FACULTY OF ENGINEERING
AND ARCHITECTURE

ELECTRONICS AND INFORMATION SYSTEMS DEPARTMENT
LIQUID CRYSTALS AND PHOTONICS RESEARCH GROUP

LIQUID CRYSTALS AND LIGHT EMITTING MATERIALS FOR PHOTONIC APPLICATIONS

Kristiaan Neyts April 2018 Lecture series at WAT in Warsaw

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nb-photonics
Center for Nano- and Biophotonics
Ghent University

Liquid Crystals and Photonics

OVERVIEW

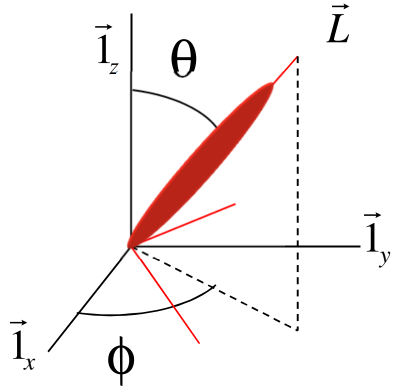
Liquid crystal properties (10h)

Properties of nematic liquid crystals
Nematic order parameter
Polarization and dielectric constant
Elastic energy
Surface alignment
Electrical energy
Jones matrix method
Variable phase retarder
VAN mode
IPS mode
TN mode

DIELECTRIC TENSOR

Dielectric tensor in laboratory axes?

$$\overline{\overline{\varepsilon}} = \begin{pmatrix} \varepsilon_\perp & 0 & 0 \\ 0 & \varepsilon_\perp & 0 \\ 0 & 0 & \varepsilon_{//} \end{pmatrix} \qquad \vec{L} = \begin{pmatrix} \cos\phi\sin\theta \\ \sin\phi\sin\theta \\ \cos\theta \end{pmatrix}$$



$$\overline{\overline{\varepsilon}} = \begin{pmatrix} \varepsilon_\perp + (\varepsilon_{//} - \varepsilon_\perp)\cos^2\phi\sin^2\theta & (\varepsilon_{//} - \varepsilon_\perp)\sin\phi\cos\phi\sin^2\theta & (\varepsilon_{//} - \varepsilon_\perp)\cos\phi\sin\theta\cos\theta \\ (\varepsilon_{//} - \varepsilon_\perp)\sin\phi\cos\phi\sin^2\theta & \varepsilon_\perp + (\varepsilon_{//} - \varepsilon_\perp)\sin^2\phi\sin^2\theta & (\varepsilon_{//} - \varepsilon_\perp)\sin\phi\sin\theta\cos\theta \\ (\varepsilon_{//} - \varepsilon_\perp)\cos\phi\sin\theta\cos\theta & (\varepsilon_{//} - \varepsilon_\perp)\sin\phi\sin\theta\cos\theta & \varepsilon_\perp + (\varepsilon_{//} - \varepsilon_\perp)\cos^2\theta \end{pmatrix}$$

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REFRACTIVE INDICES

Ordinary and extra-ordinary indices:

$$n_e = \sqrt{\frac{\varepsilon_{//}}{\varepsilon_0}}; \quad n_o = \sqrt{\frac{\varepsilon_{\perp}}{\varepsilon_0}}$$

optical frequencies:

$$\begin{cases} 1.5 < n_e, n_o < 2.2 \\ 0 < n_e - n_o < 0.6 \end{cases}$$

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For light propagation with *k*-vector at an angle θ from *L*

$$n^{(2)} = \left(\frac{\cos^2\theta}{n_o^2} + \frac{\sin^2\theta}{n_e^2} \right)^{-\frac{1}{2}}$$

PRINCIPLE OF VIRTUAL WORK

Internal energy in the system

$$\begin{cases} W_{electric} = \int_{vol} \frac{1}{2}\vec{D}\cdot\vec{E}\,dV = \frac{1}{2}V\cdot Q \\ W_{magnetic} = \int_{vol} \frac{1}{2}\vec{B}\cdot\vec{H}\,dV = \frac{1}{2}I\cdot\Phi \end{cases}$$

cst *V* over a capacitor with charge *Q*

cst *I* over a gap with flux Φ

virtual work

$$VdQ + Id\Phi = d\left(\tfrac{1}{2}V\cdot Q\right) + d\left(\tfrac{1}{2}I\cdot\Phi\right) + dW_{elastic} + dA$$

$$0 = -\tfrac{1}{2}d\left(VQ\right) - \tfrac{1}{2}d\left(I\Phi\right) + dW_{elastic} + dA$$

$$0 = d\int_{vol}\left(-\tfrac{1}{2}\vec{D}\cdot\vec{E}\right)dV + d\int_{vol}\left(-\tfrac{1}{2}\vec{B}\cdot\vec{H}\right)dV + dW_{elastic} + dA$$

$$0 = d\int_{vol}\underbrace{\left(f_{electric} + f_{magnetic} + f_{elastic}\right)}_{\text{energy density}}dV + dA$$

dissipation>0

energy density

integral should be minimal for stability

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ELASTIC ENERGY

Requirements for LC elastic energy?

-zero energy for homogeneous director *L* of the LC

-continuum theory requires small deformations on molecular scale

-energy is a scalar, independent of system of axes

-energy should have inversion symmetry (*L*/-*L* in nematic)

small deformations

therefore: only first derivatives

of the director *L* :

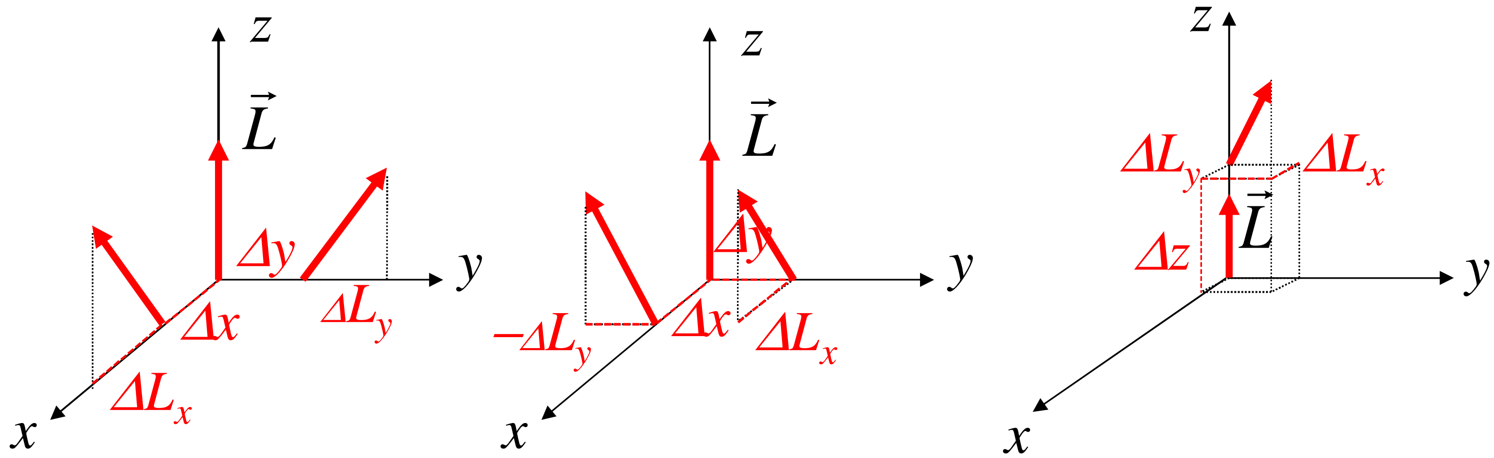
$$\frac{\partial L_x}{\partial x} \quad \frac{\partial L_y}{\partial x} \quad \frac{\partial L_z}{\partial x}$$

$$\frac{\partial L_x}{\partial y} \quad \frac{\partial L_y}{\partial y} \quad \frac{\partial L_z}{\partial y}$$

$$\frac{\partial L_x}{\partial z} \quad \frac{\partial L_y}{\partial z} \quad \frac{\partial L_z}{\partial z}$$

ELASTIC ENERGY

Elastic energy density is related to
deformation of the director *L* (in the origin: *L* along *z*-axis)



Splay

$$\frac{\partial L_x}{\partial x};\frac{\partial L_y}{\partial y}$$

Twist

$$\frac{\partial L_x}{\partial y};\frac{\partial L_y}{\partial x}$$

Bend

$$\frac{\partial L_x}{\partial z};\frac{\partial L_y}{\partial z}$$

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ELASTIC ENERGY

	Splay	Twist	Bend
our example (L//z)	$\frac{\partial L_x}{\partial x};\frac{\partial L_y}{\partial y}$	$\frac{\partial L_x}{\partial y};\frac{\partial L_y}{\partial x}$	$\frac{\partial L_x}{\partial z};\frac{\partial L_y}{\partial z}$

$$\nabla \cdot \vec{L} = \frac{\partial L_x}{\partial x} + \frac{\partial L_y}{\partial y} + \frac{\partial L_z}{\partial z}$$

$$\nabla \times \vec{L} = \left(\frac{\partial L_z}{\partial y} - \frac{\partial L_y}{\partial z}\right)\mathbf{e}_x + \left(\frac{\partial L_x}{\partial z} - \frac{\partial L_z}{\partial x}\right)\mathbf{e}_y + \left(\frac{\partial L_y}{\partial x} - \frac{\partial L_x}{\partial y}\right)\mathbf{e}_z$$

Splay	Twist	Bend
$\left(\nabla \cdot \vec{L}\right)^2$	$\left(\vec{L} \cdot \left(\nabla \times \vec{L}\right)\right)^2$	$\left(\vec{L} \times \left(\nabla \times \vec{L}\right)\right)^2$

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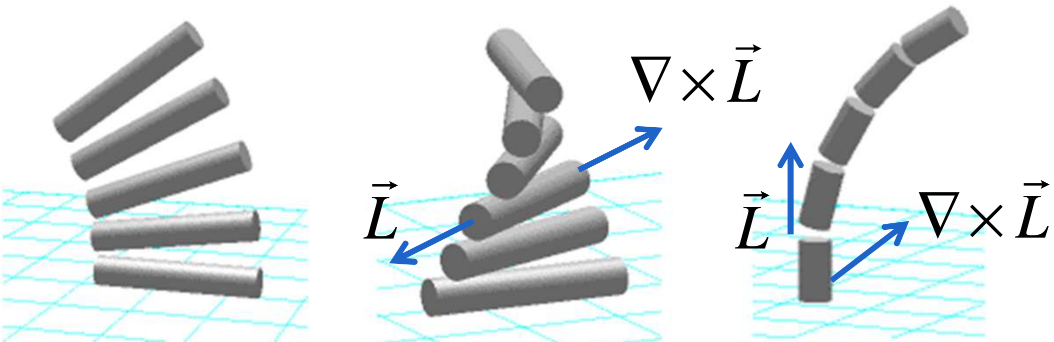
ELASTIC ENERGY

Only 3 combinations of derivatives satisfy the symmetry relations (compare with $\nabla \cdot \vec{L}$ $\nabla \times \vec{L}$) …

Splay	Twist	Bend
$\left(\nabla \cdot \vec{L}\right)^2$	$\left(\vec{L} \cdot \left(\nabla \times \vec{L}\right)\right)^2$	$\left(\vec{L} \times \left(\nabla \times \vec{L}\right)\right)^2$

$$f_{elastic} = \tfrac{1}{2}\left[K_{11}\left(\nabla \cdot \vec{L}\right)^2 + K_{22}\left(\vec{L} \cdot \left(\nabla \times \vec{L}\right)\right)^2 + K_{33}\left(\vec{L} \times \left(\nabla \times \vec{L}\right)\right)^2\right]$$

K: elastic constants (in pN)



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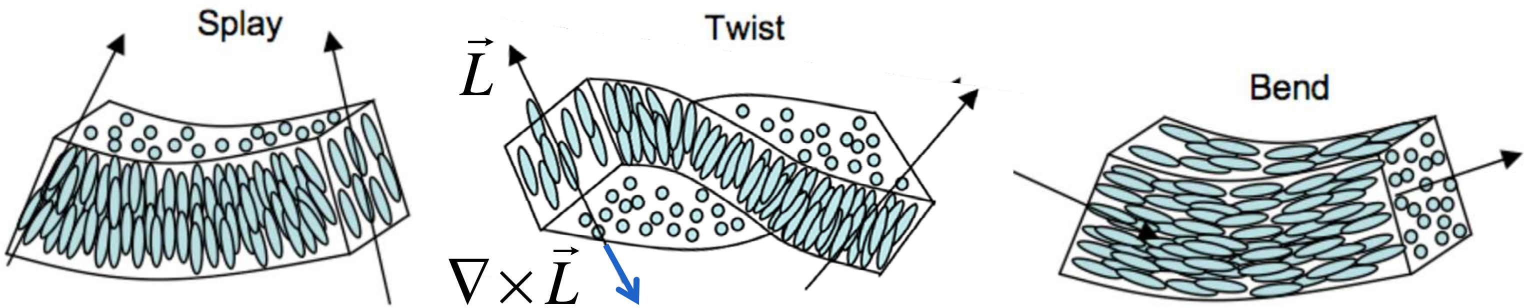
ELASTIC ENERGY

Elastic energy for chiral liquid crystal

lowest energy when: $\vec{L}\cdot\left(\nabla\times\vec{L}\right)=-q_0$ right handed CLC: q_0>0

$$f_{elastic}=\tfrac{1}{2}\left[K_{11}\left(\nabla\cdot\vec{L}\right)^2+K_{22}\left(\vec{L}\cdot\left(\nabla\times\vec{L}\right)+q_0\right)^2+K_{33}\left(\vec{L}\times\left(\nabla\times\vec{L}\right)\right)^2\right]$$

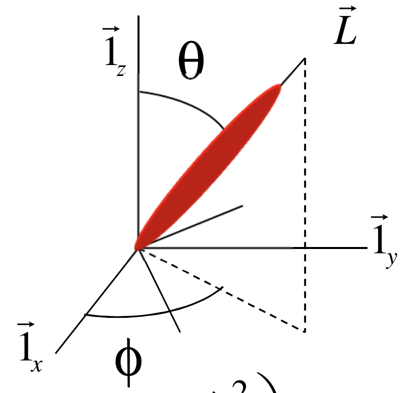


right handed twist

$\vec{L}\cdot\left(\nabla\times\vec{L}\right)<0$

ELASTIC ENERGY

In a **1D geometry** (*L* depending only on *z*)



$$\vec{L} = \begin{pmatrix} \cos\phi(z)\sin\theta(z) \\ \sin\phi(z)\sin\theta(z) \\ \cos\theta(z) \end{pmatrix}$$

only $\dfrac{\partial}{\partial z}$

$$f_{elastic} = \tfrac{1}{2}\left(K_1 \left(\nabla \cdot \vec{L}\right)^2 + K_2 \left(\vec{L} \cdot \left(\nabla \times \vec{L}\right)\right)^2 + K_3 \left(\vec{L} \times \left(\nabla \times \vec{L}\right)\right)^2 \right)$$

after calculation: ...

$$f_{elastic} = \tfrac{1}{2}\left(K_1 \left(\sin\theta \frac{\partial\theta}{\partial z}\right)^2 + K_2 \left(\sin^2\theta \frac{\partial\phi}{\partial z}\right)^2 + K_3 \left(\left(\cos\theta \frac{\partial\theta}{\partial z}\right)^2 + \left(\cos\theta\sin\theta \frac{\partial\phi}{\partial z}\right)^2 \right) \right)$$

single *K* approximation: $f_{elastic} \approx \tfrac{1}{2} K \left(\left(\nabla \cdot \vec{L}\right)^2 + \left(\nabla \times \vec{L}\right)^2 \right)$

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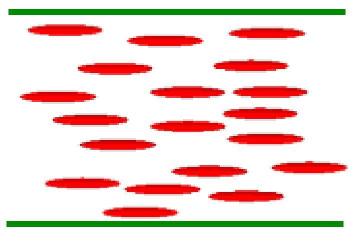
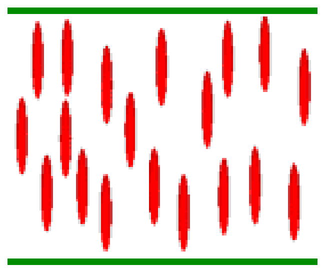
INTERFACE INTERACTION

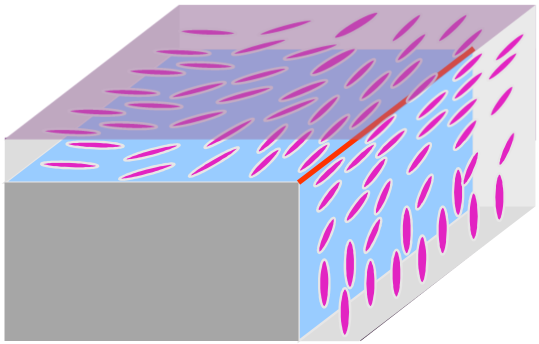
- most surfaces prefer planar alignment:
  parallel with interface
  (glass, water, silicon)

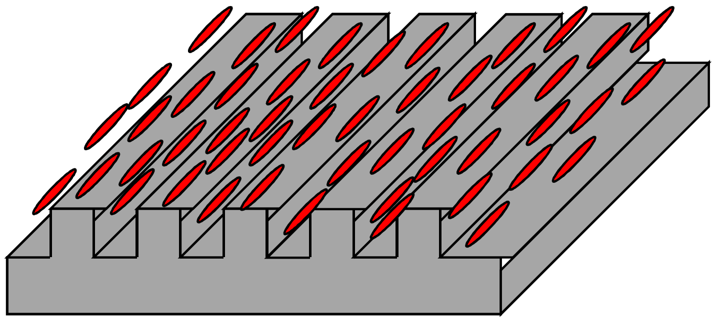


- some surfaces prefers homeotropic alignment:
  perpendicular to interface
  (air)



- azimuthal alignment with a structure





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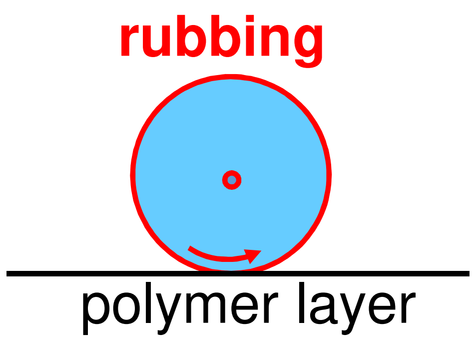
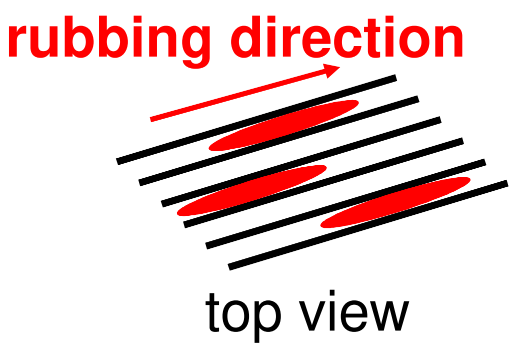
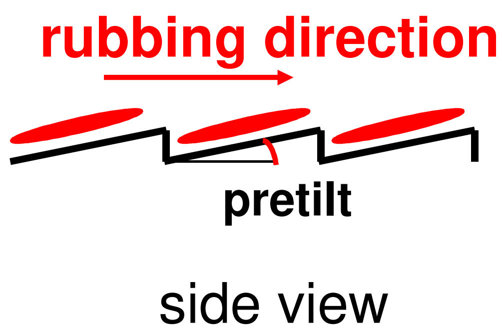
INTERFACE INTERACTION

spin coating of a polymer layer
provides parallel alignment
azimuthal angle: by rubbing







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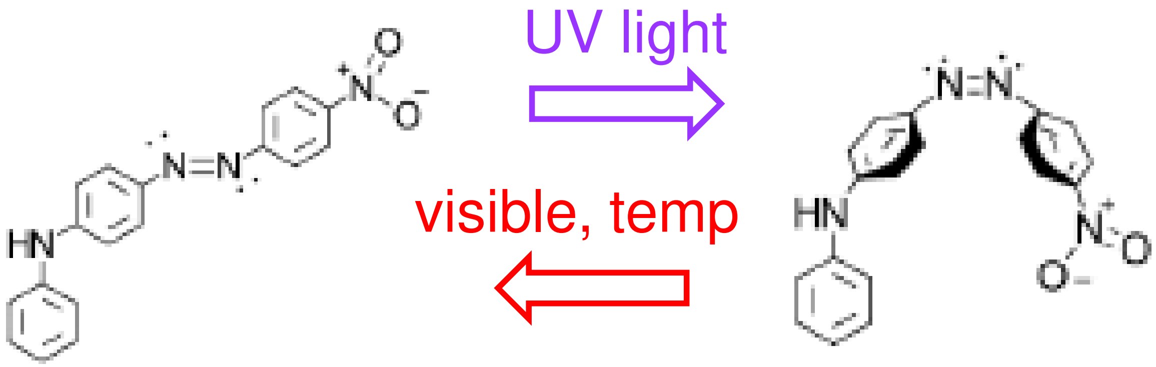
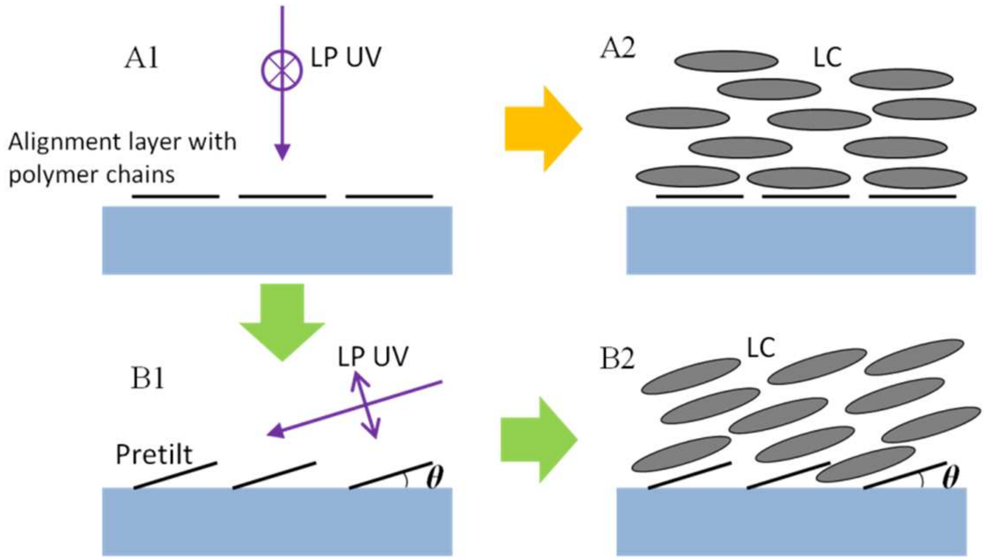
INTERFACE INTERACTION

azo-materials
ground state
E-isomer
'trans'



excited
Z-isomer
'cis'

photo-alignment
with azo dye
polymer ⊥
to *E* field



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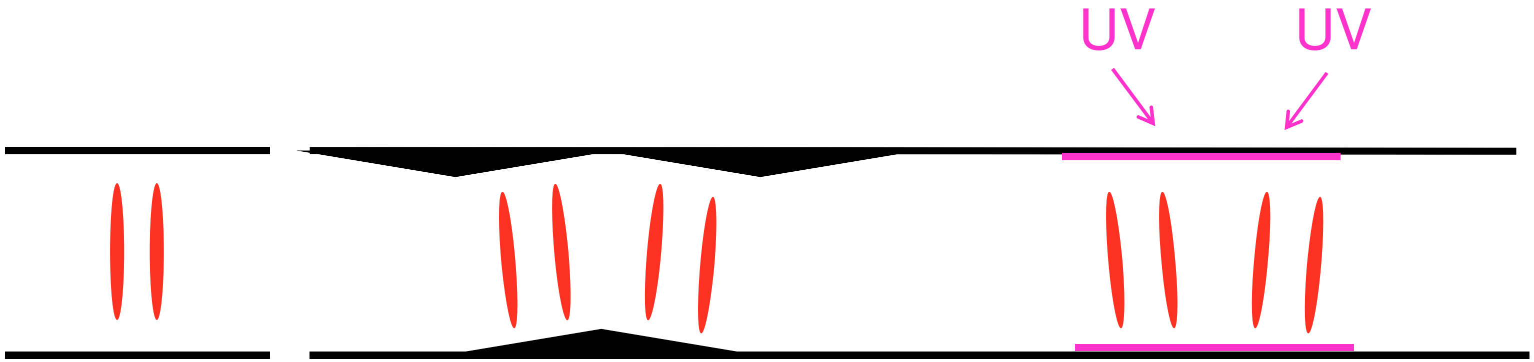
VERTICALLY ALIGNED LC MODE

Reproducible reorientation

how to define the azimuth ϕ of reorientation?

methods to determine ϕ



homeotropic alignment
ϕ not determined

protrusions

photo-aligned

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INTERFACE INTERACTION

- Strong anchoring

surface fixes the director $\vec{L}$ at the interface: $\vec{L}_{pref}$

- Weak anchoring

a deviation leads to a surface energy:

- one preferred direction $\vec{L}_{pref}$ with minimal energy

$$f_{surface} = \tfrac{1}{2} K_s \left(1 - \left(\vec{L} \cdot \vec{L}_{pref}\right)^2\right)$$

- parallel alignment (no preferred azimuth)

$$f_{surface} = \tfrac{1}{2} K_s \left(1 - \left(\vec{L} \times \vec{L}_{\perp}\right)^2\right)$$

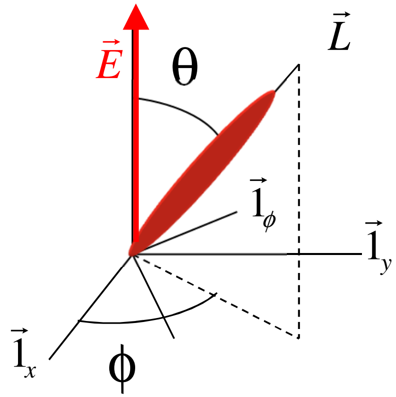
ELECTRIC ENERGY

Electric energy density (with source)

$$f_{electric} = -\tfrac{1}{2}\vec{D}\cdot\vec{E} = -\tfrac{1}{2}\left(\overline{\overline{\varepsilon}}\vec{E}\right)\vec{E} = -\tfrac{1}{2}\varepsilon_{\perp}E^{2} - \tfrac{1}{2}\Delta\varepsilon\left(\vec{L}\cdot\vec{E}\right)^{2}$$

$$\overline{\overline{\varepsilon}}\vec{E} = \varepsilon_{\perp}\vec{E} + \Delta\varepsilon\left(\vec{L}\vec{L}\right)\vec{E} = \varepsilon_{\perp}\vec{E} + \Delta\varepsilon\vec{L}\left(\vec{L}\cdot\vec{E}\right)$$

$$\begin{cases} \vec{L}\cdot\vec{E} = E\cos\theta \\ \vec{L}\times\vec{E} = -E\sin\theta\,\vec{1}_{\phi} \end{cases}$$



given field E (for example V/d)

Δε>0: lowest energy when L and E are parallel

Δε<0: lowest energy when L and E are perpendicular

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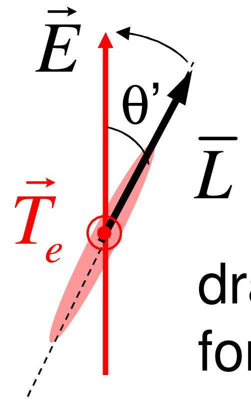
ELECTRIC TORQUE

Electric field tries to align the director *L* along *E*

$$\overline{T}_e = \overline{P}\times\overline{E} = \overline{D}\times\overline{E}$$
$$= \left(\overline{\overline{\varepsilon}}\,\overline{E}\right)\times\overline{E}$$
$$= \left(\varepsilon_\perp \overline{\overline{I}} + \Delta\varepsilon \overline{L}\,\overline{L}\right)\overline{E}\times\overline{E}$$
$$= \Delta\varepsilon\left(\overline{L}\cdot\overline{E}\right)\overline{L}\times\overline{E}$$



drawing for Δε>0

$$\begin{cases} \vec{L}\cdot\vec{E} = E\cos\theta \\ \vec{L}\times\vec{E} = -E\sin\theta\,\vec{1}_\phi \end{cases}$$

Check:

$$\left|\vec{T}_e\right| = \left|\frac{df_{electric}}{d\theta}\right|$$

EXAMPLE: PURE TWIST

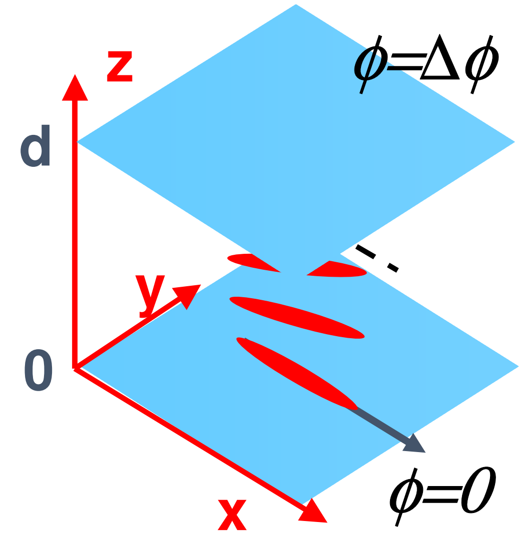
LC between substrates, strong planar anchoring

rubbing with azimuthal difference $\Delta\phi$ (assume for all z: $\theta = \pi/2$)

$$\vec{L} = \begin{pmatrix} \cos\phi(z) \\ \sin\phi(z) \\ 0 \end{pmatrix}$$

lowest energy?

ϕ **(*z*)?**



pure twist:

$$f_{elastic} = \tfrac{1}{2} K_2 \left(\vec{L}\cdot\left(\nabla\times\vec{L}\right)\right)^2 = \tfrac{1}{2} K_2 \left(\frac{\partial\phi}{\partial z}\right)^2$$

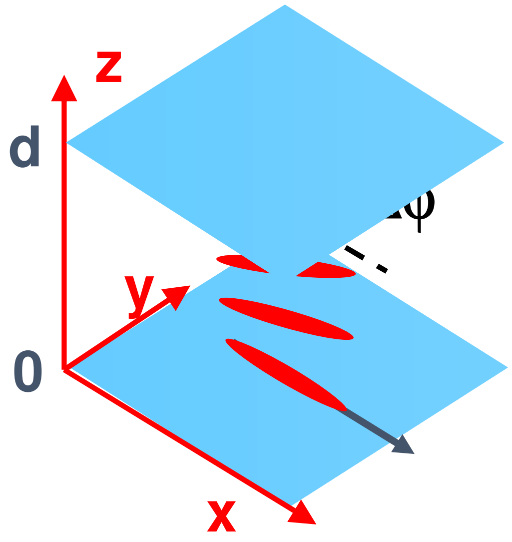
Total energy in the system (only elastic energy)

$$F_{tot} = \int_0^d f_{tot} dz = \int_0^d \tfrac{1}{2} K_2 \left(\frac{\partial\phi}{\partial z}\right)^2 dz$$

EXAMPLE: PURE TWIST

Minimizing the energy

$$F_{tot} = \int_0^d f_{tot} dz = \int_0^d \tfrac{1}{2} K_2 \left(\frac{\partial \phi}{\partial z} \right)^2 dz$$



Variational problem

find $f_{tot}\left(\phi(z), \phi'(z)\right)$ that minimizes $\int f_{tot}\left(\phi, \phi'\right) dz$

$\phi(z)$ is the solution of the Euler-Lagrange equation:

$$\frac{\partial f_{tot}}{\partial \phi} - \frac{d}{dz}\frac{\partial f_{tot}}{\partial \phi'} = 0 \qquad f_{tot} = \tfrac{1}{2} K_2 \phi'^2$$

Solution: $\phi(z) = z\dfrac{\Delta\phi}{d}$ $\qquad F_{tot} = \tfrac{1}{2} K_2 \dfrac{\Delta\phi^2}{d}$