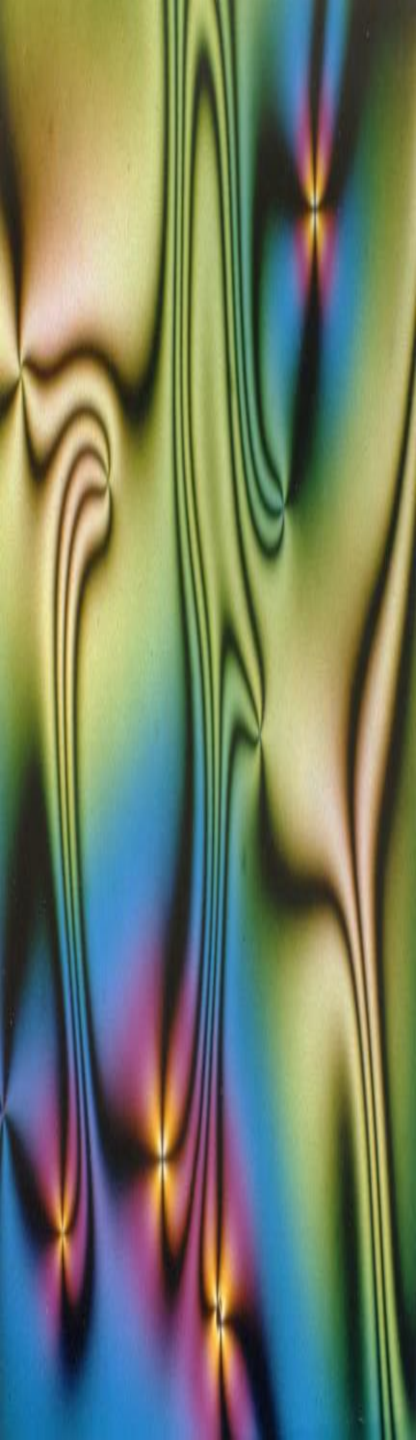


The Mathematics of Liquid Crystals – Multi-Faceted Approaches, Challenges and Applications for Future Technologies

Apala Majumdar

University of Strathclyde

Piscopia Seminar
23rd February

A bit about myself…

- Professor of Applied Mathematics, University of Strathclyde, United Kingdom
- https://www.strath.ac.uk/staff/majumdarapalaprofessor/
- https://themajumdargroup.wordpress.com/
- Expertise: **mathematics of materials science and liquid crystals, applications in science and technology**
- Core skills: variational methods, nonlinear partial differential equations, asymptotics and modelling
- Highly **interdisciplinary research agenda** – worked with physicists, chemists and researchers from industry (Hewlett Packard and Merck)
- International Connections: **IIT Delhi, IIT Bombay, Peking University, University of Luxembourg, University of Verona (Italy).**

Places I have worked in…

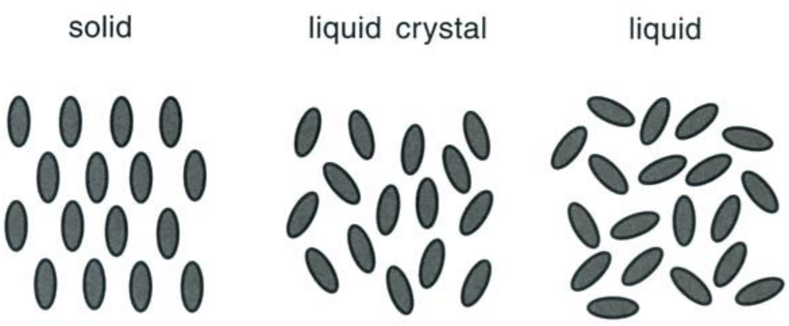
- ✓ PhD from University of Bristol in Applied Mathematics.
- ✓ CASE student with Hewlett Packard.

- ✓ Research Fellowship at University of Oxford

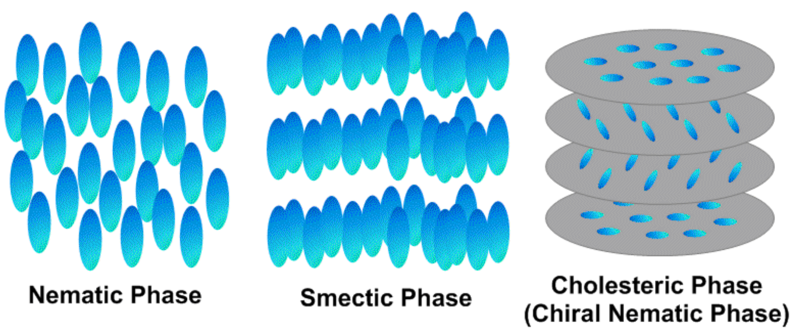
- ✓ University of Bath
- ✓ Director of Centre for Nonlinear Mechanics (2018-2019)
- ✓ Led a Bath-Chile-Mexico network spanning 2 Universities in Chile (CMM, Catholic University of Chile) and 1 University in Mexico (UNAM).

- ✓ University of Strathclyde

https://www.strath.ac.uk/staff/majumdarapalaprofessor/



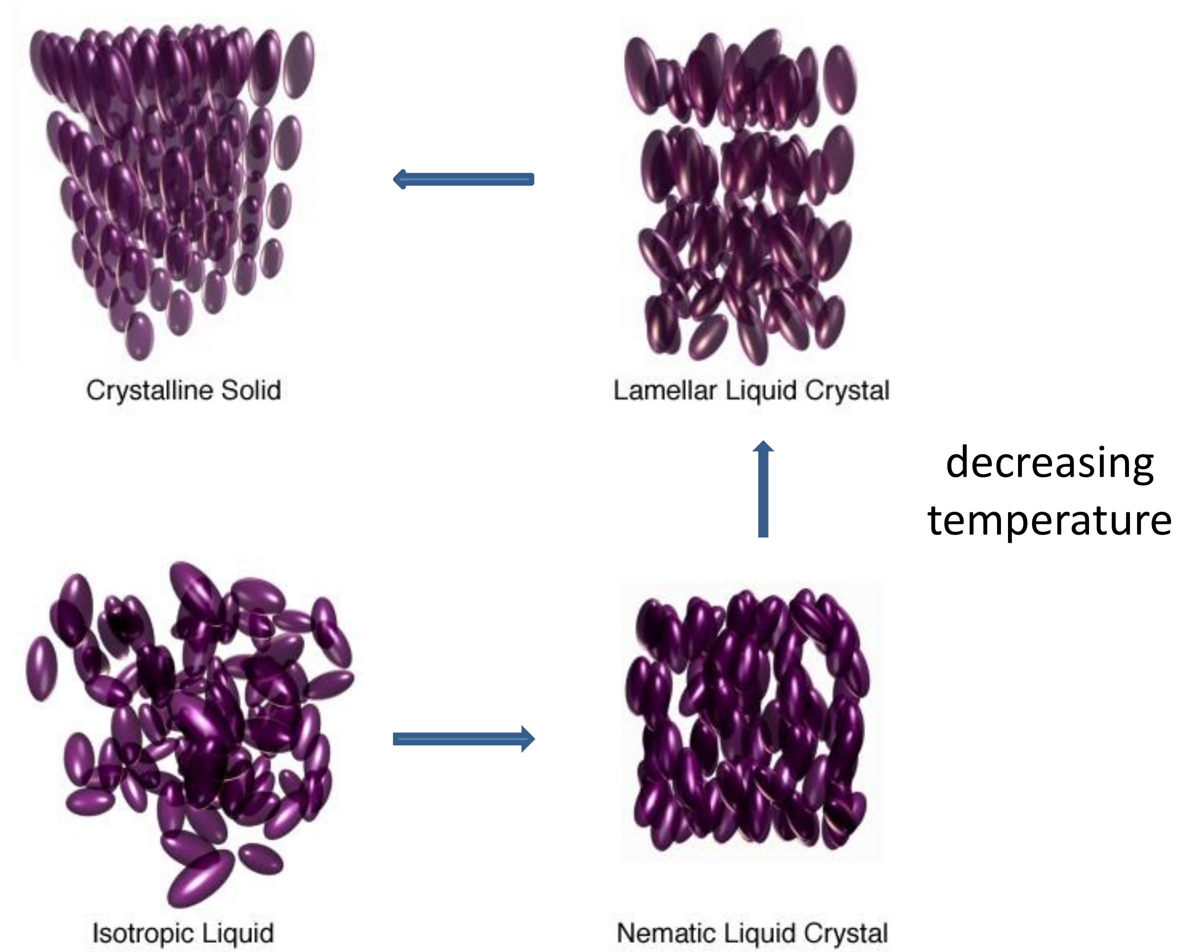
(Felix, et al., 2015)



(tokyo chemical industry)

Liquid Crystals – what are they?

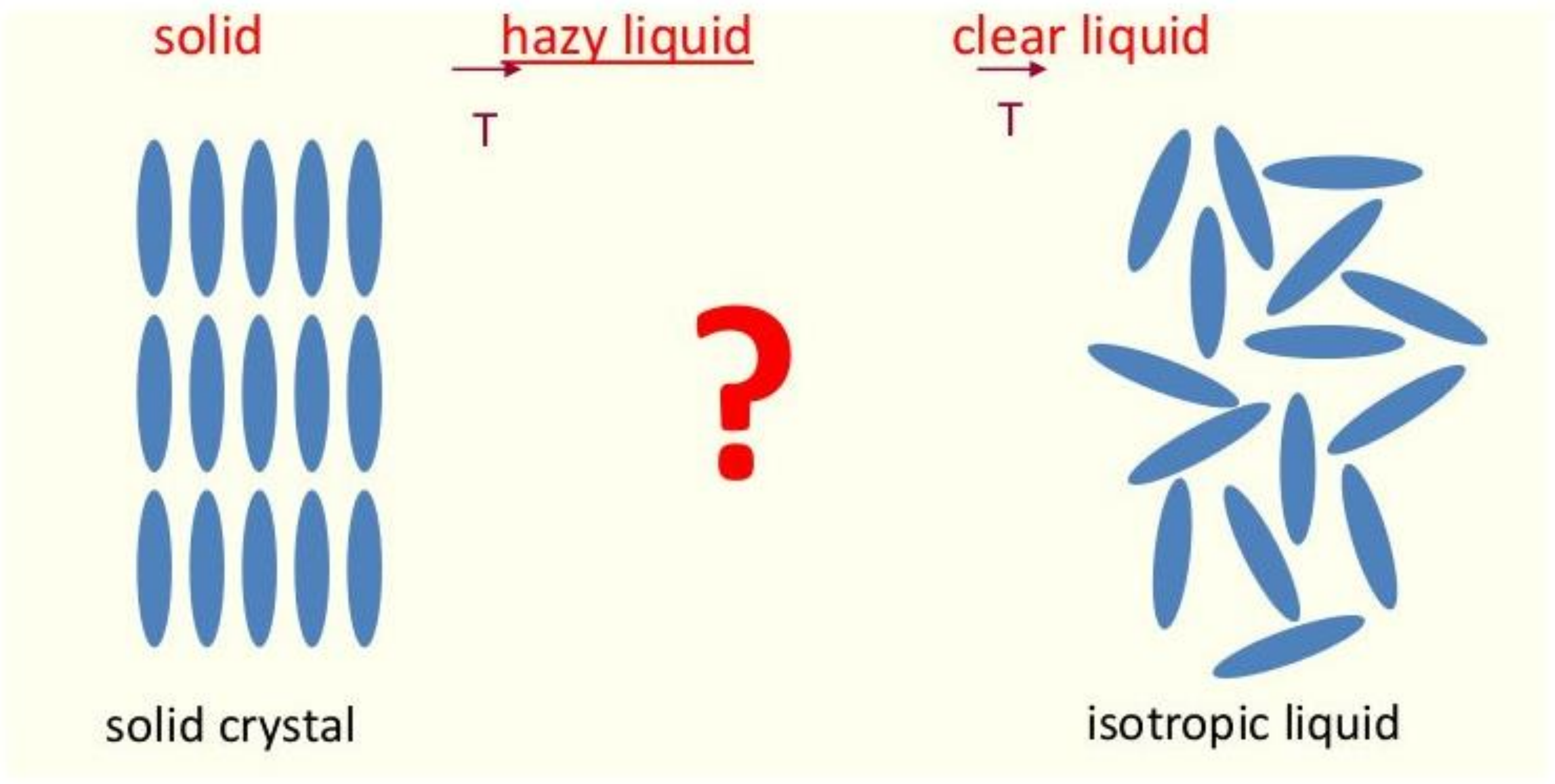
- Mesogenic phases of matter



- Intermediate between solids and liquids

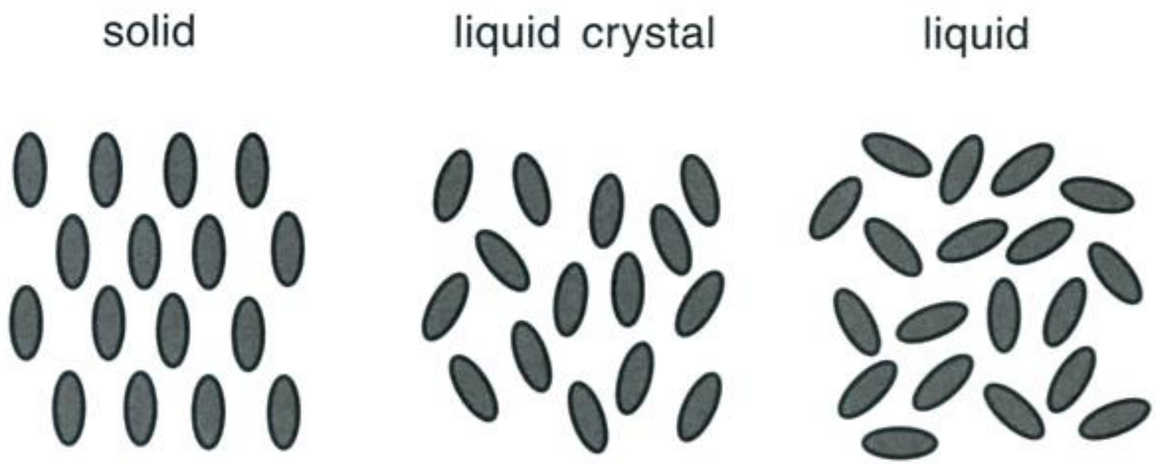
History

- Discovered by Reinitzer in 1888 : two melting points for cholesterol! !

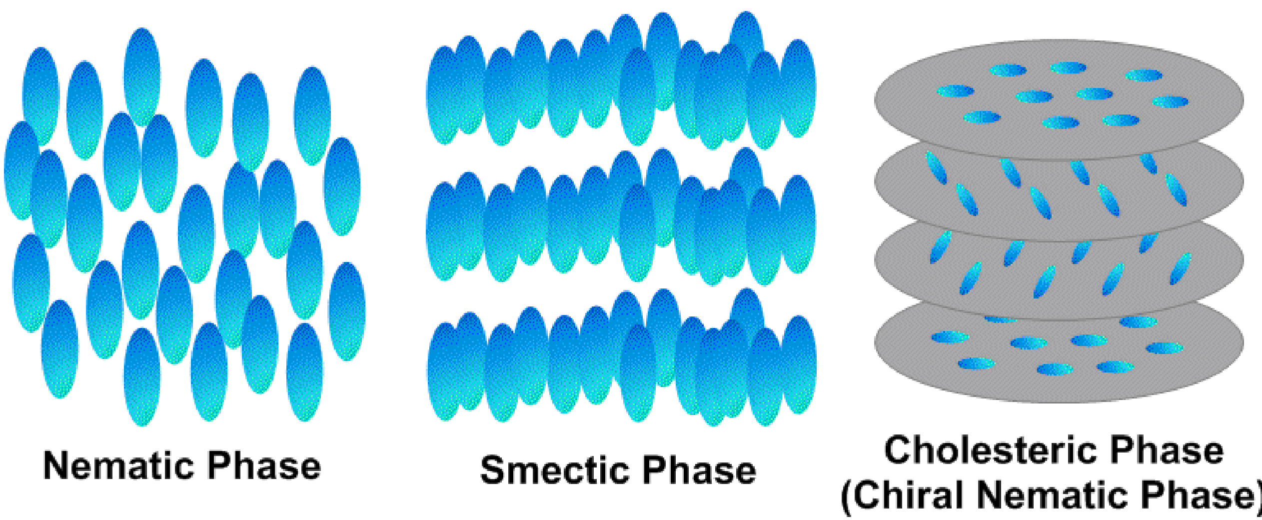


Courtesy: Peter Palffy-Muhoray Lectures at Colorado - Boulder

Liquid Crystals – what are they?



(Felix, et al., 2015)



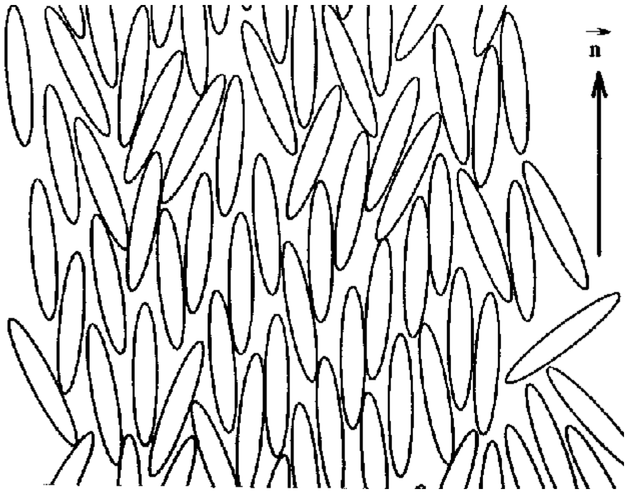
(tokyo chemical industry)

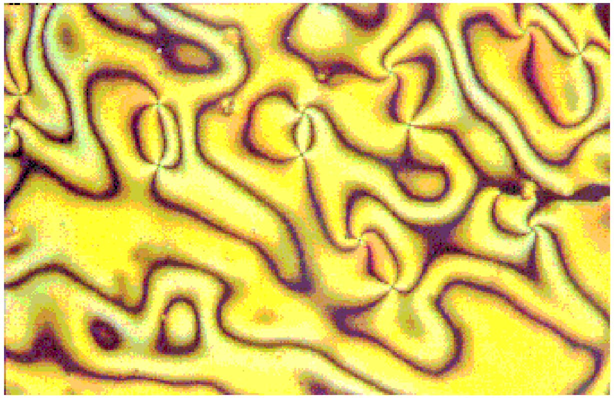
Nematic Liquid Crystals

The constituent molecules have

• no positional order (flow about freely) but

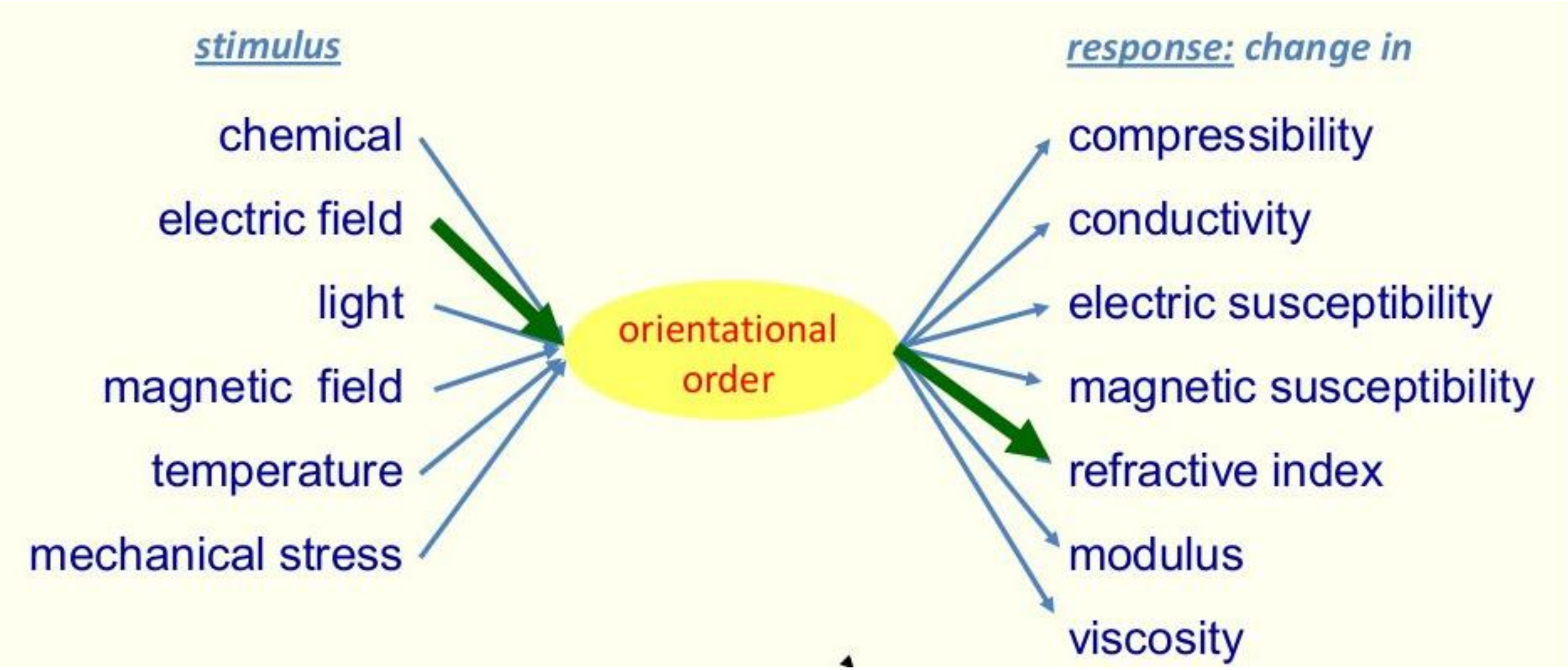
• tend to align along certain locally preferred directions i.e. exhibit long-range orientational ordering.





Nematic – greek word for `thread'.

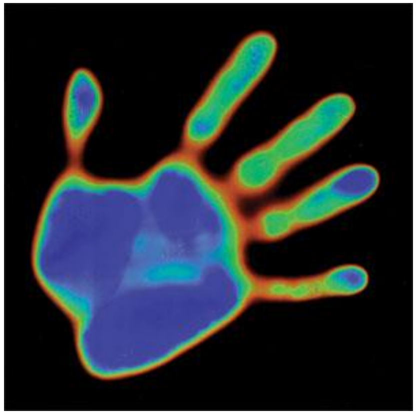
Key word: anisotropy!!!

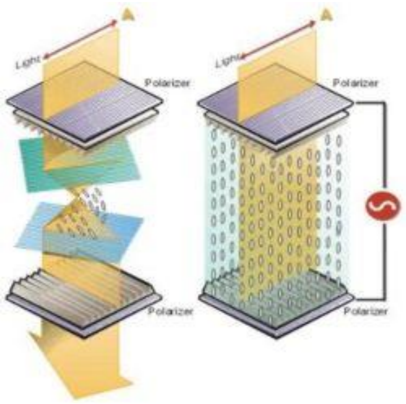


Courtesy: Images from Peter Palffy-Muhoray's lectures at Colorado – Boulder (*Physics Today 60 (9), 54 (2007)*)

Applications

- Soft materials: weak perturbations lead to mesoscopic or macroscopic responses $\Rightarrow$ array of applications !!

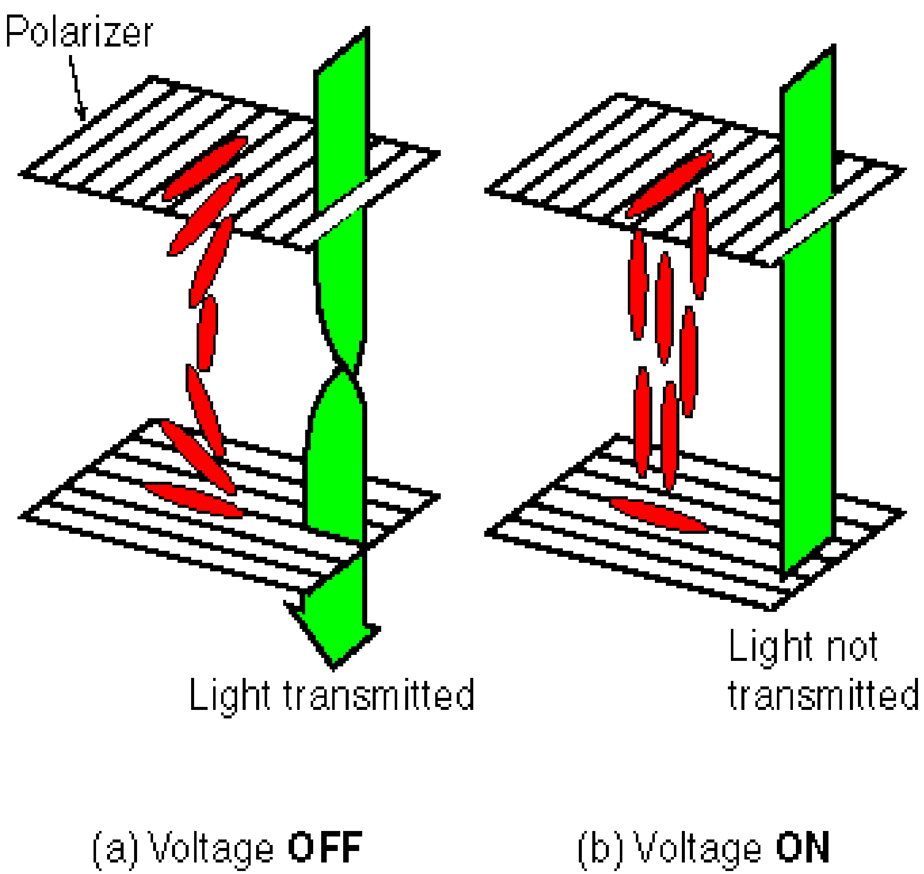




Display Applications

Key properties:-

- Anisotropic birefringent fluids – strong coupling to incident light
- Sensitive to external electric and magnetic fields .



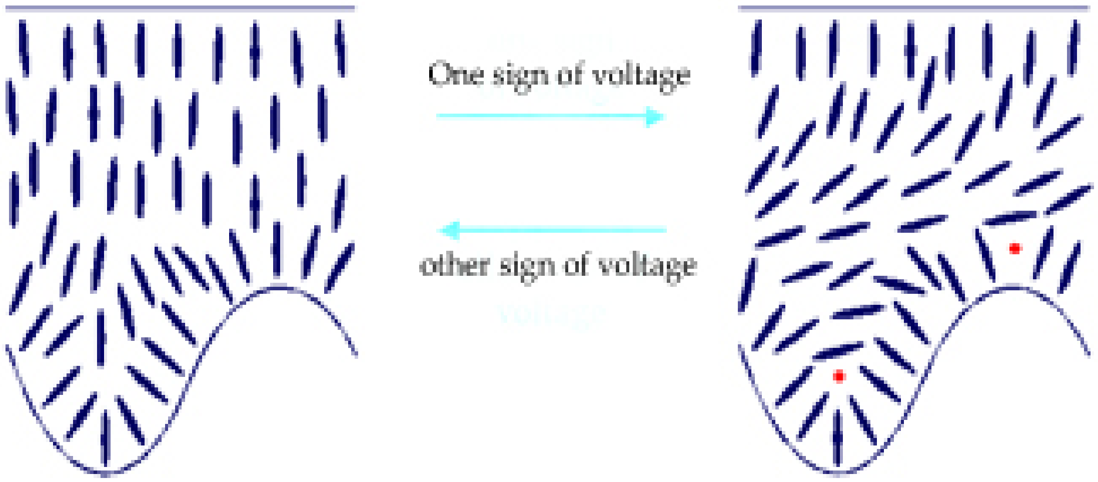
Twisted Nematic Liquid Crystal Display – a monostable liquid crystal display.

Bistable displays

Working principle:

• locally stable bright and dark states without an electric field

• power is needed to switch between distinct states but not to maintain them

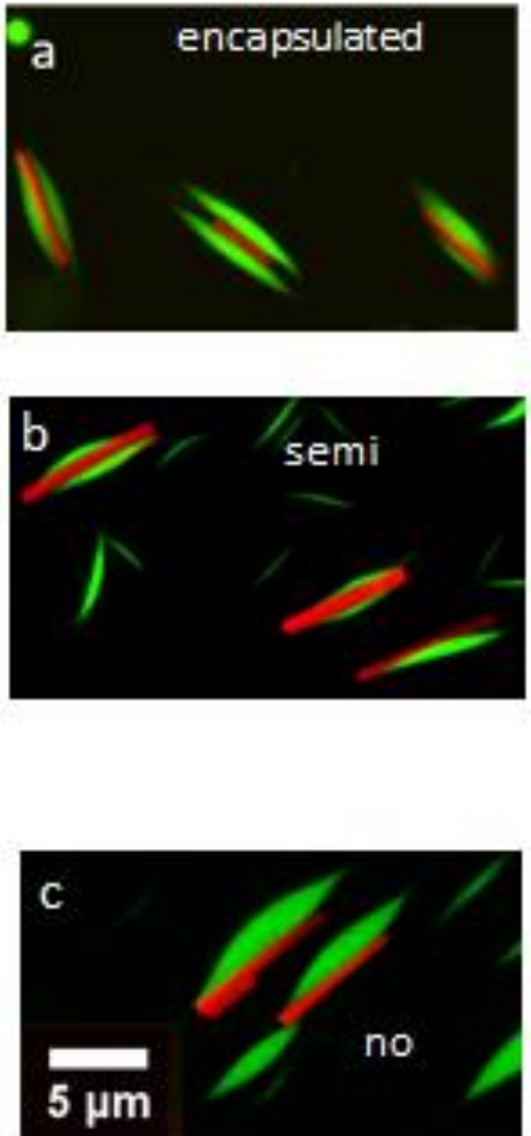


Zenithally Bistable Nematic Device

www.eng.ox.ac.uk

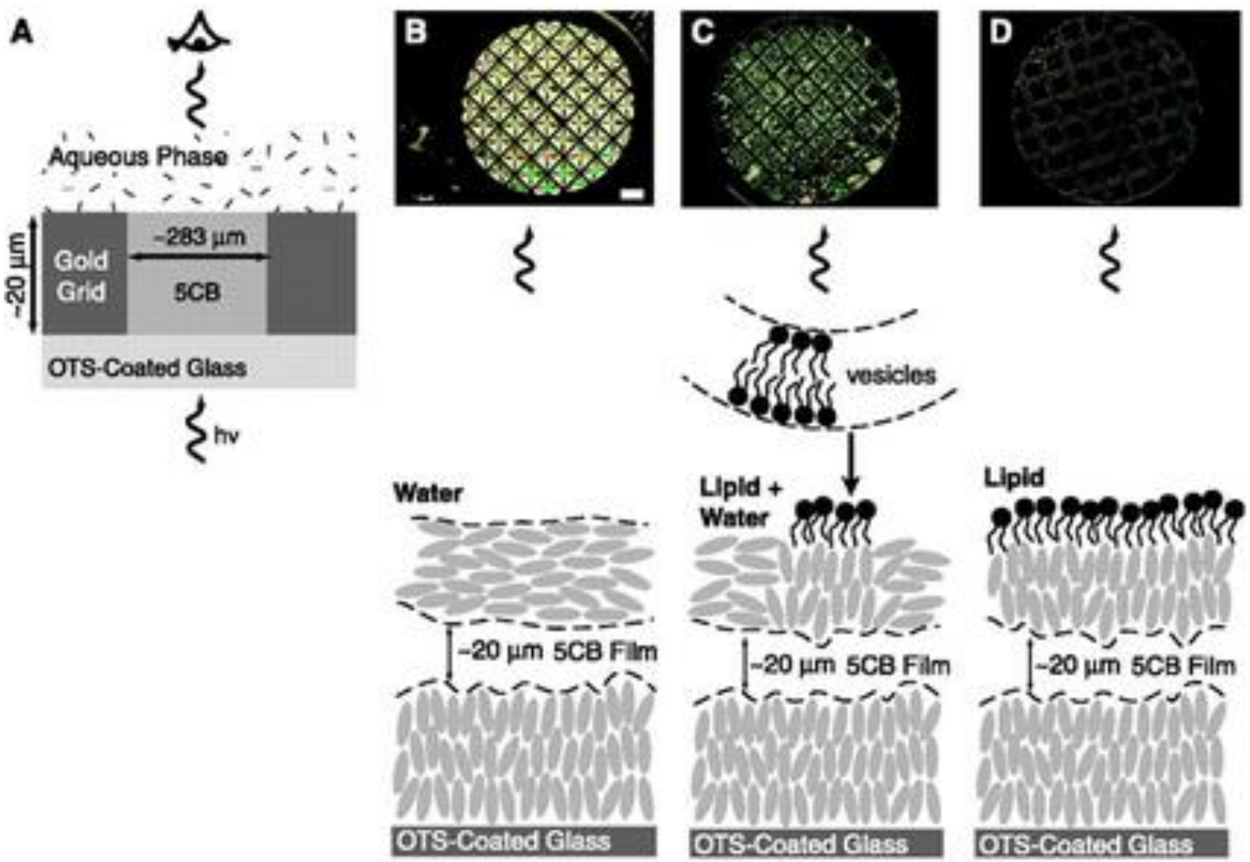
• larger, higher resolution displays with much reduced power consumption.

Pathological Studies: bacterium encapsulated by viral tactoids



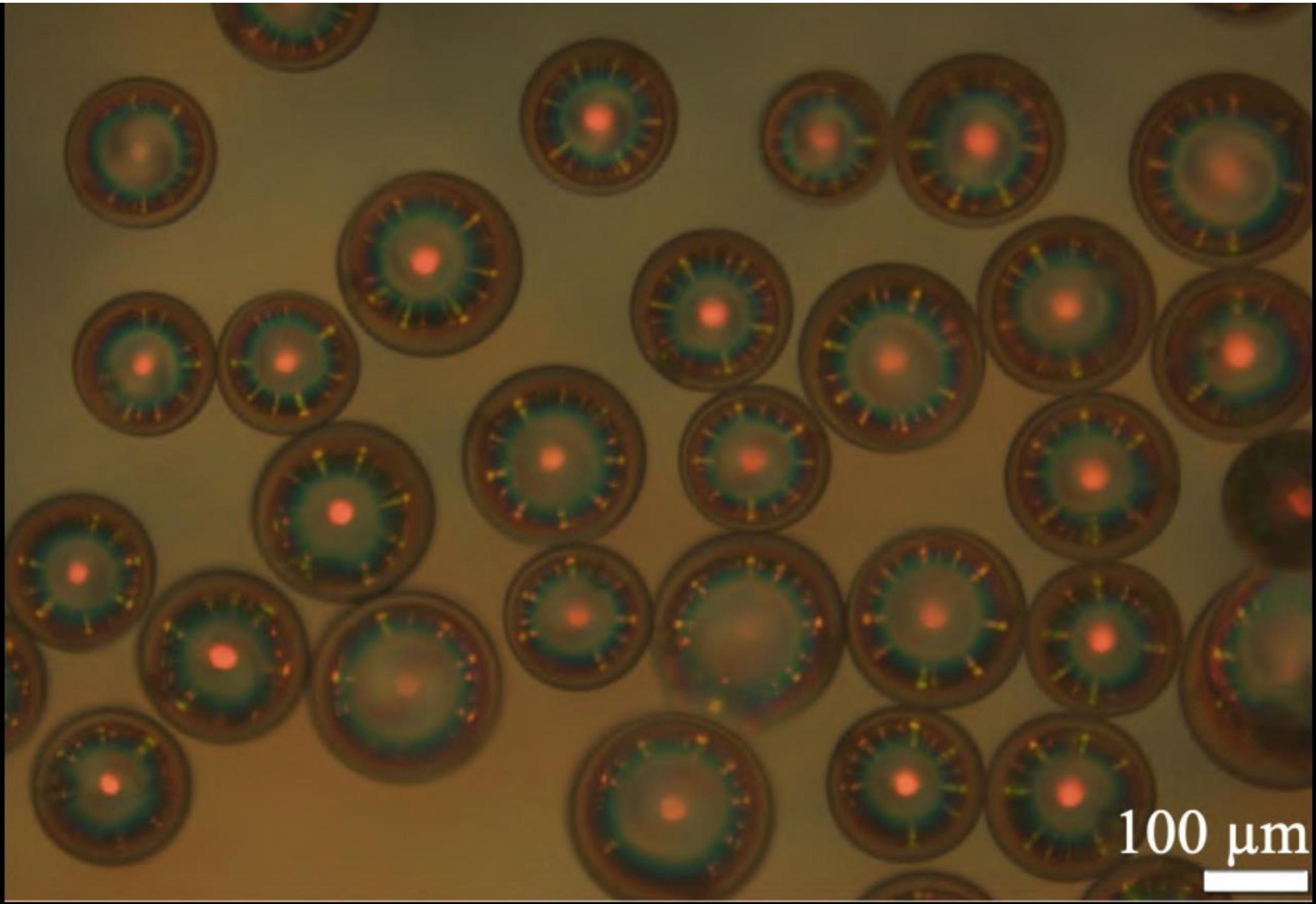
Figures provided by Iago Grobas, Mariana De Silva, Dirk Aarts (University of Oxford); Modelling – Yucen Han, Lei Zhang and Apala Majumdar

Use in sensors…



https://nlabbottcornell.weebly.com/research.html

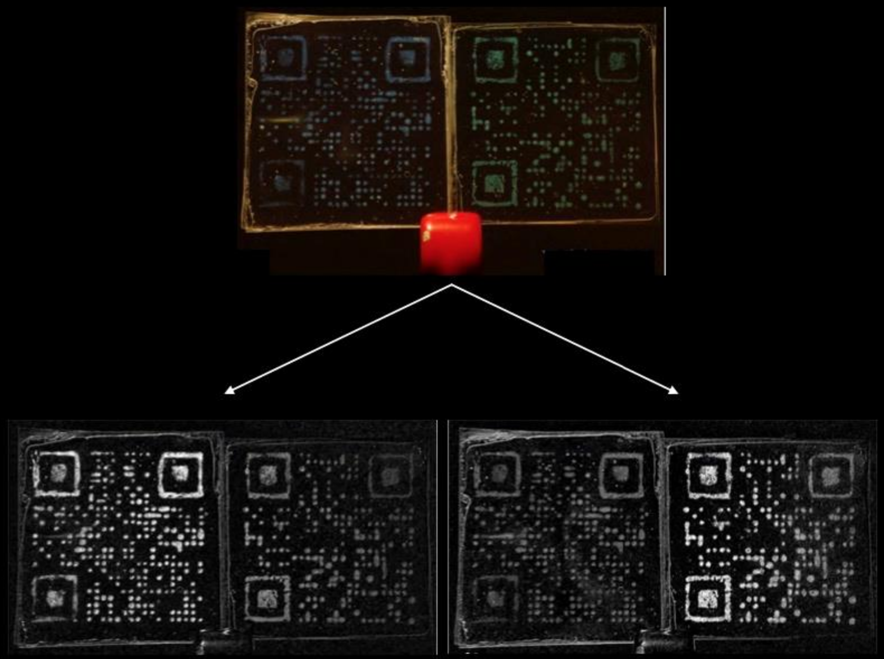
Applications in counterfeiting....



M. Schwartz et *al.*, *Multifunct. Mater.* **4**, 022002 (2021)

Applications in counterfeiting….

QR-codes made using CSR droplets



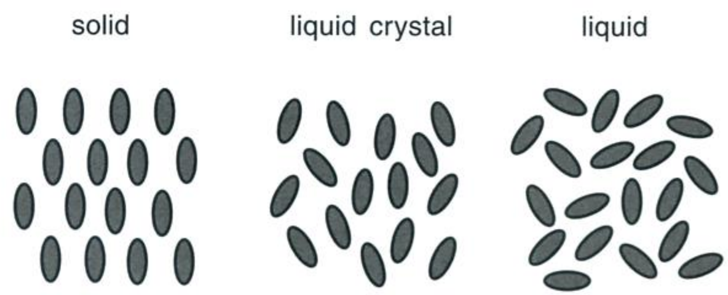
M. Schwartz et *al.*, *Multifunct. Mater.* **4**, 022002 (2021)

Liquid Crystals are a fascinating playground for mechanics, geometry, modelling and analysis to meet physics and real-life applications.

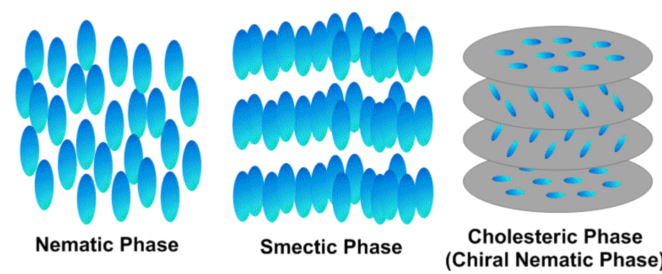
- Real opportunity for new mathematics-driven approaches to new materials, optimal design, optimal performance and efficient methodologies.

UK Liquid Crystal Research

- ✓ University of Strathclyde (large theory group)
- ✓ University of Glasgow
- ✓ University of Aberdeen
- ✓ Scottish Microelectronics Centre, University of Edinburgh
- ✓ Heriot Watt and Dundee
- ✓ New Scottish Network for Liquid Crystals led by Strathclyde
- ✓ Strathclyde-funded Reading Group for junior researchers in liquid crystals and soft matter
- ✓ Links well with the UK wide Durham-Oxford-Strathclyde network on anisotropic materials and the premier British Liquid Crystal Society
- ✓ Other UK centres of excellence – Leeds, Birmingham, Durham, Oxford, Bristol, Southampton …



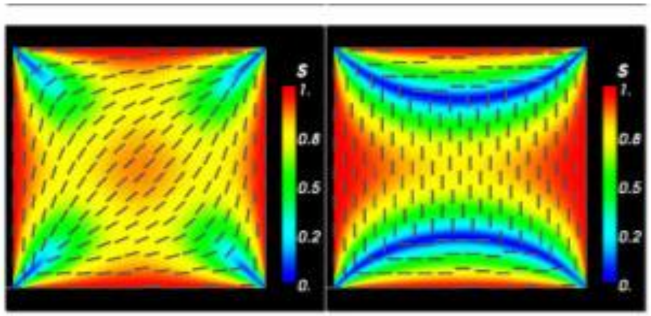
(Felix, et al., 2015)



(tokyo chemical industry)

Format of talk:

- A brief review of Mathematical Theories for Nematic Liquid Crystals
- Oseen-Frank Theory
- Landau-de Gennes Theory
- 2D Polygons
- 3D Shells
- Questions?

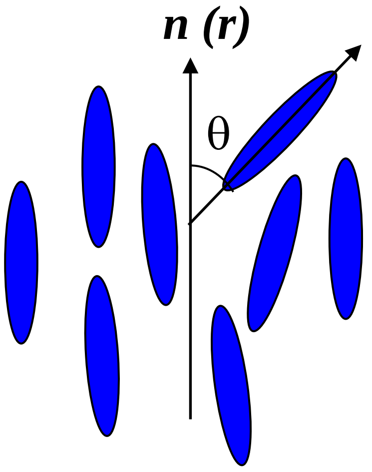


2D pattern formation in NLC-filled square domains.

Important mathematical parameters -

Nematic liquid crystals are anisotropic liquids with preferred directions of molecular alignment. The preferred alignment directions constitute the first set of important parameters.

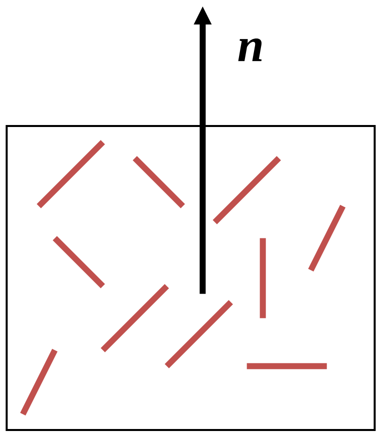
Simplest model – think of nematic molecules as being elongated rods with a single preferred direction of alignment such that all directions perpendicular to this distinguished direction are physically equivalent.



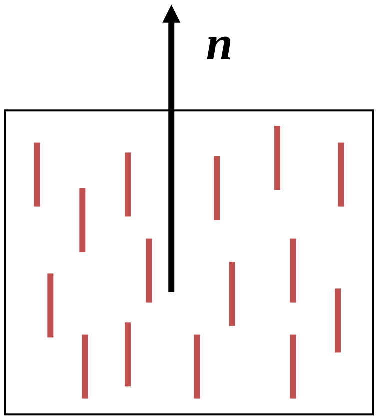
n (r) : preferred direction of orientation of the long molecular axes.

Scalar order parameter “S”:

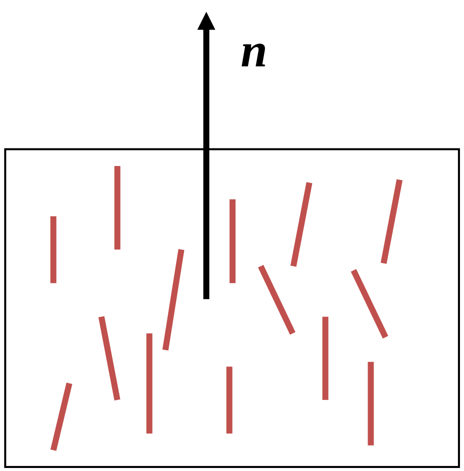
a measure of the degree of alignment of the molecules.



S = 0; no alignment



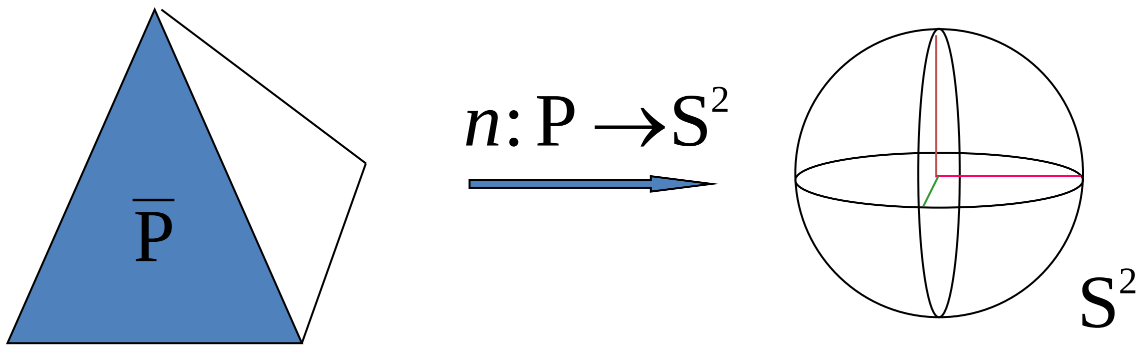
S = 1; perfect alignment



S ≈ 0.5; typical liquid crystal.

The Oseen-Frank Theory for Nematic Liquid Crystals

- assume constant value of scalar order parameter
- describe preferred direction by a unit-vector field ***n(r)***

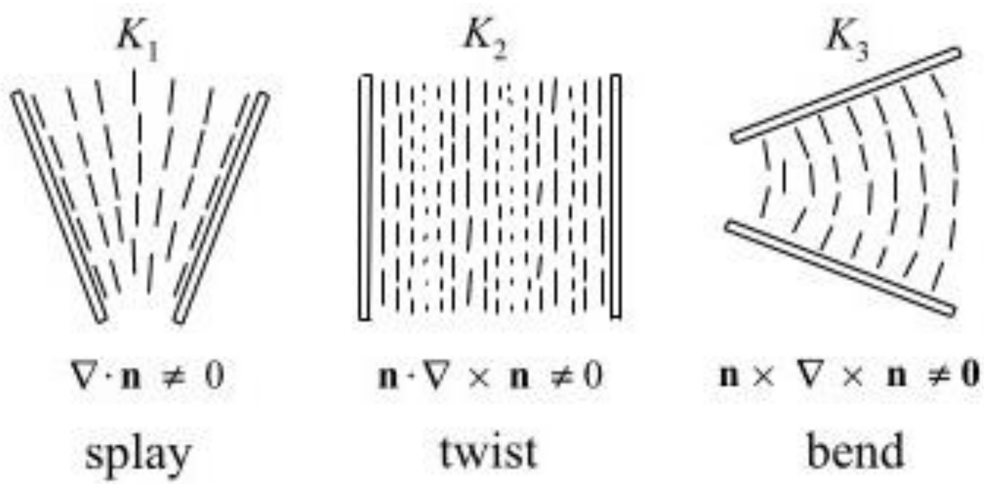


- just two degrees of freedom to describe a three-dimensional unit-vector field

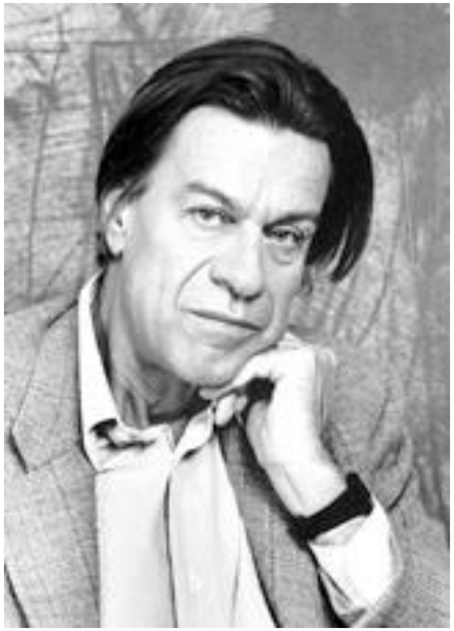
The Oseen-Frank theory…

- Describe the nematic phase by a unit-vector field.
- Does not account for the equivalence between ***n*** and ***–n***.

$$E[\mathbf{n}] := \iiint_\Omega \frac{1}{2}\left(K_1(\nabla\cdot\mathbf{n})^2 + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n})^2 + K_3(\mathbf{n}\times\nabla\times\mathbf{n})^2\right) + \frac{1}{2}(K_2+K_4)\left(\nabla\cdot[(\mathbf{n}\cdot\nabla)\mathbf{n} - (\nabla\cdot\mathbf{n})\mathbf{n}]\right)\, d\Omega,$$



The Landau-de Gennes Theory



The Nobel Prize in Physics in 1991 was awarded to Pierre-Gilles de Gennes for "for discovering that methods developed for studying order phenomena in simple systems can be generalized to more complex forms of matter, in particular to liquid crystals and polymers“.

The Landau-de Gennes Theory

• General continuum theory that can account for all nematic phases and physically observable singularities.

•Define macroscopic order parameter that distinguishes nematic liquid crystals from conventional liquids, in terms of anisotropic macroscopic quantities such as the magnetic susceptibility and dielectric anisotropy.

• The **Q** – tensor order parameter is a symmetric, traceless 3×3 matrix.

$$Q = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{12} & Q_{22} & Q_{23} \\ Q_{13} & Q_{23} & -Q_{11} - Q_{22} \end{pmatrix}$$

- De Gennes' 1991 Nobel prize in Physics

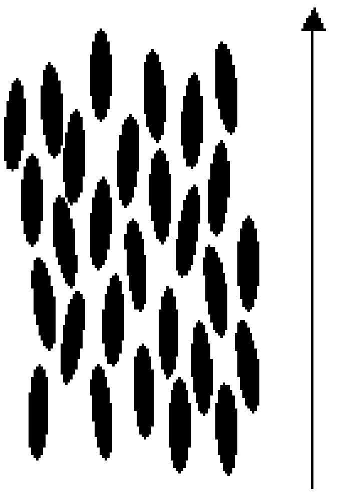
  "for discovering that methods developed for studying order phenomena in simple systems can be generalized to more complex forms of matter, in particular to liquid crystals and polymers"

Five degrees of freedom.

Eigenvalues of the Q-tensor and LC Phases

$$Q = \lambda_1 n \otimes n + \lambda_2 m \otimes m + \lambda_3 p \otimes p$$

$$\sum_{i=1}^{3} \lambda_i = 0$$



- isotropic – triad of zero eigenvalues

$$\lambda_1 = \lambda_2 = \lambda_3 = 0 \qquad \Rightarrow \qquad Q = 0$$

- uniaxial – a pair of equal non-zero eigenvalues; OF theory is a special uniaxial case with constant eigenvalues

$$\lambda_2 = \lambda_3 = -\lambda; \lambda_1 = 2\lambda \quad \Rightarrow \quad Q = 3\lambda\left(n \otimes n - \frac{1}{3} I \right)$$

- biaxial – three distinct eigenvalues and two locally preferred directions of molecular alignment.

The Landau-de Gennes energy functional

The physically observable configurations are modelled by minimizers of the Landau-de Gennes liquid crystal energy functional subject to the imposed boundary conditions.

In the absence of any external fields and surface effects, the simplest form of the Landau-de Gennes energy is given by

$$I[Q] = \int_{\Omega} f_B(Q) + w(Q, \nabla Q)\, dV$$

The thermotropic potential : -

$$f_B(Q) = \frac{a}{2} \operatorname{tr} Q^2 - \frac{b}{3} \operatorname{tr} Q^3 + \frac{c}{4} \left(\operatorname{tr} Q^2\right)^2 + C(a,b,c)$$

$$a = \alpha\left(T - T^*\right) \qquad \alpha, b, c, T^* > 0$$

- non-convex , non-negative potential with multiple critical points
- dictates preferred phase of liquid crystal – isotropic/ uniaxial/ biaxial?

The Thermotropic Potential

$$\mathrm{f_B}(\mathrm{Q}) = \frac{\mathrm{a}}{2}\,\mathrm{tr}\,Q^2 \;-\; \frac{\mathrm{b}}{3}\,\mathrm{tr}\,Q^3 + \frac{\mathrm{c}}{4}\left(\mathrm{tr}\,Q^2\right)^2 + C(a,b,c)$$

$$\mathrm{a} = \alpha\left(T - T^*\right) \qquad \alpha, \mathrm{b}, \mathrm{c}, \mathrm{T}^* > 0$$

- Compute critical points of this quartic polynomial as a function of the temperature

$$\mathrm{f_B}(\lambda_1, \lambda_2, \lambda_3) = \frac{\mathrm{a}}{2}\sum_{i=1}^{3}\lambda_i^2 \;-\; \frac{\mathrm{b}}{3}\sum_{i=1}^{3}\lambda_i^3 + \frac{\mathrm{c}}{4}\left(\sum_{i=1}^{3}\lambda_i^2\right)^2 + C(a,b,c)$$

$$\sum_{i=1}^{3}\lambda_i = 0$$

$$\frac{\partial \mathrm{f_B}(\lambda_1, \lambda_2, \lambda_3)}{\partial \lambda_\mathrm{i}} - \delta\lambda_\mathrm{i} = 0 \quad \Rightarrow \quad \lambda_\mathrm{i} = \lambda_\mathrm{j} \quad i \neq j$$

All critical points are either uniaxial or isotropic for all temperatures.

The Thermotropic Potential

All critical points are either uniaxial or isotropic for all temperatures

$$Q = S\left(n \otimes n - \frac{I}{3}\right) \qquad n \in S^2$$

- Compute minimizers of bulk potential by looking at the critical points of the thermotropic potential restricted to uniaxial tensors.

$$f_B(S) = \frac{a}{3}S^2 - \frac{2b}{27}S^3 + \frac{c}{9}S^4 + C(a,b,c)$$

- $S_1 = 0$, the isotropic state, is globally stable for $a > \frac{b^2}{27c}$, metastable for $0 < a < \frac{b^2}{27c}$ and unstable for $a < 0$.
- $S_1 = \frac{1}{4c}\left(-b + \sqrt{b^2 - 24ac}\right)$, the nematic state, is globally stable for $a < \frac{b^2}{27c}$, metastable for $\frac{b^2}{27c} < a < \frac{b^2}{24c}$ and not defined for $a > \frac{b^2}{24c}$.
- $S_1 = \frac{1}{4c}\left(-b - \sqrt{b^2 - 24ac}\right)$ is metastable (but has a negative value) for $a < 0$, unstable for $\frac{b^2}{27c} < a < \frac{b^2}{24c}$ and not defined for $a > \frac{b^2}{24c}$.

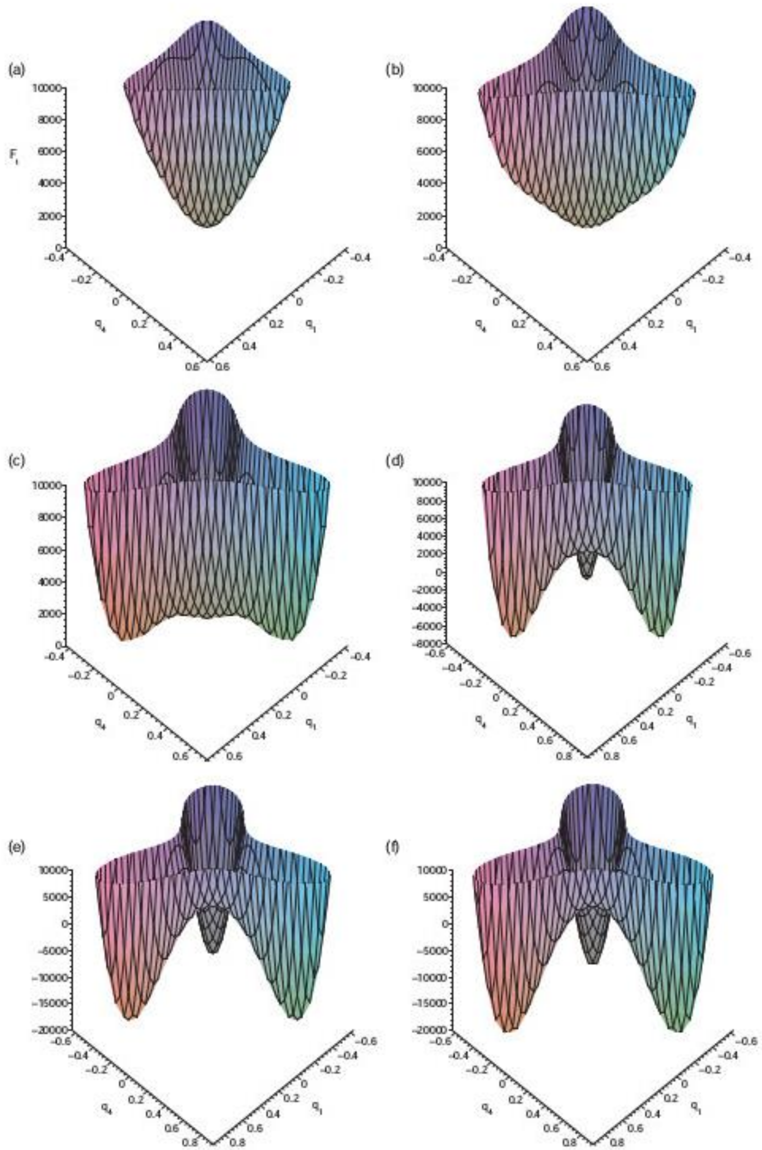


FIG. 7: The thermotropic potential for parameters $\alpha = 0.042 \times 10^6 \mathrm{Nm}^{-2}\mathrm{K}^{-1}$, $b = -0.64 \times 10^6 \mathrm{Nm}^{-2}$, $c = 0.35 \times 10^6 \mathrm{Nm}^{-2}$ [7] and (a) $\Delta T = 2.0$, (b) $\Delta T = 1.5$, (c) $\Delta T = 1.0$, (d) $\Delta T = 0.5$, (e) $\Delta T = 0.0$, (f) $\Delta T = -0.1$. At high temperatures (a,b) only the isotropic state is stable and at low temperature (d,e,f) the three uniaxial states are stable. At intermediate temperatures (c) both the isotropic and all three nematic states are stable.

$$f_B(S) = \frac{a}{3} S^2 - \frac{2b}{27} S^3 + \frac{c}{9} S^4 + C(a,b,c)$$

Introduction to Q-tensor theory 2014

Nigel J. Mottram, Christopher J.P. Newton

The Landau-de Gennes Euler Lagrange Equations

The physically observable configurations correspond to minimizers of the Landau-de Gennes liquid crystal energy subject to the imposed boundary conditions.

The Euler-Lagrange equations in the one-constant case :

$$w(Q, \nabla Q) = L|\nabla Q|^2$$

$$w(Q, \nabla Q) = L_1|\nabla Q|^2 + L_2 Q_{ij,j} Q_{ik,k}$$

$$\Delta Q_{ij} = \frac{1}{L}\left(A Q_{ij} - B\left(Q_{ip}Q_{pj} - \frac{1}{3}(trQ^2)\delta_{ij}\right) + C(trQ^2)Q_{ij}\right) \quad i,j = 1,2,3$$

$$\Delta Q_{ij} + \frac{L_2}{2}\left(Q_{ik,kj} + Q_{jk,ki} - \frac{2}{3}\delta_{ij}Q_{kl,kl}\right) = \frac{\lambda^2}{L}\left\{A Q_{ij} - B\left(Q_{ik}Q_{kj} - \frac{1}{3}\delta_{ij}\mathrm{tr}\mathbf{Q}^2\right) + C Q_{ij}\mathrm{tr}\mathbf{Q}^2\right\},$$

✓ System of nonlinear, coupled partial differential equations

What can mathematics tell us?

$$\Delta Q_{ij} = \frac{1}{L}\left(AQ_{ij} - B\left(Q_{ip}Q_{pj} - \frac{1}{3}(trQ^2)\delta_{ij}\right) + C(trQ^2)Q_{ij}\right) \quad i,j = 1,2,3$$

- ✓ Physically relevant/ observable states ⇔ Energy minimizers
- ✓ Energy minimizers ⇔ Classical Solutions of Euler-Lagrange Equations
- ✓ Asymptotic Analysis ⇒ Defect Sets
- ✓ Non- Energy Minimising Solutions ⇒ Switching Mechanisms

- ✓ **Modelling experiments and applications**
- ✓ **Predicting and Designing New Systems**
- ✓ **Control of Static and Dynamic Phenomena**

What can mathematics do for LC devices:

- **Stable states**

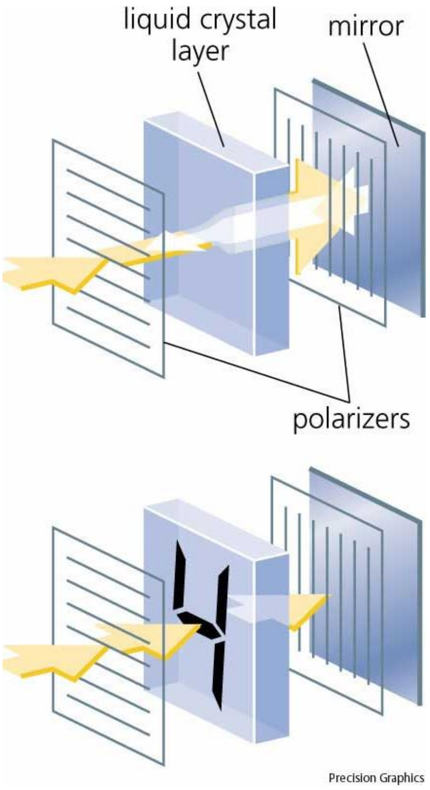
▪ structure
▪ multiplicity
▪ defects

- **Optical properties**?

Inverse problems

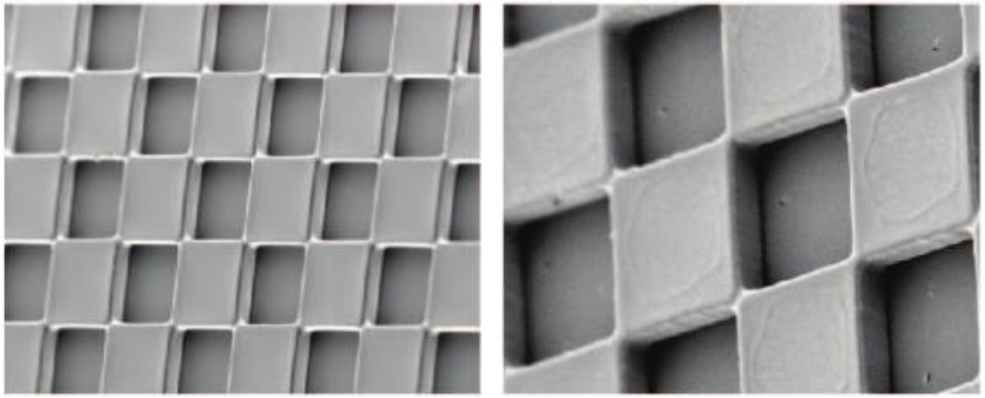
- **Switching mechanisms**

Estimates for switching times – relate to image control and refresh times?



See [1] A.Majumdar, C.J.P.Newton, J.M.Robbins and M.Zyskin, 2007 Topology and bistability in liquid crystal devices. Phys. Rev. E, 75, 051703--051714.
[2] Raisch, A. and Majumdar, A., 2014. Order reconstruction phenomena and temperature-driven dynamics in a 3D zenithally bistable device. *EPL (Europhysics Letters)*, 107 (1), 16002.
[3] M.Robinson, C.Luo, P.Farrell, R.Erban, and A.Majumdar 2017 From molecular to continuum modelling of bistable liquid crystal devices. Liquid Crystals, Volume 44, Issue 14-15, 2267-2284.
[4] H.Kusumaatmaja and A.Majumdar, 2015 Free energy pathways of a Multistable Liquid Crystal Device. Soft Matter 11 (24), 4809-4817.

A Toy Problem: The Planar Bistable LC Device



Tsakonas, Davidson, Brown, Mottram , Appl. Phys. Lett. 90, 111913 (2007)

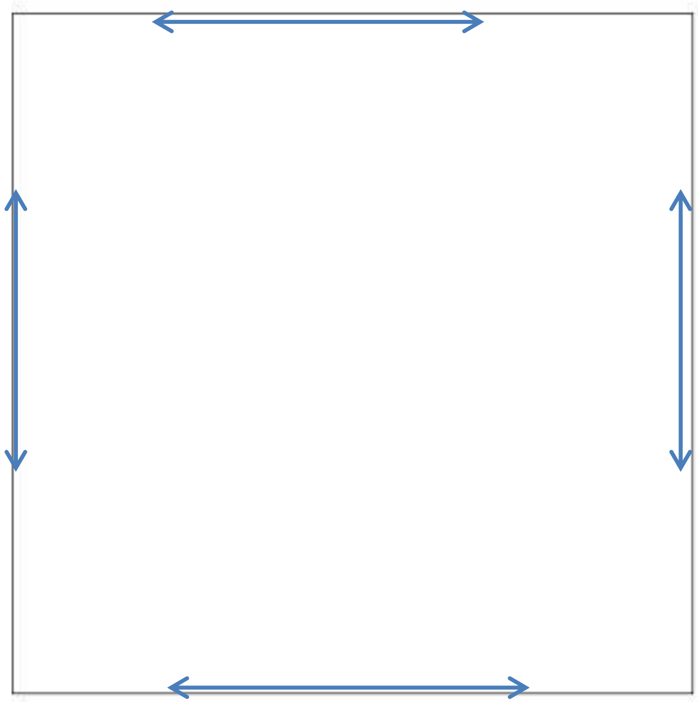
- Micro-confined liquid crystal system.

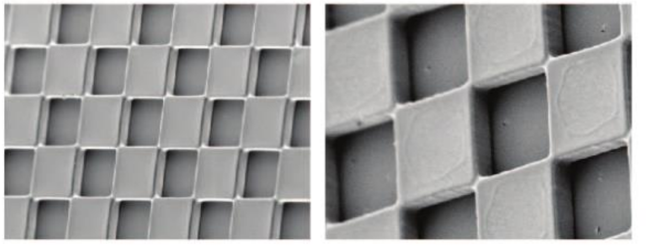
- Array of nematic liquid crystal-filled square / rectangular wells with dimensions between 20×20×12 microns and 80×80×12 microns.

- Surfaces treated to induce planar or tangential anchoring.

Boundary Conditions

• Top and bottom surfaces treated to have tangent boundary conditions – liquid crystal molecules in contact with these surfaces are in the plane of the surfaces.



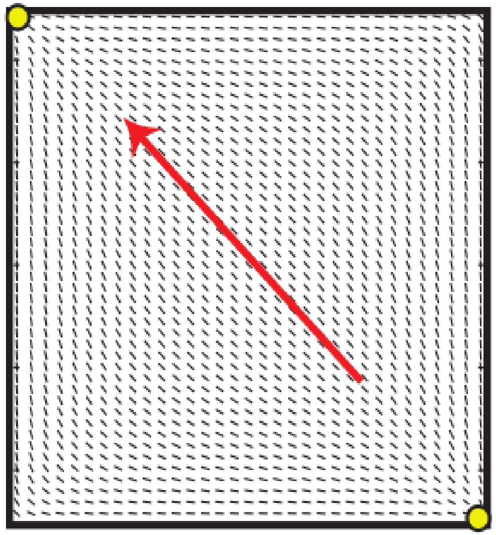


Tsakonas, Davidson, Brown, Mottram 2007

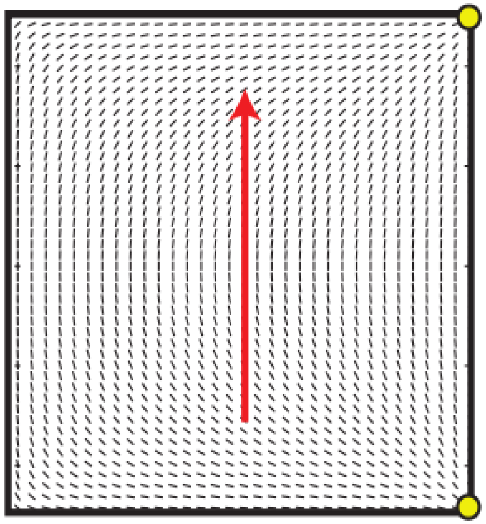
Chong Luo, Apala Majumdar and Radek Erban, 2012 **"Multistability in planar liquid crystal wells",** Physical Review E, Volume 85, Number 6, 061702

Kralj, S. and Majumdar, A., 2014. Order reconstruction patterns in nematic liquid crystal wells. *Proceedings of the Royal Society of London Series A - Mathematical Physical and Engineering Sciences*, 470 (2169), 20140276.

Bistability: two experimentally observed states



Tsakonas, Davidson, Brown, Mottram 2007



- Diagonal state – nematic alignment along one of the square diagonals
- Rotated state – rotation by π radians between a pair of parallel edges.

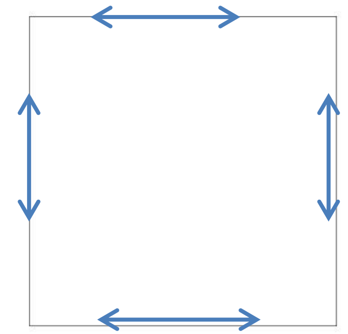
Modelling details

- We look for a particular kind of solution of the form

$$\mathbf{Q} = (q_3+q_1)\vec{e}_x\otimes\vec{e}_x+(q_3-q_1)\vec{e}_y\otimes\vec{e}_y+q_2(\vec{e}_x\otimes\vec{e}_y+\vec{e}_y\otimes\vec{e}_x)-2q_3\vec{e}_z\otimes\vec{e}_z,$$

- planar degenerate boundary conditions on top and bottom surfaces

- planar strong anchoring on lateral surfaces in xz- and yz-planes

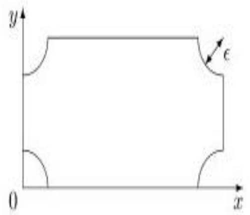


λ

$$\mathbf{Q}_s(0,y,z) = \mathbf{Q}_s(R,y,z) = \frac{S_{eq}}{3}\left(-\vec{e}_x\otimes\vec{e}_x+2\vec{e}_y\otimes\vec{e}_y-\vec{e}_z\otimes\vec{e}_z\right)$$

$$\mathbf{Q}_s(x,0,z) = \mathbf{Q}_s(x,R,z) = \frac{S_{eq}}{3}\left(2\vec{e}_x\otimes\vec{e}_x-\vec{e}_y\otimes\vec{e}_y-\vec{e}_z\otimes\vec{e}_z\right).$$

$$S_{eq} = \frac{b+\sqrt{b^2-24ac}}{4c}$$

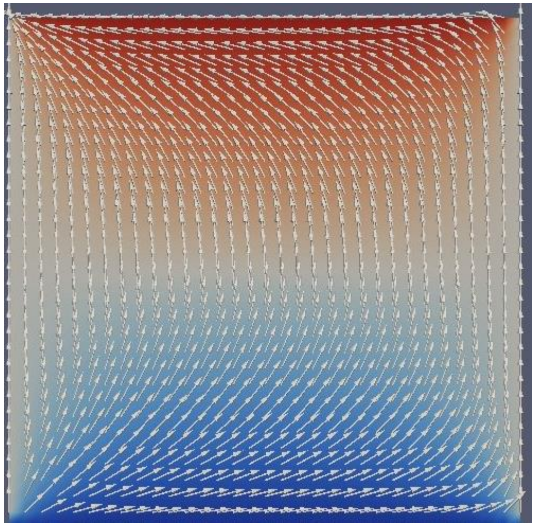


Chong Luo, Apala Majumdar and Radek Erban, 2012 **"Multistability in planar liquid crystal wells",** Physical Review E, Volume 85, Number 6, 061702

Kralj, S. and Majumdar, A., 2014. Order reconstruction patterns in nematic liquid crystal wells. *Proceedings of the Royal Society of London Series A - Mathematical Physical and Engineering Sciences*, 470 (2169), 20140276.

Large micron-sized wells

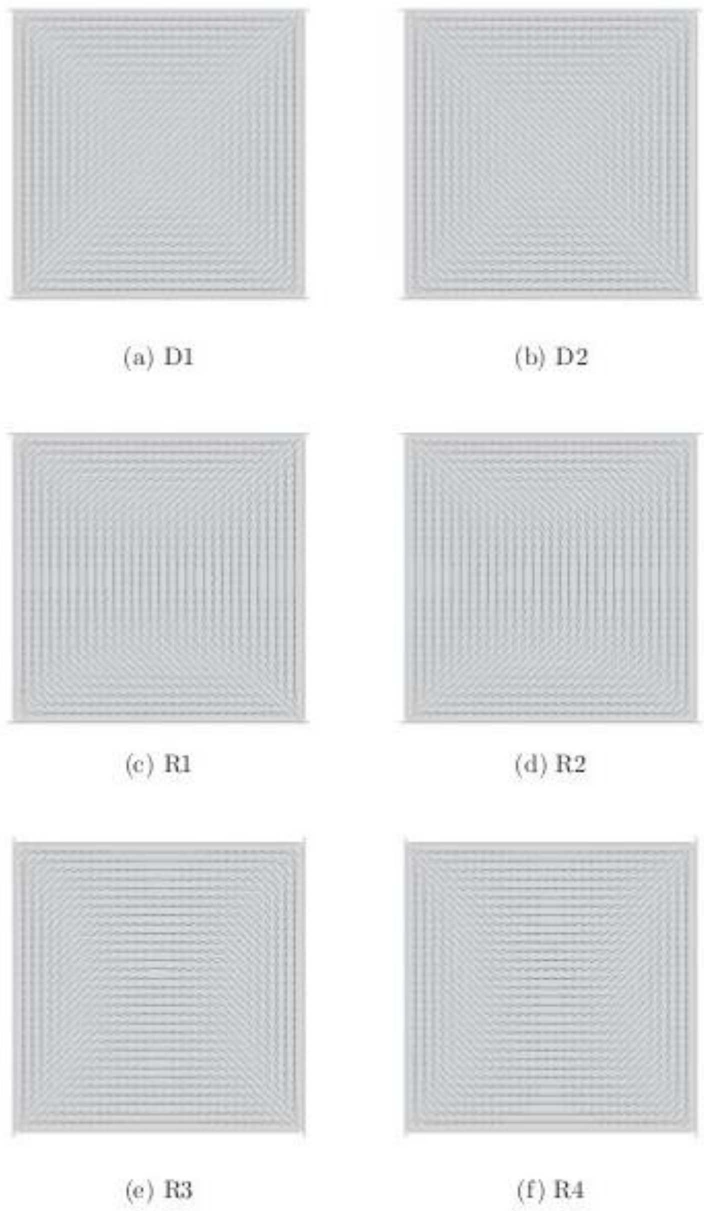
- Minimize the Landau-de Gennes energy with a surface potential to account for the planar boundary conditions.
- Recover six different stable states – two of the diagonal type and four of the rotated type.
- Stable states are effectively uniaxial everywhere away from the vertical edges, or the vertices of the bottom cross-section.



Chong Luo, Apala Majumdar and Radek Erban, 2012 **"Multistability in planar liquid crystal wells",** Physical Review E, Volume 85, Number 6, 061702
Kralj, S. and Majumdar, A., 2014. Order reconstruction patterns in nematic liquid crystal wells. *Proceedings of the Royal Society of London Series A - Mathematical Physical and Engineering Sciences*, 470 (2169), 20140276.

Dirichlet conditions on Lateral Surfaces

We find six different solutions : two diagonal and four rotated solutions.



Chong Luo, Apala Majumdar and Radek Erban, **"Multistability in planar liquid crystal wells",** *Physical Review E,* Volume 85, Number 6, 061702, 15 pages (2012)

Kusumaatmaja, H. and Majumdar, A., 2015. Free energy pathways of a multistable liquid crystal device. *Soft Matter*, 11 (24), pp. 4809-4817.

Structural Uniaxial-Biaxial Transitions

- Competition between two length scales: square length `R' and bare biaxial correlation length, which is typically on the nano-meter scale

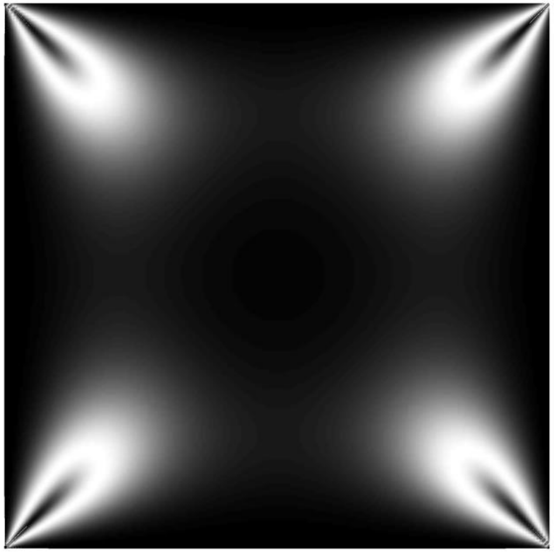
$$\xi_b^{(0)} = 2\sqrt{LC}/B$$

- Introduce ratio

$$\eta = R/\xi_b = \sqrt{\tau}R/\xi_b^{(0)}.$$

- τ : measure of temperature

- Large η : predominantly uniaxial textures with biaxial rims around square vertices; recover diagonal and rotated solutions



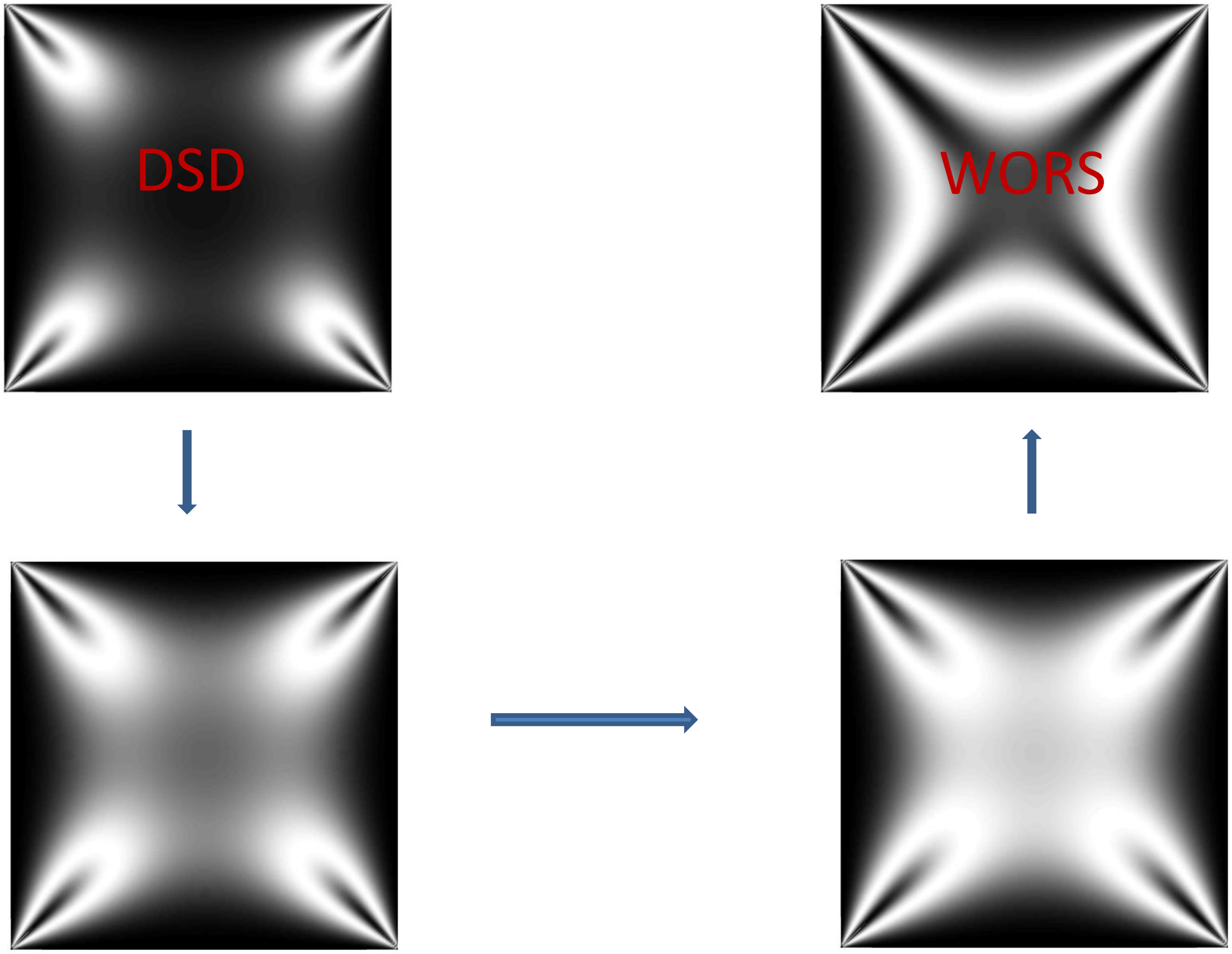
$$\beta^2 = 1 - 6\frac{\left(trQ^3\right)^2}{\left(trQ^2\right)^3}$$

$$0 \leq \beta^2 \leq 1$$

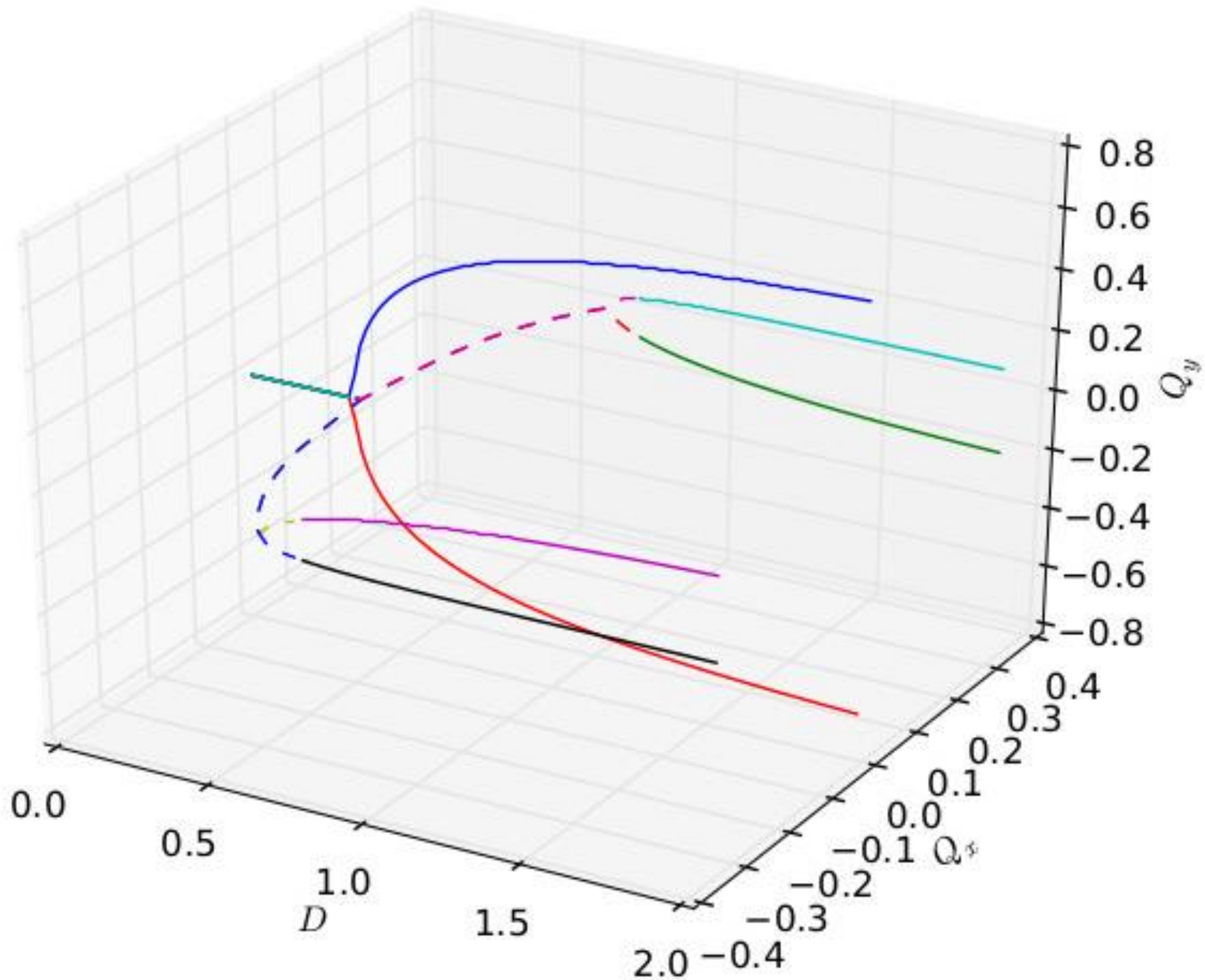
$$\beta^2 = 0 \Rightarrow uniaxial$$

Decrease the ratio η: new structures for sub micron-sized wells

- Well Order Reconstruction Structure (WORS) at critical $\eta \sim 7$

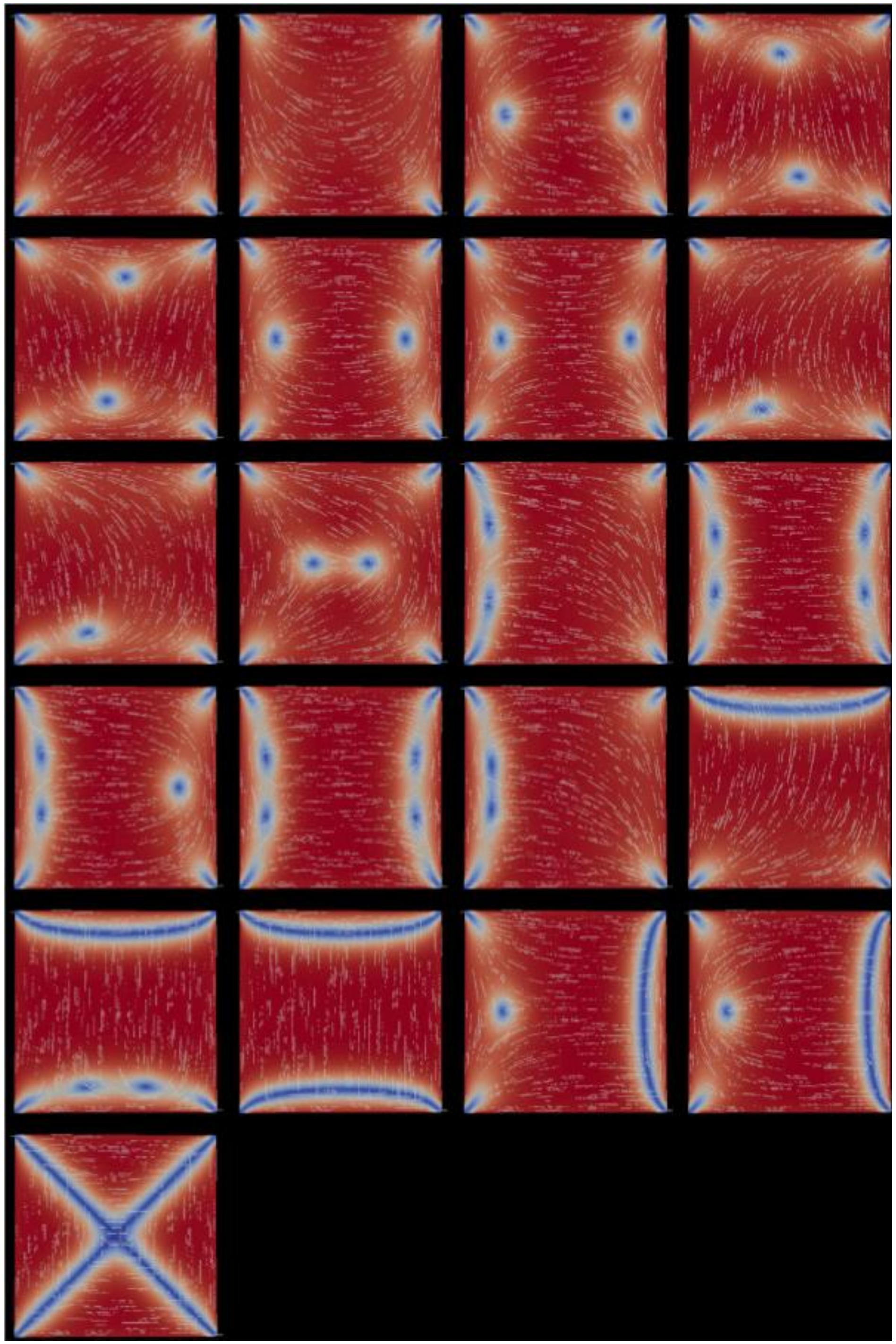


A detailed bifurcation plot



Unique solution for small squares; six distinct solution branches for large squares – two diagonal and four rotated.

[From molecular to continuum modelling of bistable liquid crystal devices](http://www.tandfonline.com/doi/abs/10.1080/02678292.2017.1290284)
Martin Robinson, Chong Luo, Patrick E. Farrell, Radek Erban & Apala Majumdar.
http://www.tandfonline.com/doi/abs/10.1080/02678292.2017.1290284



Look for critical points (not just minimizers) of

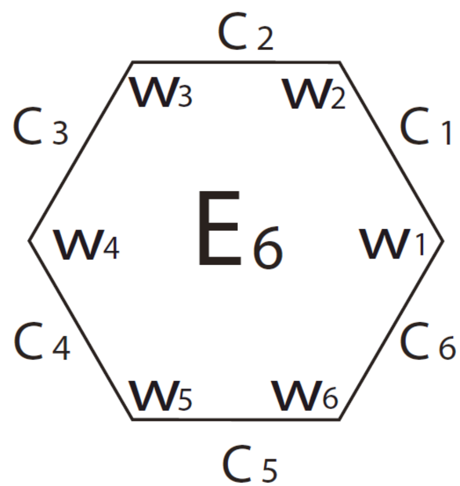
$$J[q_1,q_2] := \int_\Omega \left(|\nabla q_1|^2 + |\nabla q_2|^2 \right) dA + $$
$$+ \int_\Omega \frac{\lambda^2}{L} \left(\frac{-B^2}{2C} \left(q_1^2 + q_2^2\right) + C\left(q_1^2 + q_2^2\right)^2 \right) dA$$

21 other critical points found using numerical deflation techniques for intermediate values of λ.

[From molecular to continuum modelling of bistable liquid crystal devices](http://www.tandfonline.com/doi/abs/10.1080/02678292.2017.1290284)
Martin Robinson, Chong Luo, Patrick E. Farrell, Radek Erban & Apala Majumdar
http://www.tandfonline.com/doi/abs/10.1080/02678292.2017.1290284

P. E. Farrell, Á. Birkisson, and S. W. Funke, "Deflation techniques for finding distinct solutions of nonlinear partial differential equations," *SIAM Journal on Scientific Computing*, vol. 37, p. A2026–A2045, 2015.

Reduced LdG Approaches on Regular Polygons



- Work with a reduced order parameter write $\mathbf{P}$ in terms of nematic scalar order parameter, s and direction $\mathbf{n} = (\cos\gamma, \sin\gamma)$,

$$\mathbf{P} = 2s\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{2}\mathbf{I_2}\right).$$

so that

$$P_{11} = s\cos(2\gamma),\ \ P_{12} = s\sin(2\gamma).$$

- Impose Dirichlet tangent boundary conditions for **P.**

Reduced Approaches contd.

- We can write $\mathbf{P}$ in terms of nematic scalar order parameter, s and direction $\mathbf{n} = (\cos\gamma, \sin\gamma)$,

$$\mathbf{P} = 2s\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{2}\mathbf{I_2}\right).$$

so that

$$P_{11} = s\cos(2\gamma),\ P_{12} = s\sin(2\gamma).$$

- The reduced Landau-de Gennes free energy is given by

$$\mathrm{E}[\mathbf{Q}] = \int_\Omega [\frac{\lambda^2}{L}\left(-\frac{B^2}{4C}tr\mathbf{P}^2 + \frac{C}{4}(tr\mathbf{P}^2)^2\right) + \frac{1}{2}|\nabla\mathbf{P}|]\mathrm{d}A$$

- The corresponding Euler-Lagrange equations are

$$\Delta P_{11} = \frac{2C\lambda^2}{L}\left({P_{11}}^2 + {P_{12}}^2 - \frac{B^2}{4C^2}\right)P_{11},$$

$$\Delta P_{12} = \frac{2C\lambda^2}{L}\left({P_{11}}^2 + {P_{12}}^2 - \frac{B^2}{4C^2}\right)P_{12}.$$

See Maity, Majumdar and Nataraj, IMA Journal of Numerical Analysis, 41 (2020), 1130–1163.

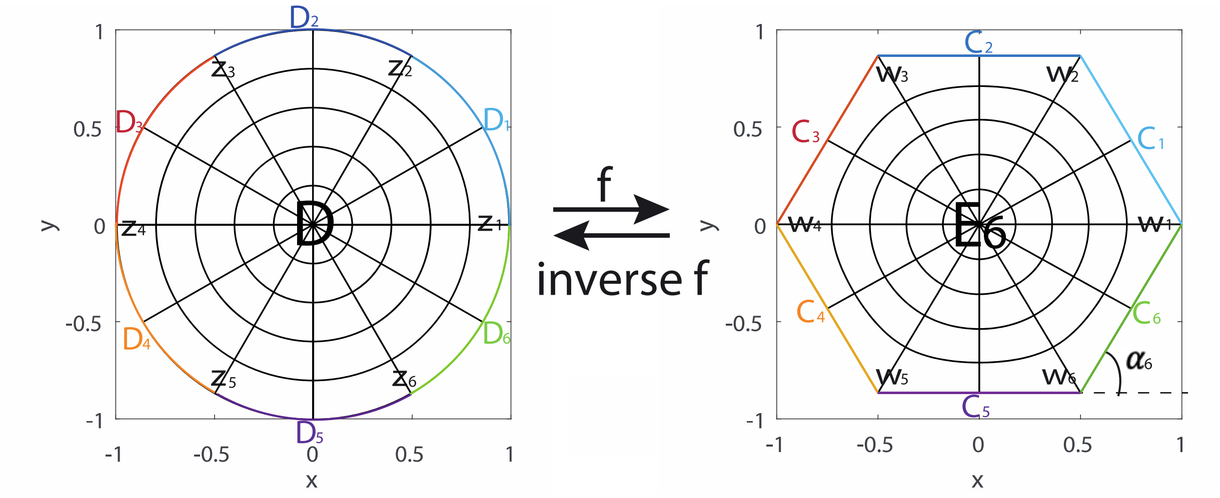
Nano-scale geometries ($\lambda \to 0$)

- **Proposition:** *Let $\mathbf{P}^\lambda \in H^1(\bar{\Omega}, S_0)$ be a solution of the reduced LdG Euler-Lagrange equation (4) for $\lambda > 0$, subject to the boundary condition (5) on $\partial\Omega$. Then as $\lambda \to 0, \mathbf{P}^\lambda$ uniformly converges to the unique solution of the Laplace equation*

$$\Delta P_{11}^0 = 0,$$
$$\Delta P_{12}^0 = 0,$$

subject to the same Dirichlet condition.

Fang, Majumdar, Zhang, 2020

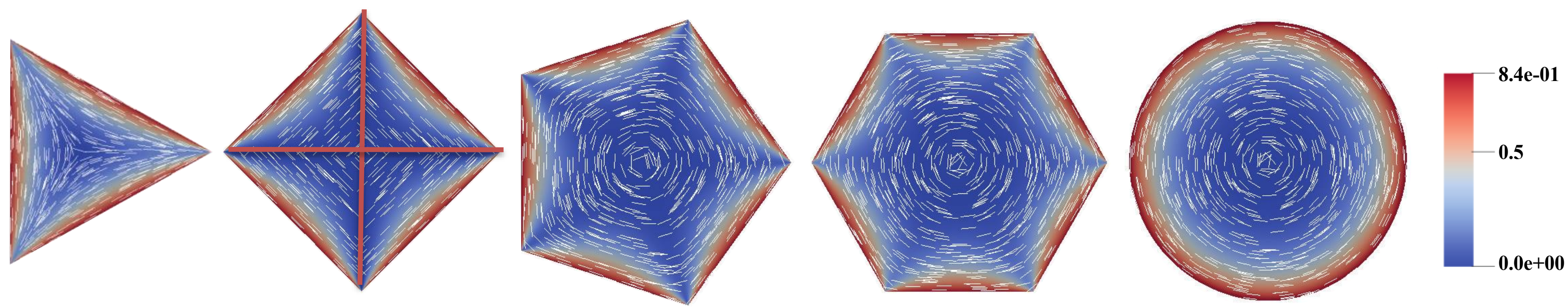


Nano-scale geometries ($\lambda \to 0$)

Proposition: *Let $P_R = (P_{11}, P_{12})$ be the unique Ring solution of*

$$\Delta P_{11}^0 = 0,$$
$$\Delta P_{12}^0 = 0.$$

Then $P_{11}(0,0) = P_{12}(0,0) = 0$ at the center of all regular polygons E_K. However, $P_R(x,y) \neq (0,0)$ for $(x,y) \neq (0,0)$, for all E_K with $K \neq 4$, i.e. the WORS (Well Order Reconstruction Solution) is a special case of P_R on E_4 such that $P_R = (0,0)$ on the square diagonals.



$-\frac{1}{2}$ point defect | line defect | +1 point defect | +1 point defect | +1 point defect

- Y. Han, A. Majumdar, L. Zhang, 2020 A Reduced Study for Nematic Equilibria on Two-Dimensional Polygons, SIAM Journal on Applied Mathematics, Vol. 80, No. 4, pp. 1678–1703.

Multistability for Large Polygons

“splay” vertices
γ^{∞} rotates by $\frac{2\pi}{K}$

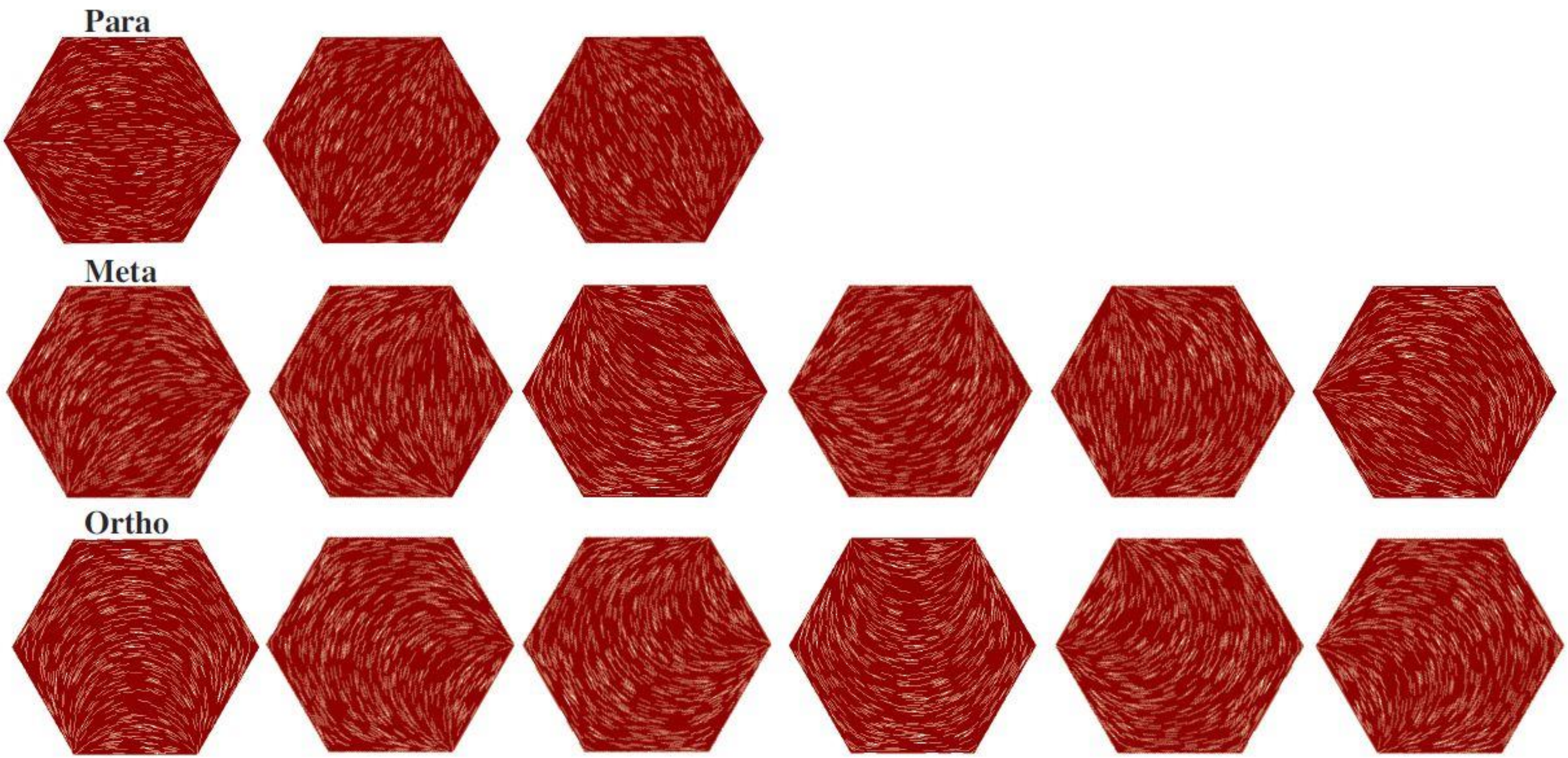
“bend” vertices
γ^{∞} rotates by $\frac{2\pi}{K}$

To satisfy $deg(\mathbf{n}_b, \partial E_K) = 0$, we have 2 “splay” vertices and $(K-2)$ “bend” vertices. Hence, we have at least $\binom{K}{2}$ stable states on the regular polygon with K edges.

Remark: There may be stable states with $deg(\mathbf{n}_b, \partial E_K) \neq 0$.

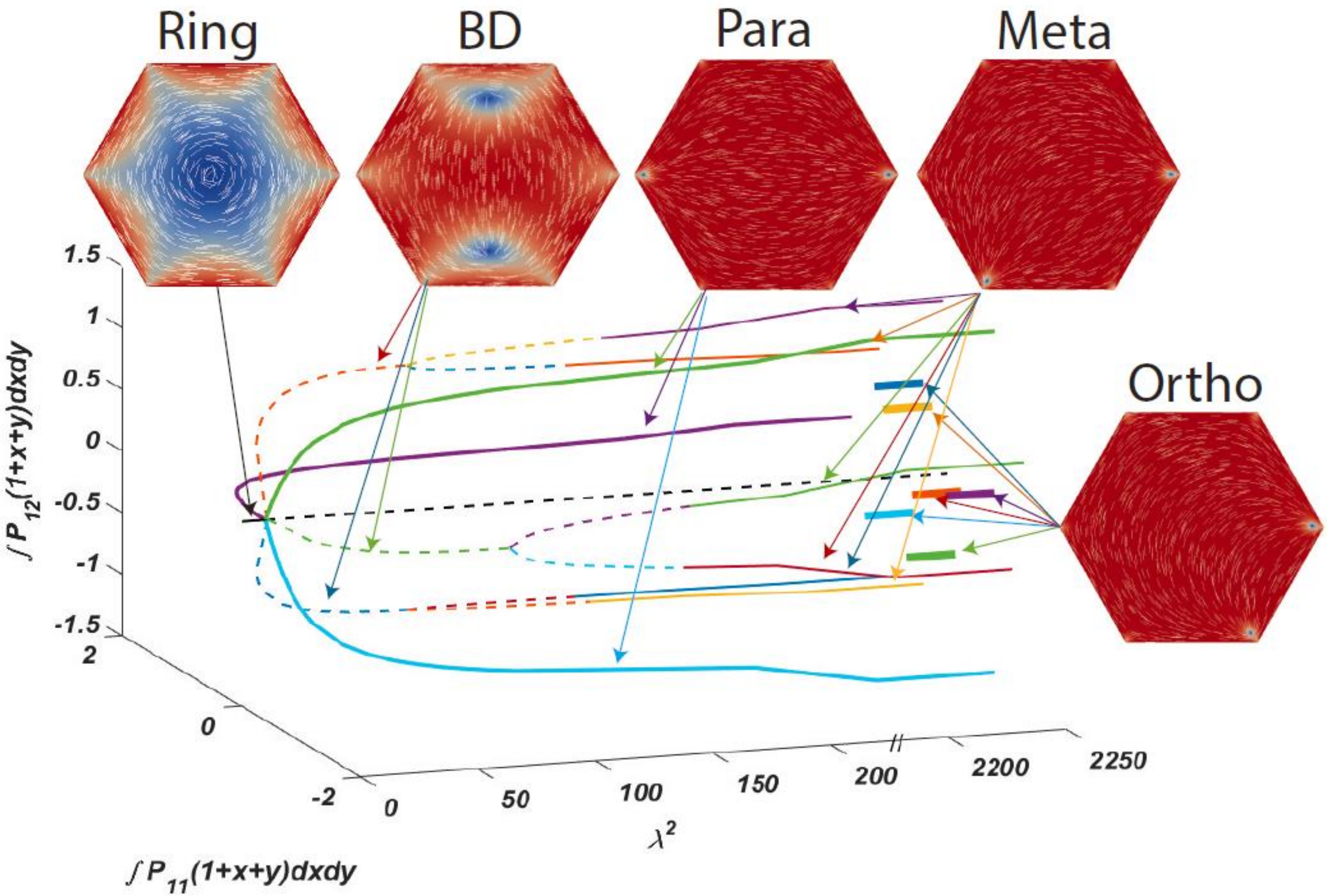
15 stable states on large hexagon

When $K = 6$, $\binom{K}{2} = 15$, we have three Para, six Meta, and six Ortho states.



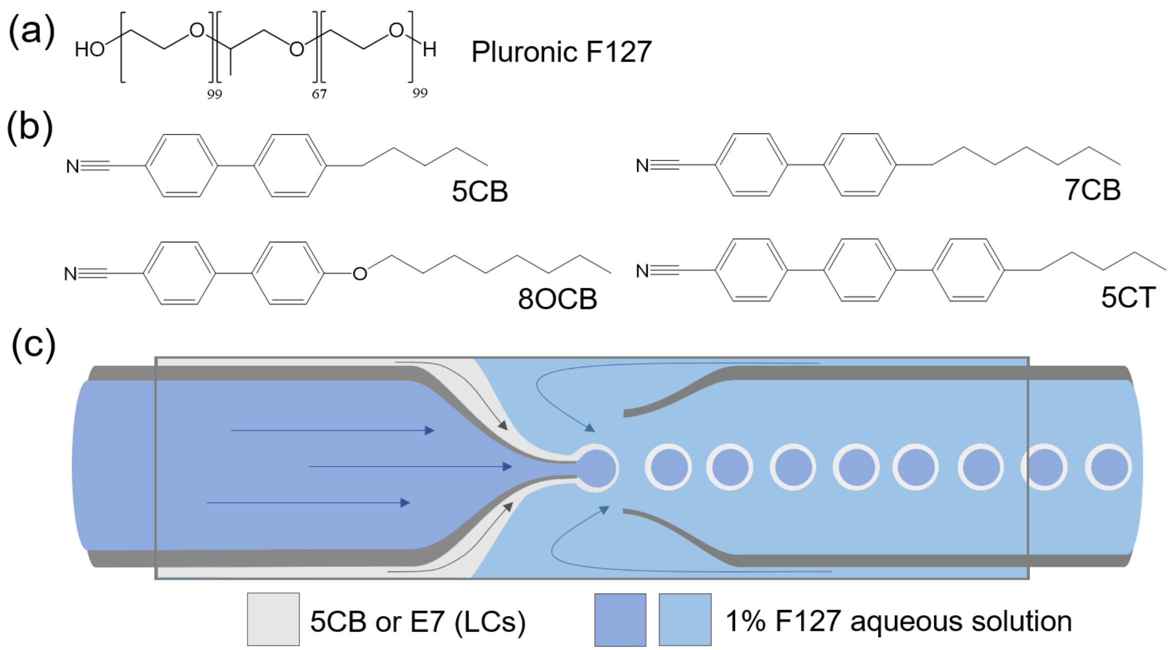
- Y. Han, A. Majumdar, L. Zhang, 2020 A Reduced Study for Nematic Equilibria on Two-Dimensional Polygons, SIAM Journal on Applied Mathematics, Vol. 80, No. 4, pp. 1678–1703.

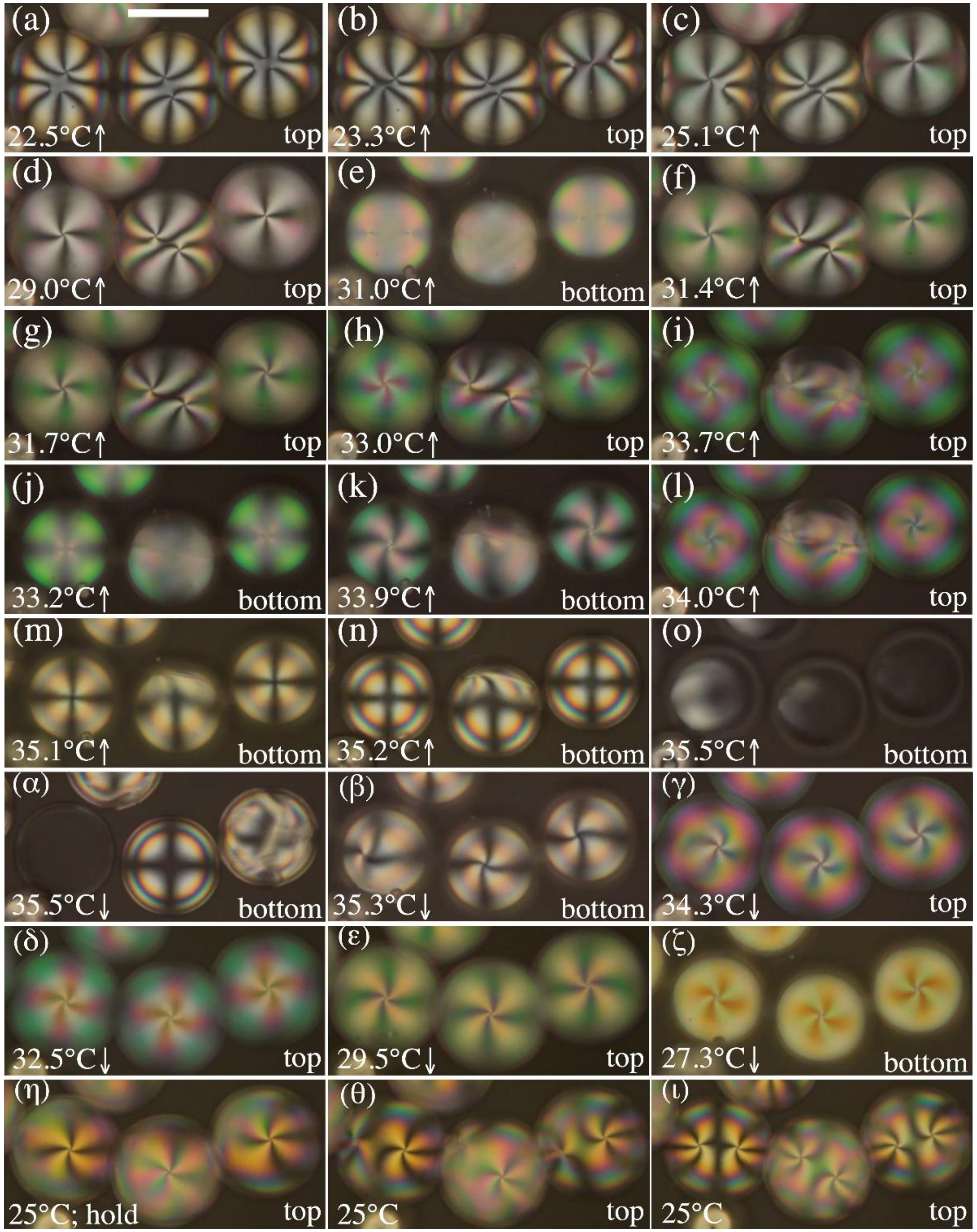
Bifurcation Diagram on a Hexagon as a function of Edge Length



Multistability and Heating Transitions for 3D nematic shells

- ✓ J. Noh, Y. Wang, H. Liang, V. Jampani, A. Majumdar and J. Lagerwall, *Dynamic tuning of the director field in liquid crystal shells using block copolymers,* Physical Review Research, 2 (2020), 033160.





- ✓ Heating transitions from a fully tangential nematic shell, to a hybrid shell and then to a normally aligned nematic shell.

MODELLING DETAILS FOR HYBRID SHELLS

$$
\begin{aligned}
F[Q] = \int_\Omega & \frac{t}{2} tr(Q^2) - \sqrt{6} tr(Q^3) + \frac{1}{2}(tr(Q^2))^2 \\
&+ \frac{\xi_R^2}{2}(Q_{ij,k}Q_{ij,k} + \eta Q_{ij,j}Q_{ik,k}) d\mathbf{x} \\
&+ \int_{D_1} \frac{w_0}{2}(Q_{ij}(\mathbf{x}) - Q^{\mathrm{s}}_{ij}(\mathbf{x}))^2 dA \\
&+ \int_{D_2} \frac{w_1}{2}\left(\widetilde{Q}_{ij} - \widetilde{Q}^{\perp}_{ij}\right)^2 dA
\end{aligned}
$$

$$
\mathbf{Q}^s(x) = s^+ \left(\nu(x) \otimes \nu(x) - \frac{1}{3}\mathbf{I}\right)
$$

$$
\widetilde{Q}^{\perp}_{ij} = P_{ik}\widetilde{Q}_{kl}P_{lj}, \quad \mathbf{P} = \mathbf{I} - \nu \otimes \nu.
$$

Heating Transition – Example I

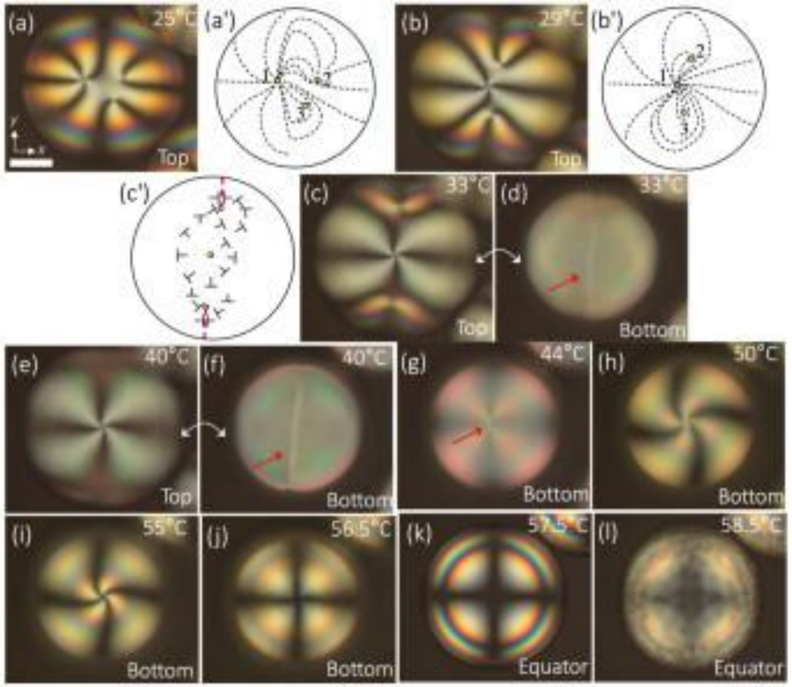


FIG. 8. Alignment transformation upon heating [(a)–(l)] of an E7 shell starting in the T2 configuration [2(+½′), +1′], stabilized by F127 on both sides. The shell is between crossed polarizers (horizontal and vertical). The focal plane is noted in each panel. We draw the ground state director field (a′) and the new one (b′) arising after a defect exchange that initiates the transformation. In (c′), the tilt direction is suggested with nails, nail head and tail signifying upwards- and downwards-pointing director, respectively (or vice versa). The π defect line is highlighted with red arrows in the micrographs and its ends reaching the top shell half are drawn as dashed red lines in c′. Scale bar: 50 μm.

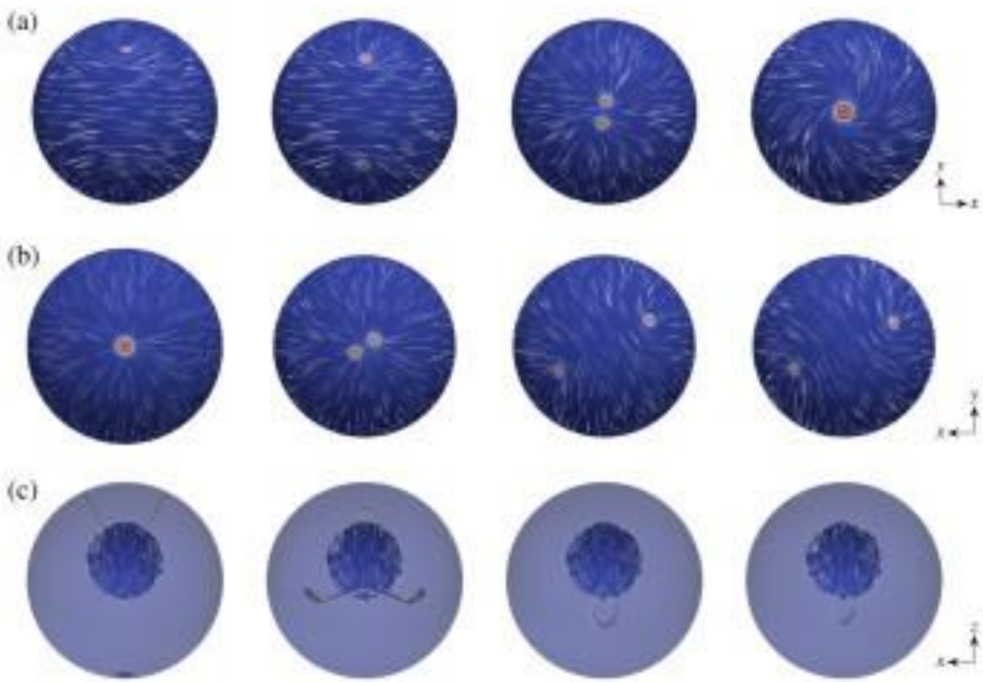


FIG. 9. Simulated trajectory of the T → H transition starting from T2 [2(+½′), +1′], with $t = -1.79$, $c = 0.2$, $\rho = 0.4$, and $\eta = 4$. We plot **n** at the inner shell boundary [left to right: simulation steps $n = 0$, 5000, 20 000, and 40 000]: (a) view from thin part, (b) view from thick part, and (c) side view.

Heating Transition – Example II

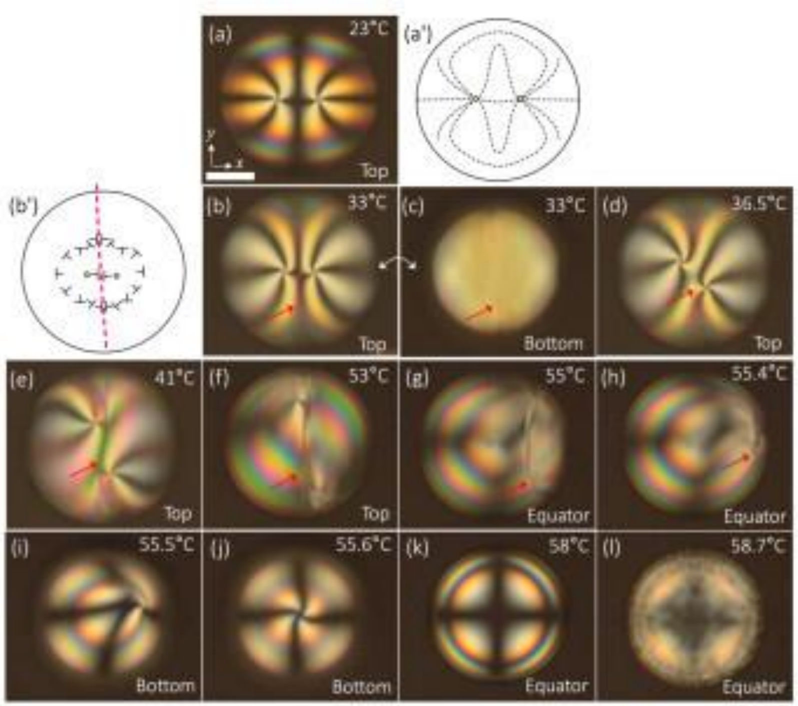


FIG. 10. Alignment transformation upon heating [(a)–(l)] of an E7 shell starting in T3 configuration [2(+1′)], stabilized by F127 on both sides. The shell is between crossed polarizers (horizontal and vertical). The focal plane is noted in each panel. The ground state director field is drawn in (a′). In (b′), the tilt direction is suggested with nails, nail head and tail signifying upwards- and downwards-pointing director, respectively (or vice versa). The π circle separating opposite tilt directions is drawn in red in b′ and highlighted with red arrows in the micrographs. Scale bar: 50 μm.

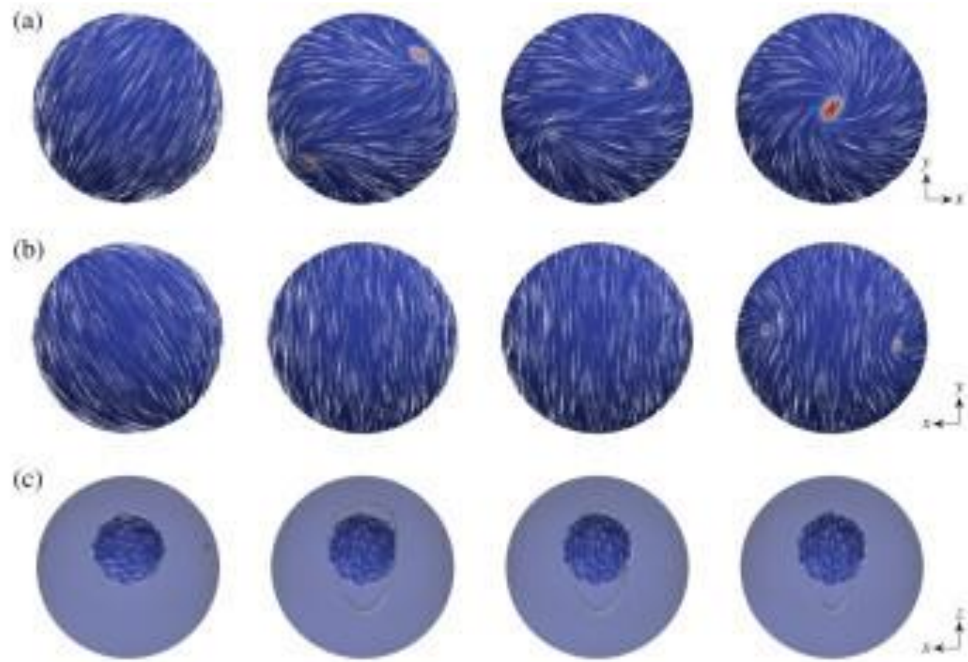


FIG. 11. Simulated trajectory of the T → H transition starting from a $+1^l$, $+1^r$ (left, right) tangential configuration, with $t = -1.79$, $c = 0.2$, $\rho = 0.4$, and $\eta = 4$; we plot $\mathbf{n}$ on the inner shell boundary [simulation steps $n = 0$, 30 000, 35 000 and 40 000 from left to right]. (a) View from the thin part, (b) view from the thick part, and (c) side view.

Heating Transition – Example III

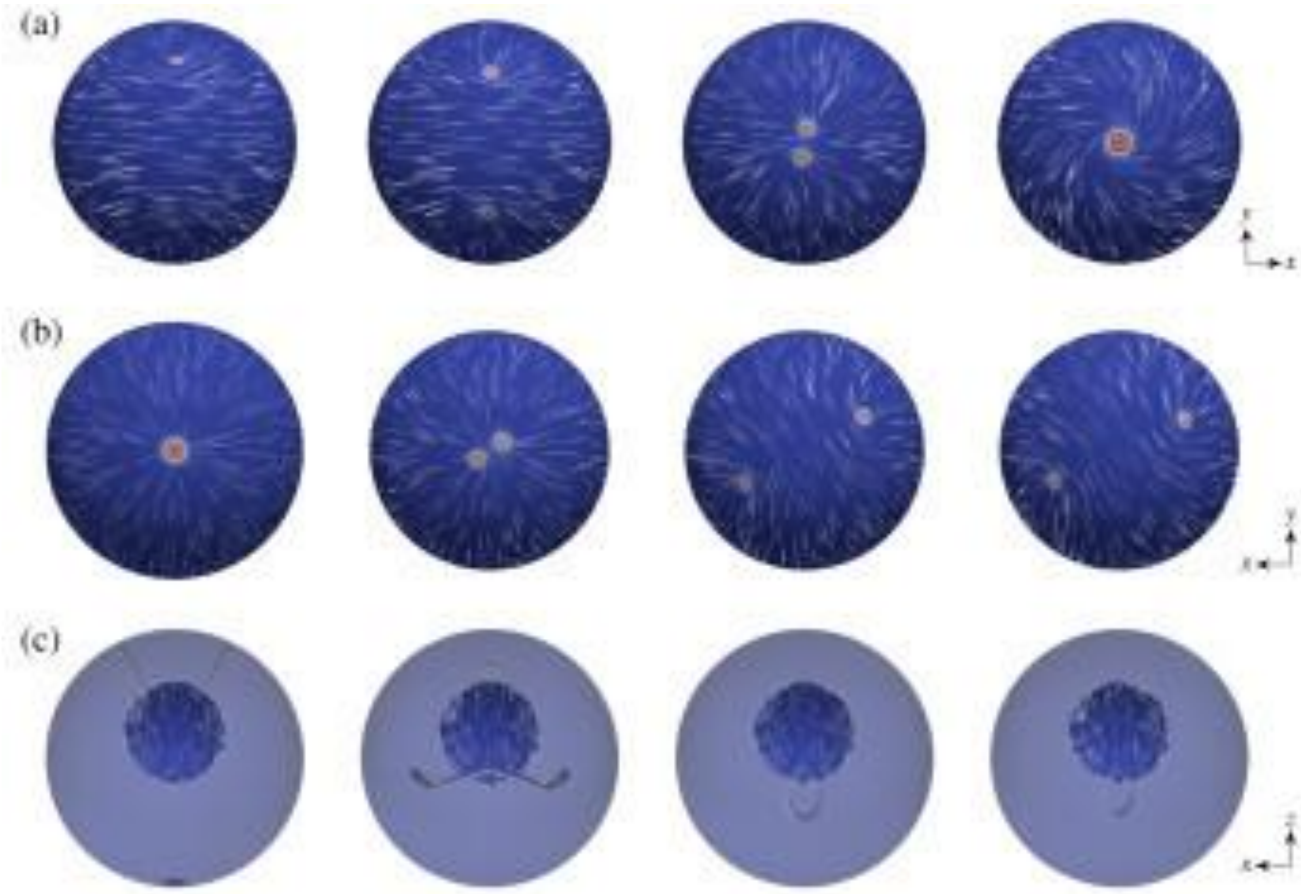


FIG. 9. Simulated trajectory of the T $\rightarrow$ H transition starting from T2 $[2(+\frac{1}{2}'), +1']$, with $t = -1.79$, $c = 0.2$, $\rho = 0.4$, and $\eta = 4$. We plot $\mathbf{n}$ at the inner shell boundary [left to right: simulation steps $n = 0$, 5000, 20 000, and 40 000]: (a) view from thin part, (b) view from thick part, and (c) side view.

$$\beta^2 = 1 - 6\frac{(tr\mathbf{Q}^3)^2}{|\mathbf{Q}|^6}$$

Why do mathematicians like these problems?

- Mathematically rich!

Topology, Calculus of Variations, Partial Differential Equations, Bifurcation Theory, Dynamical Systems, Scientific Computation, Numerical Analysis……

- Can test theoretical predictions

- Link with applications

- Interdisciplinary

- Please contact me if you want to work with me !!

Theory+ Analysis

Simulations

Experiment

Applications

Why do a PhD?

- Rich Varied Experience – scientific and interpersonal skills
- Technical Training, Advanced Problem Solving Skills
- Soft Skills – team working skills, presentation skills, analytic and numerical skills
- International Network; foreign collaborators
- Interdisciplinary
- Translate real-life problems into mathematics and vice-versa, mathematics-led advances in real life
- Real opportunity to design and lead your own work, be creative, ambitious and independent with unlimited scientific horizons!

Theory+ Analysis

Simulations

Experiment

Applications

Why do a PhD?

- Two open PhD positions in my group

Leverhulme funded PhD position - https://www.strath.ac.uk/studywithus/postgraduateresearchphdopportunities/science/mathematicsstatistics/unravellingthemysteriesofnematicsolutionlandscapes/

University of Strathclyde-funded PhD position – https://www.strath.ac.uk/studywithus/postgraduateresearchphdopportunities/science/mathematicsstatistics/softmatterwithnematicandmagneticordermodelssimulationsandapplications/

Fully funded, opportunities for travel, fantastic opportunity to work in interdisciplinary teams!
Please contact me at
apala.majumdar@strath.ac.uk

Theory+ Analysis

Simulations

Experiment

Applications

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- University of Strathclyde New Professor Fund
- DST-UKIERI Project on “Theoretical and Experimental Studies of Magnetic Nanoparticles in Anisotropic Media” with IIT Delhi (India)
- Royal Society Newton International Fellowship (Han & Majumdar)
- OCIAM Visiting Fellowship
- IMA, QJMAM, LMS
- Leverhulme Trust

and of course,

the organisers, Gemma and Tiffany, and the audience !!