Title: Topological defects of tetratic liquid-crystal order on a soft spherical surface

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Abstract: We model the orientational and positional order of tetratically shaped molecules each having four-fold structural symmetryconfined on a spherical surface. Our Monte Carlo simulation shows that at a high molecular density a tetratic orientational orderdevelops in the system accompanied by eight disclinations arranged in an anticube form on the hard spherical surface. We alsoconsider an elastic-energy model which consists of both Helfrich and Frank energies for a soft surface; the solution confirms theMonte Carlo study and further predicts the tetratic morphology that can be realized on the surface of a soft vesicle. Assumingthat the induced interaction between these disclinations are repulsive we demonstrate that the anticube structure has a lower freeenergy than for example the cubic structure.

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Topological defects of tetratic order on a soft spherical surface

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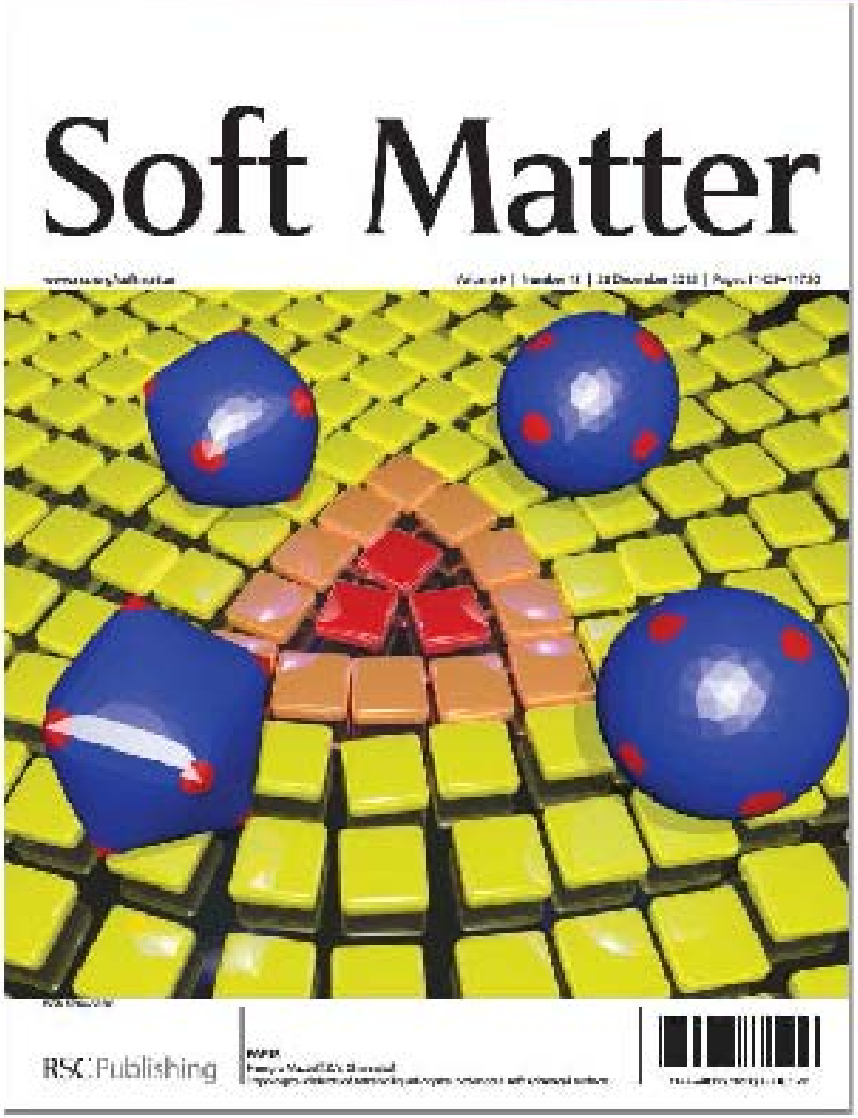

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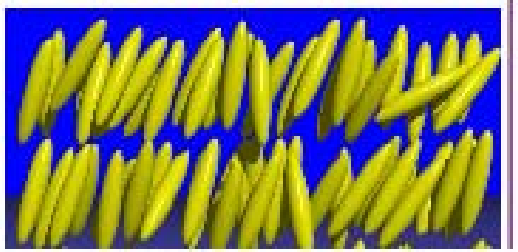
Orientational Orders

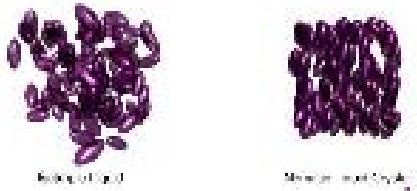
Orientational Orders



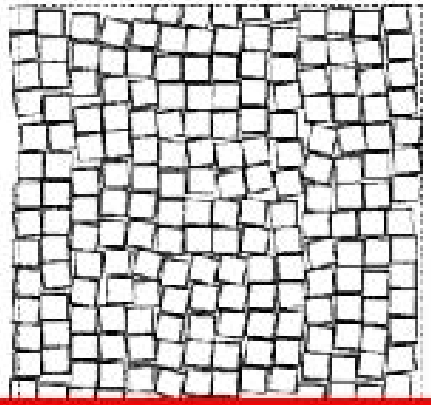
Vector(1-atic) e.g. smectic-C tilt order

XY Model

Nematic Order(2-atic) e.g. headless rods



Tetratic Order(4-atic) e.g. Hard squares

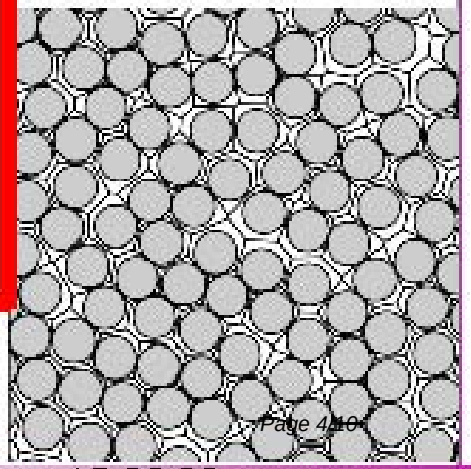


Wojciechowski & Frenkel (2004)

Avendaño & Escobedo(2012)

Zhao et.al.(2011) [Experiment]

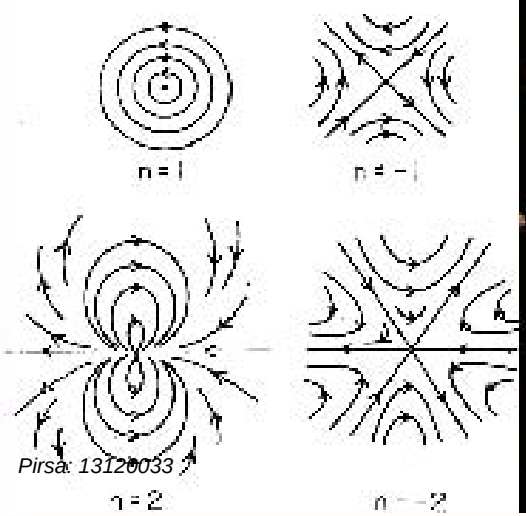
Donev et.al.(2006) [Hard rectangles]

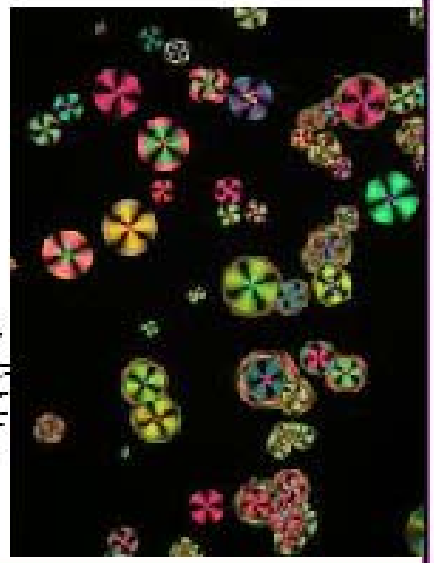


Hexatic Order(6-atic) e.g. Hard disks

Topological Defects

- Topological Defects see Review [Mermin RMP1979]
- Type of Topological Defects: Winding number
- Topological stability: Cannot be restored by continuum transformation

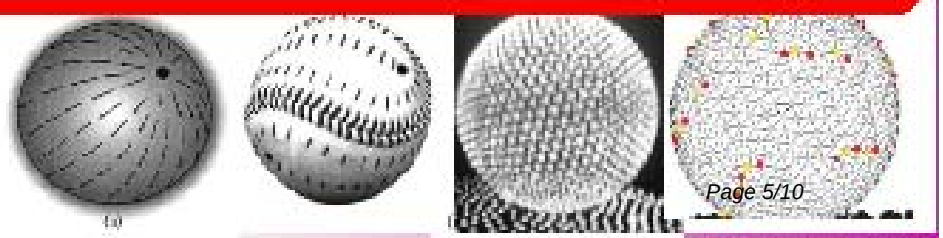




- Topological Defects are
  On Plane:
  High energy excitations
  On Sphere(or many other curved surface):
  inevitable in ground states
- Vector, nematic, hexatic defects extensively studied.

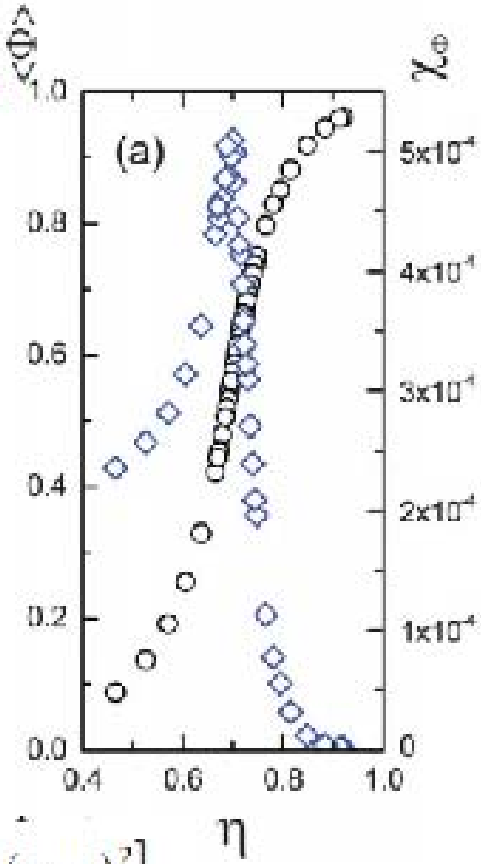
(Lubensky1992, Nelson2002, Bausch2003, Shin2008, Irvine2012.....)

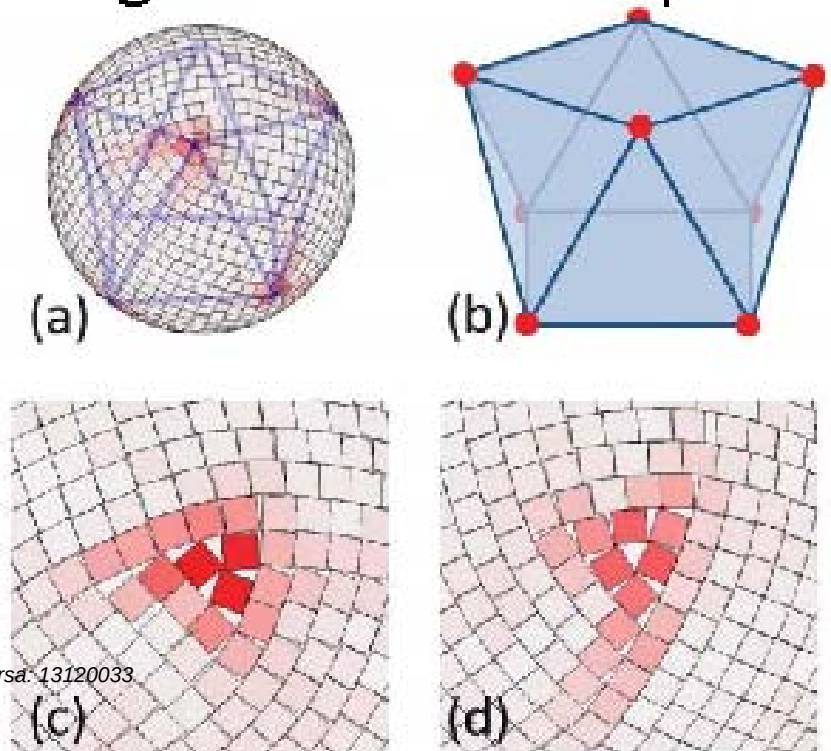
- Tetratic defect less understood



Model I: Squares On Sphere

- We employ Monte Carlo Methods to simulate hard squares confined on a sphere
- Higher density results high order get into tetratic phase at η≈0.70





$$\Phi_i = 1 - \sum_j (\mathbf{n}_i \cdot \mathbf{n}_j)^2 \left[1 - (\mathbf{n}_i \cdot \mathbf{n}_j)^2\right],$$

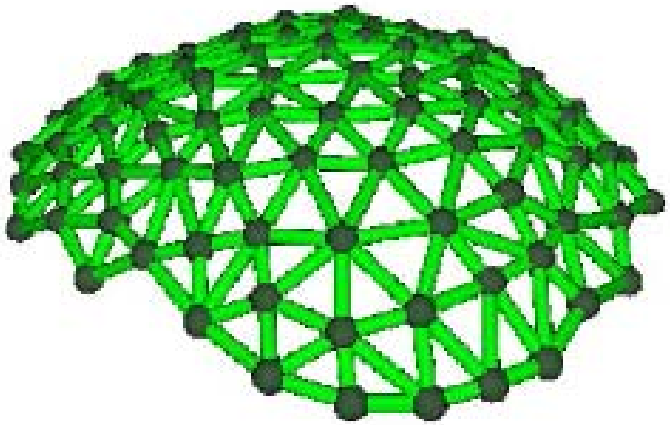
- At sufficient high density, 8 +1/4 defects form at an anticube configuration.

Model II. Elastic Model

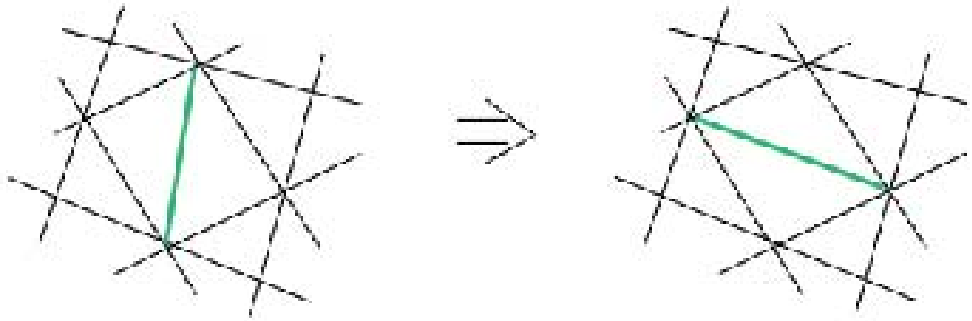
- **DTMC(Dynamic Triangulation Monte Carlo)**

  [Gompper & Kroll 2002 in statistical mechanics of membranes]

  Triangular Mesh



Dynamic triangulation:



- Using Discrete Differential Geometry to Calculate Helfrich Free Energy.

Model II. Elastic Model

- Phenomenological Model

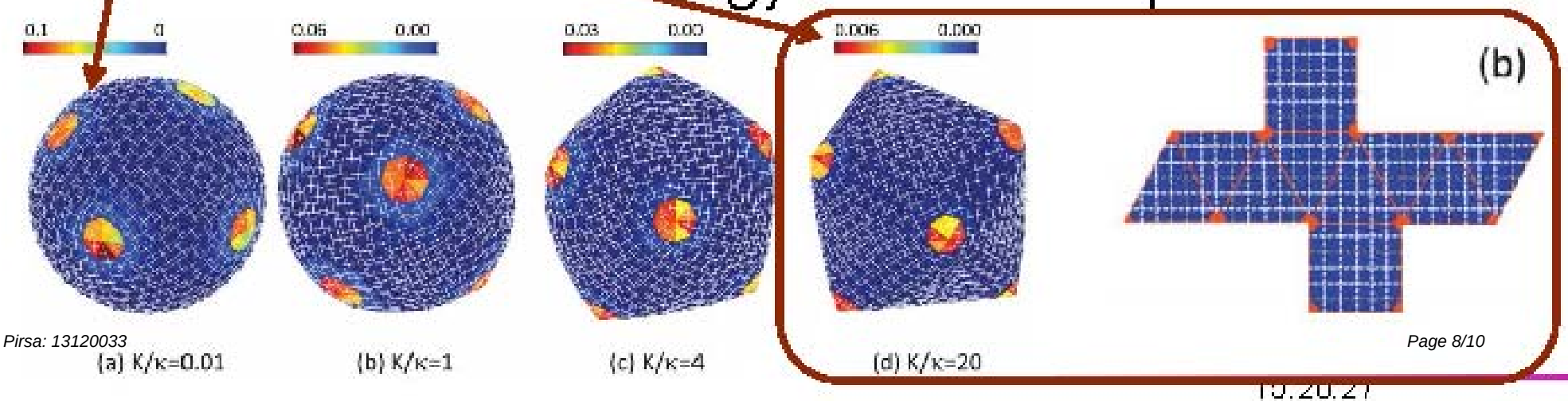
  Helfrich free energy + Frank free energy (Kardar 2008)

$$F_{\text{Helfrich}} = 2\kappa \int M^2(\mathbf{r})\mathrm{d}A \qquad F_{\text{Frank}} = K \int (D\mathbf{n}(\mathbf{r}))^2 \mathrm{d}A$$

- K<<κ: Minimize Helfrich → sphere.

  Then defect propel each other → anticube

- K>>κ: surface buckle out, Gaussian curvature all vanish → Frank energy vanish except for defects



(a) K/κ=0.01 (b) K/κ=1 (c) K/κ=4 (d) K/κ=20

Conclusion

- We examined the defect pattern of tetratic order on a spherical surface by two independent models, a Monte Carlo model in which square-shape molecules exclude from each other, and an elastic energy model in which the Helfrich and Frank energies are considered together.
- Both approaches give rise to eight defects in the tetratic order, forming the corners of an anticube.
- Illustrated how vesicle morphology changes as a function of K/κ .

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- Prof. GL Long, Prof. X. Xing and YC Su for interesting discussions.

Q&A

THANKS ALL!