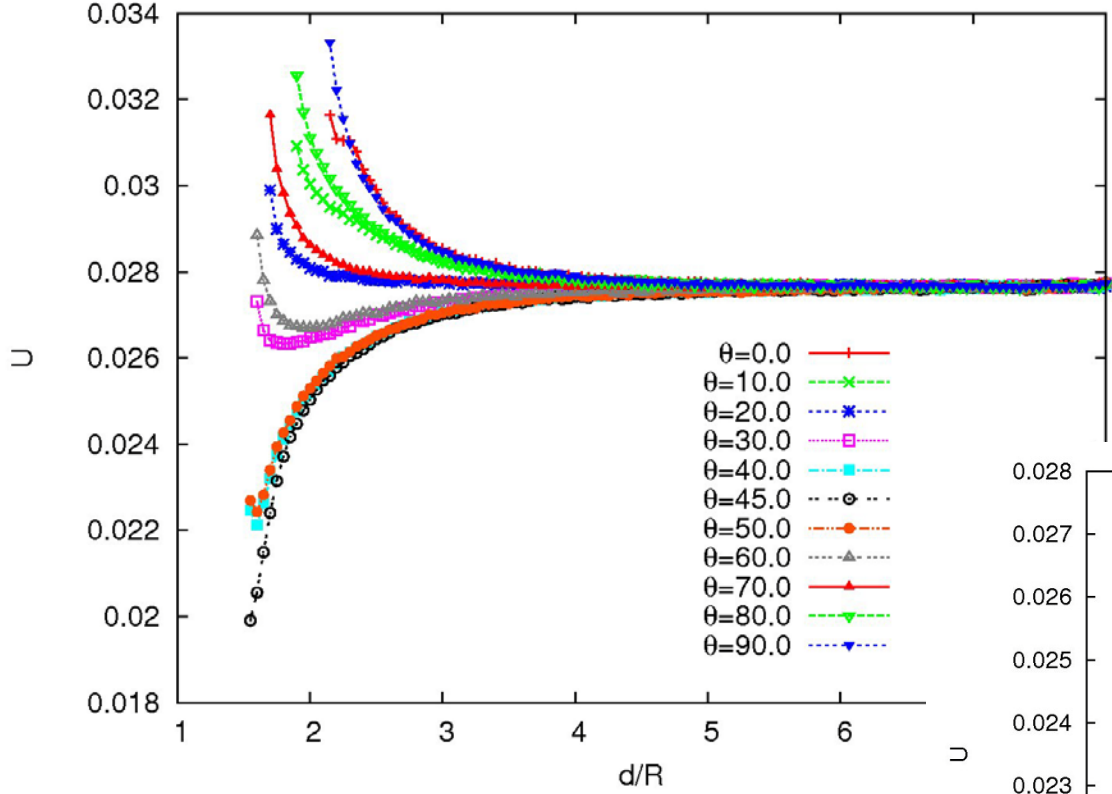
Planar anchoring

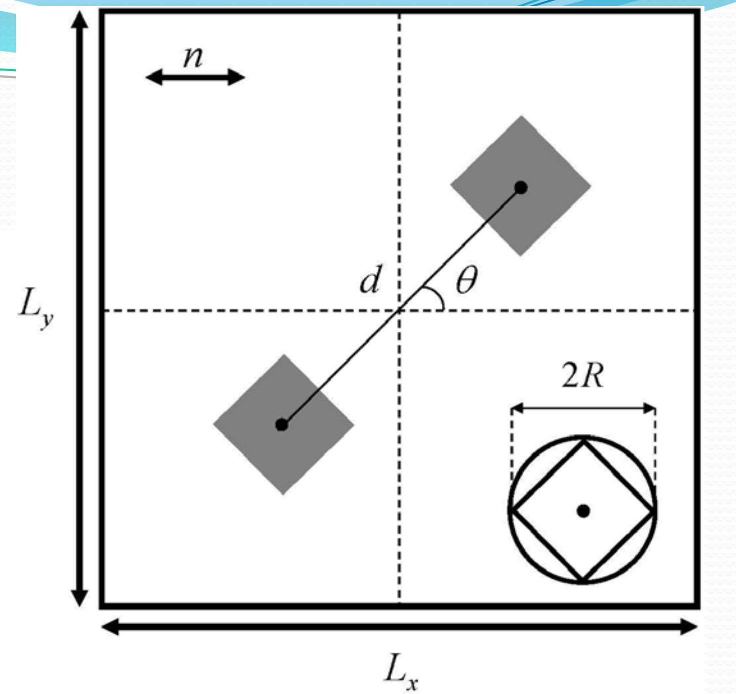


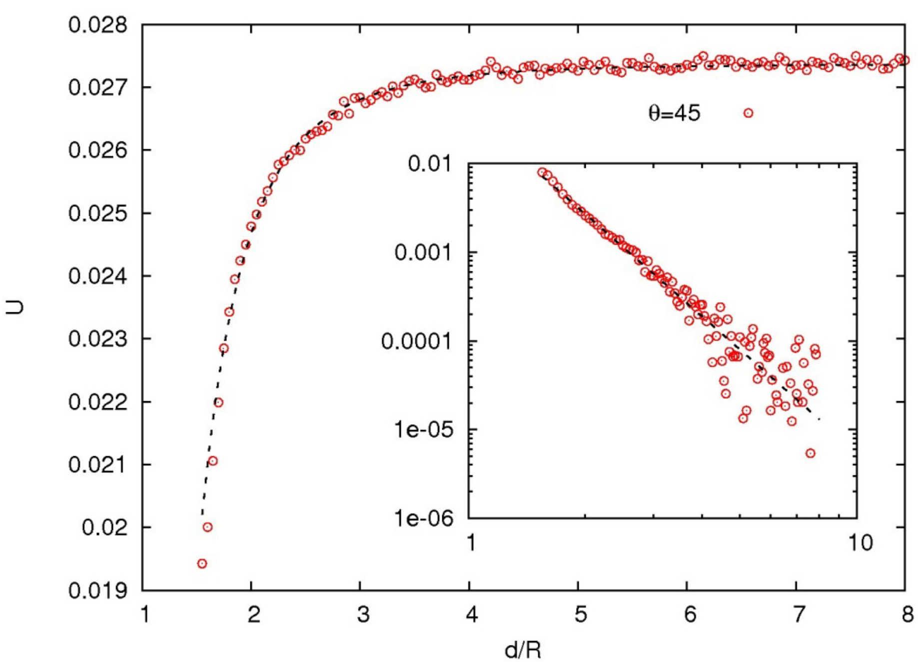


2D calculations

Planar anchoring



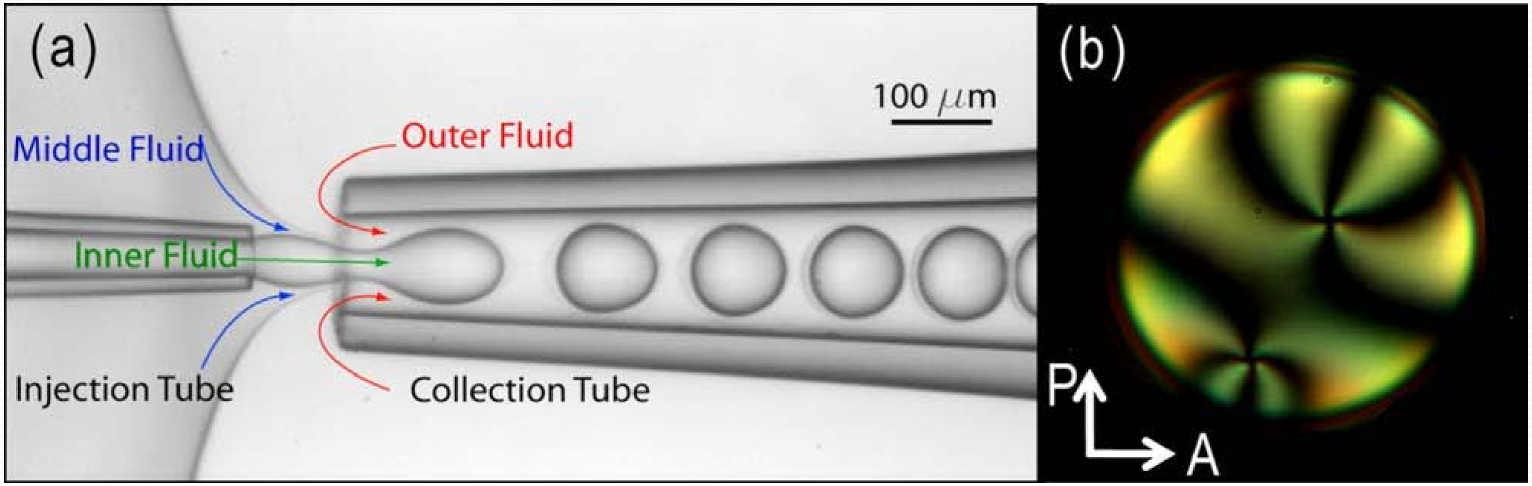




$$U(d) = a + \left(\frac{b}{d}\right)^{c}$$

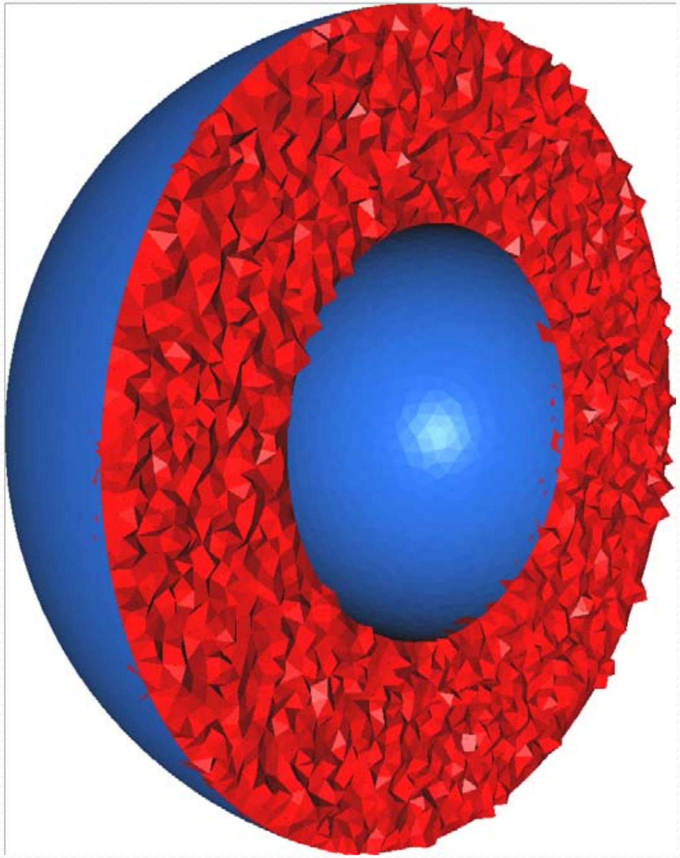
$$c = 3.78 \pm 0.06$$

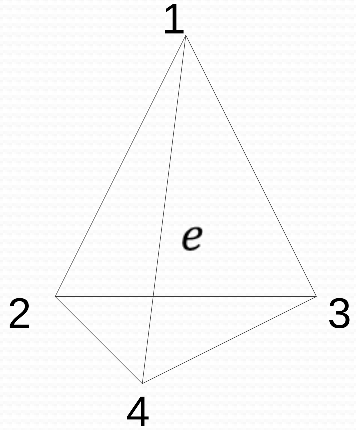
Experimental observatins



Phys Rev. E 79, 021707 (2009)

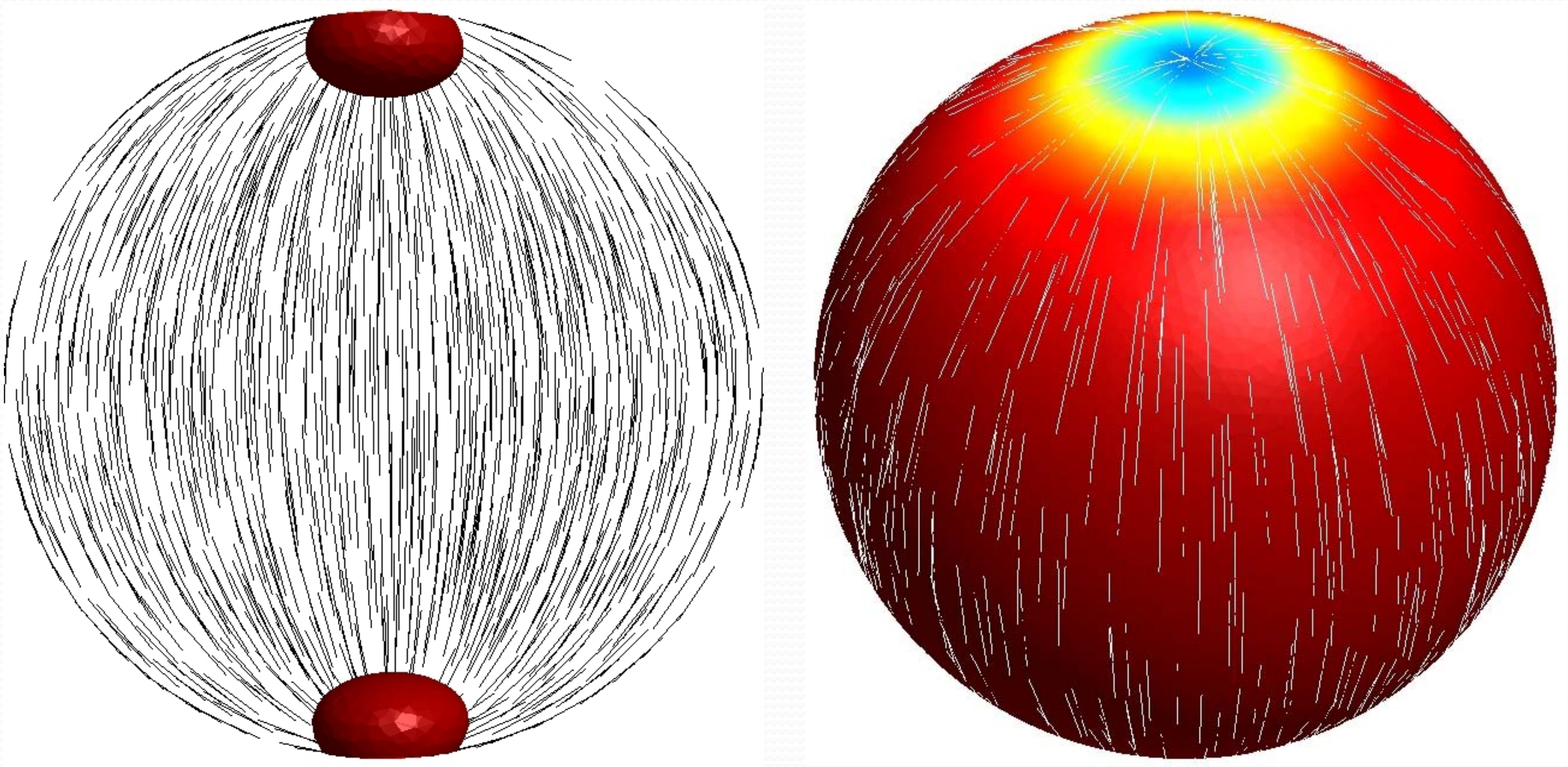
- FEM method



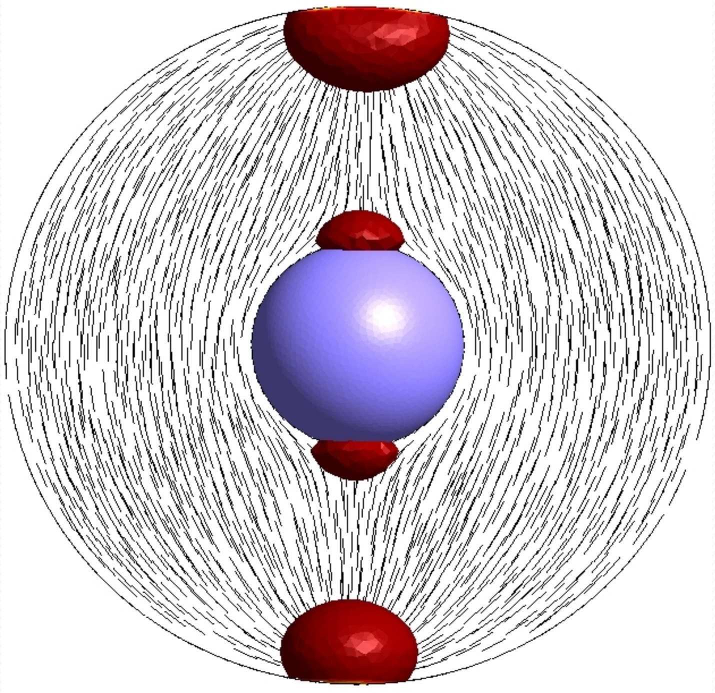


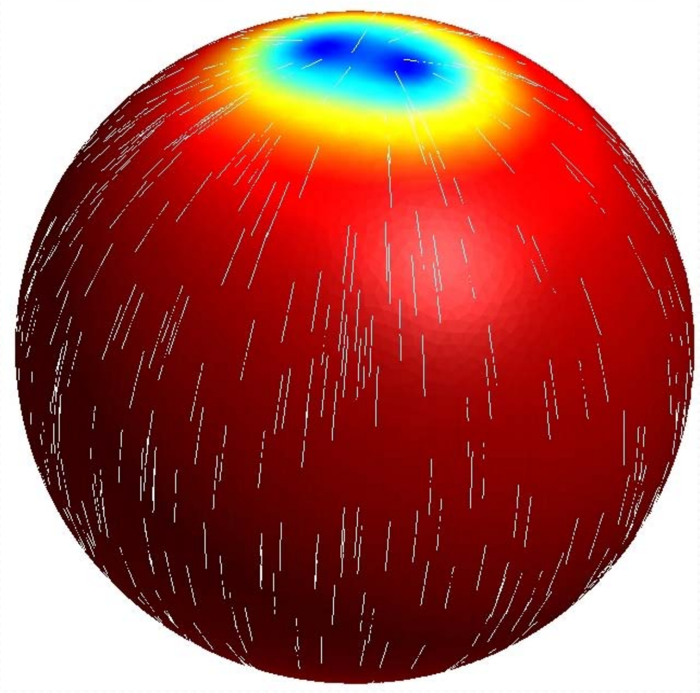
$$\varphi^e = a^e x + b^e y + c^e z + d^e$$

- Spherical droplet

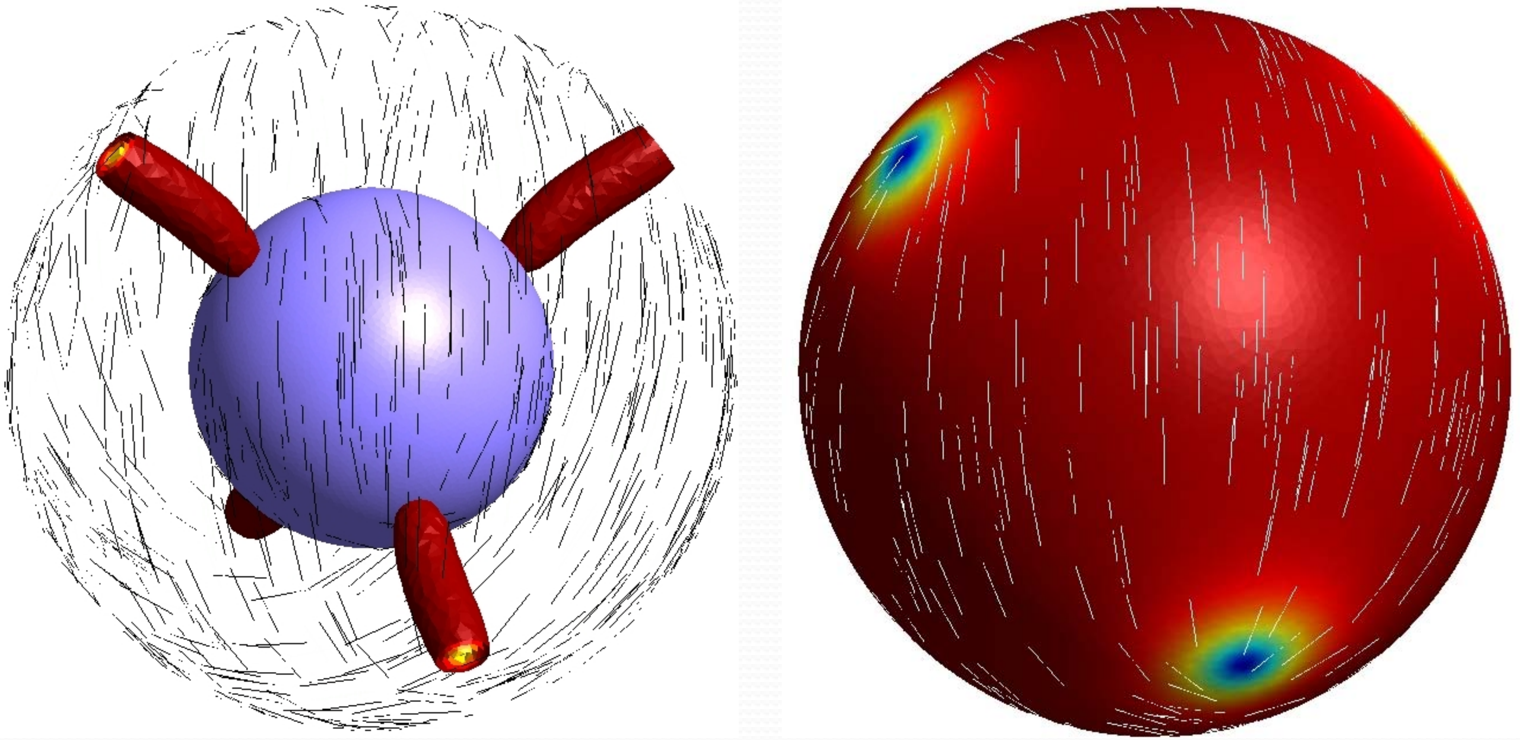


- Thick shells

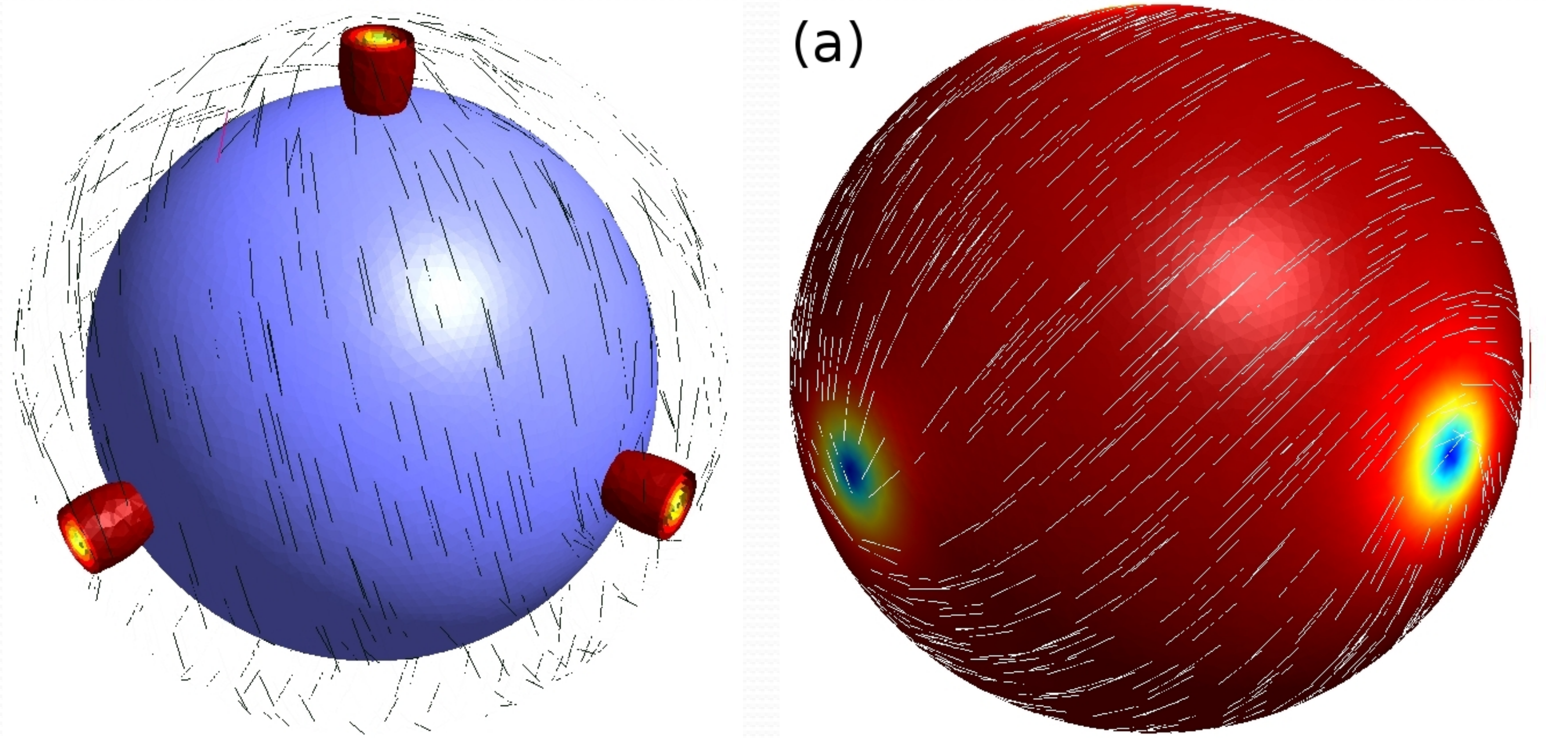


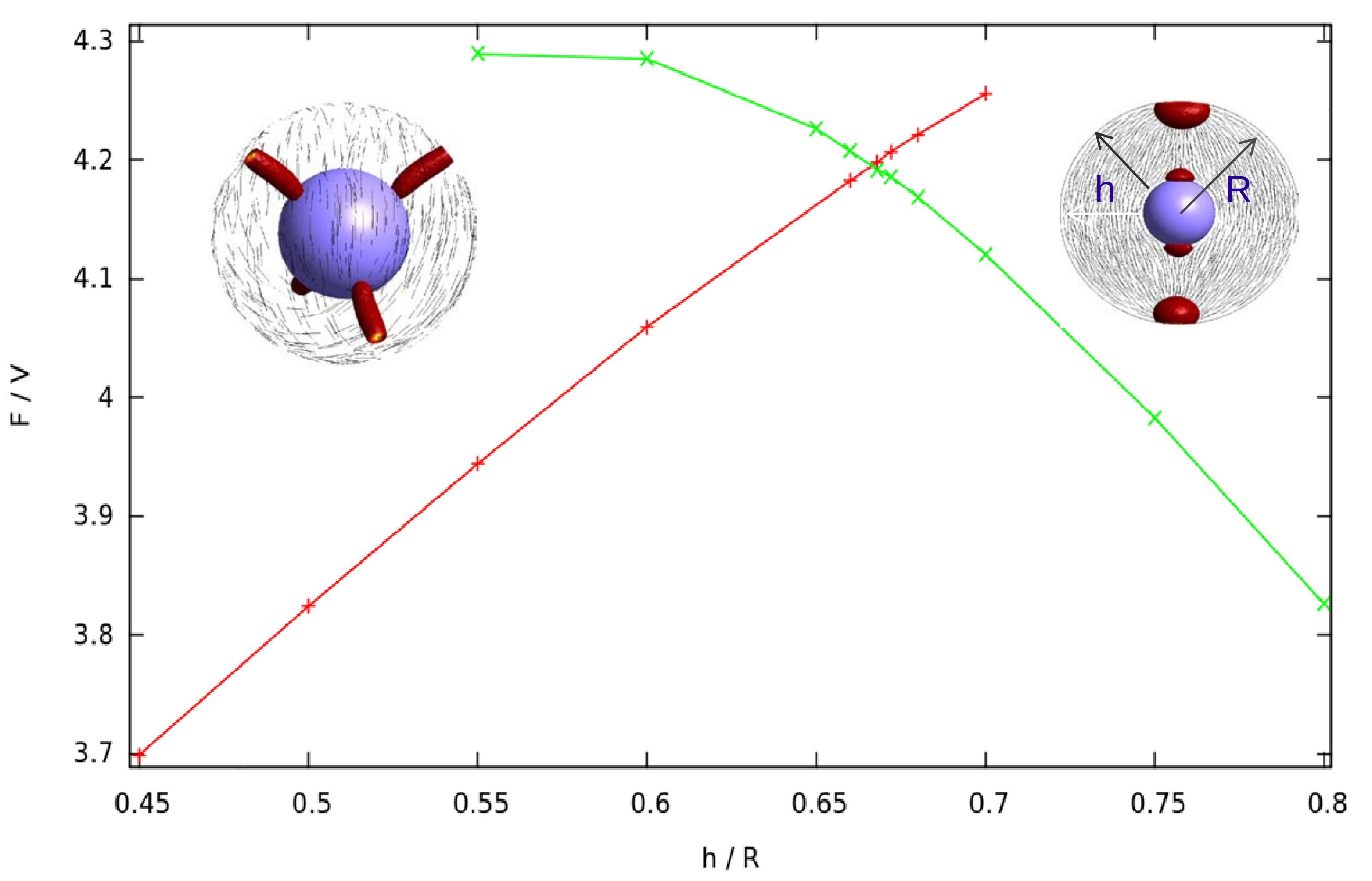


- Thin shells

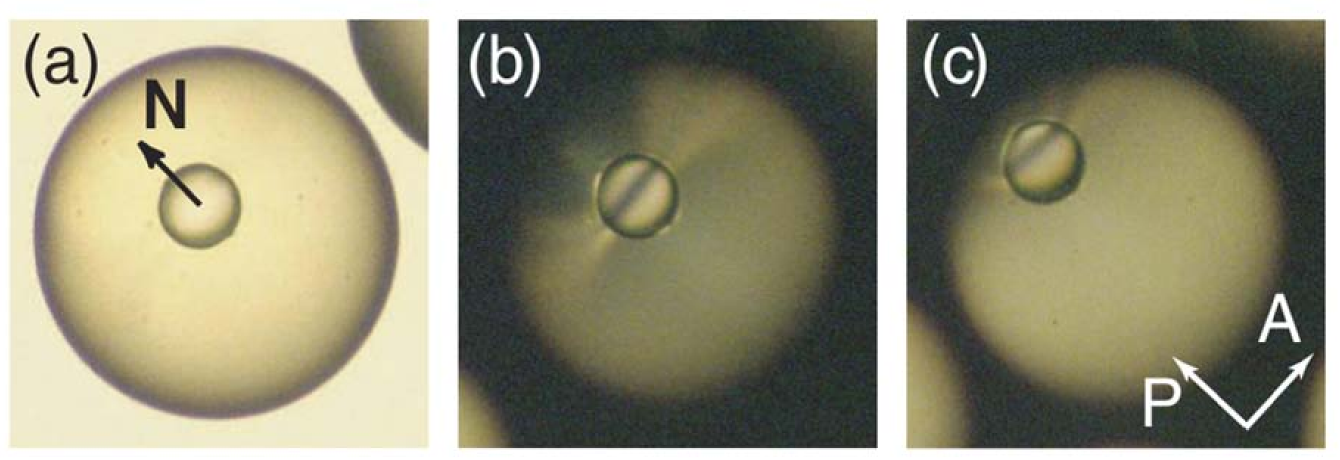


- Thin shells

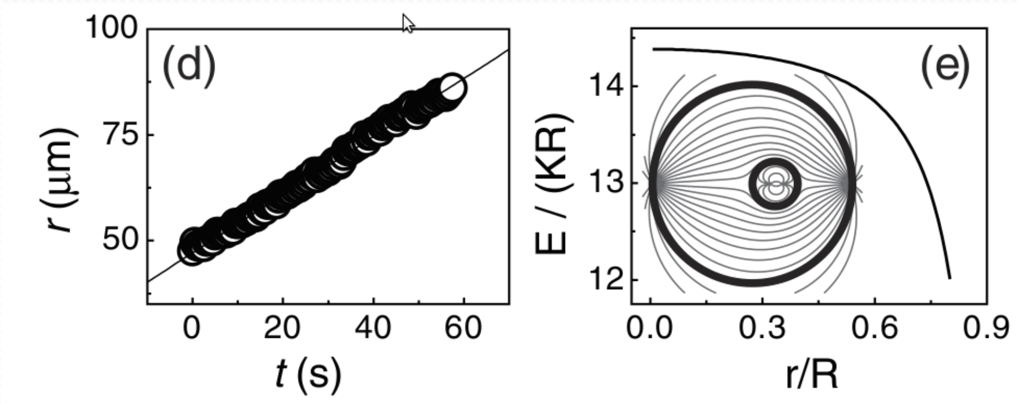




F / V
h / R
h
R
4.3
4.2
4.1
4
3.9
3.8
3.7
0.45
0.5
0.55
0.6
0.65
0.7
0.75
0.8

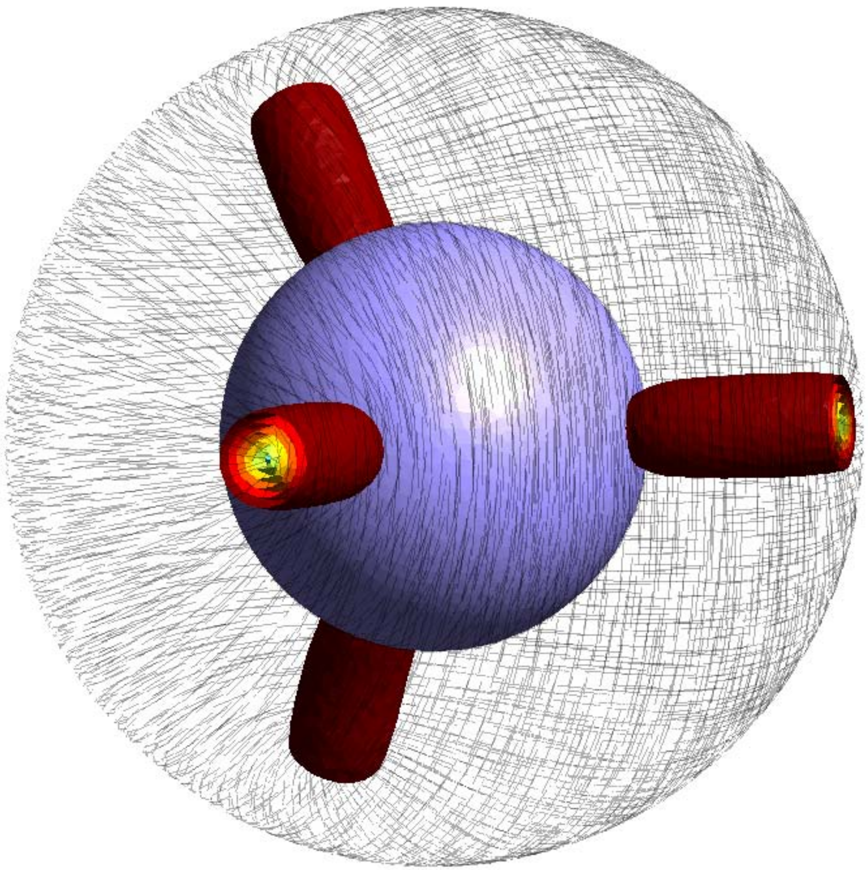


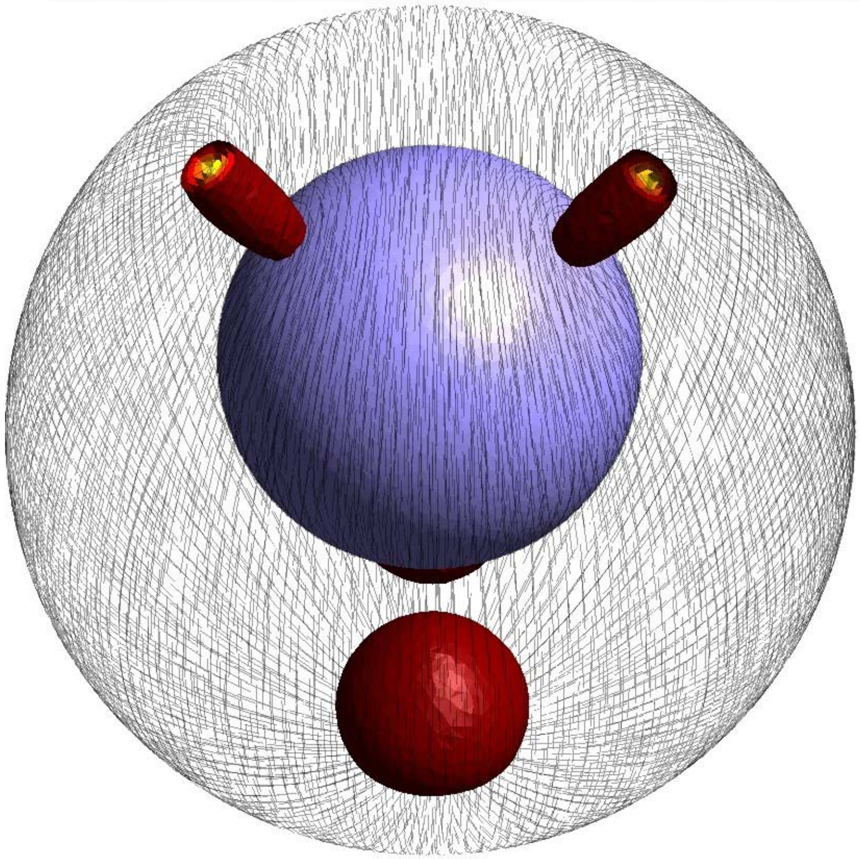
t = 0s t = 13s t = 55s



PRL 99, 157801 (2007)

- Off center spheres in thick shell





- Off center spheres in thin shell