



MAY 2014
ISSUE #63

Dear Soft Matter Colleagues,

Welcome to our May SoftMatterWorld newsletter. It's been a busy spring semester here at UC Merced and we are looking forward to the summer conference season. Let us know if you are organizing any meetings over the summer or the coming Fall and we will advertise them for you. It's free and with over 500 SMW subscribers around the world it's a good way to get the word out.

COMPLEX ORDERED PATTERNS IN MECHANICAL INSTABILITY INDUCED GEOMETRICALLY FRUSTRATED TRIANGULAR CELLULAR STRUCTURES

Sung Hoon Kang, Sicong Shan, Andrej Košmrlj, Wim L. Noorduin, Samuel Shian, James C. Weaver, David R. Clarke, and Katia Bertoldi, *Phys. Rev. Lett.* 112, 098701.

Geometric frustration is the term that describes a system that is unable to manifest a homogeneous pattern, or to find a single ground state. The authors give the example of a square and a triangle, both with an antiferromagnetic spin at each corner. The square is able to deform uniformly into a single ground state, while the triangle, having 3 corners each occupied by a binary spin, has 8 ground states to choose from (figure 1). Due to geometric constraints, local order varies throughout the system.

The authors, working out of Harvard, have modeled such systems, which seemingly cannot have ordered patterns on a large scale because of geometric frustration. In their model, the beams of the triangles could buckle up or down. They found that the buckling directions tend to want to balance out in order to minimize the free energy of the system. In symmetric systems, neighboring beams could bend the same direction, being balanced out by the next nearest neighbors bending opposite each other, producing patterns that can be seen in figure 1b. When allowing for a second buckling mode of the beams, whether the resulting pattern was chiral

or symmetric depended on the energy associated with the second buckling, which was shared between two triangles. When the half the energy cost of the second mode (since it's shared) was greater than the cost of the first bend, a symmetric pattern was the lowest energy configuration. The opposite situation led to a chiral pattern. Their experimental observations, as seen in the figure, agree with the predictions of their models.

Coupling between elasticity and geometric frustration in these systems allows for the formation of complex ordered symmetric or chiral patterns. Specific configurations could be controlled by varying the porosity of the system. The symmetric and chiral patterns could also be controlled by varying the aspect ratio of the beams of the triangles. The researchers suggest future work can focus on further exploring this phenomenon, and that simple changes in geometry of the elastic structures can create easily observable effects.

The full paper can be found here in [Physical Review Letters](#).

Michael Lane

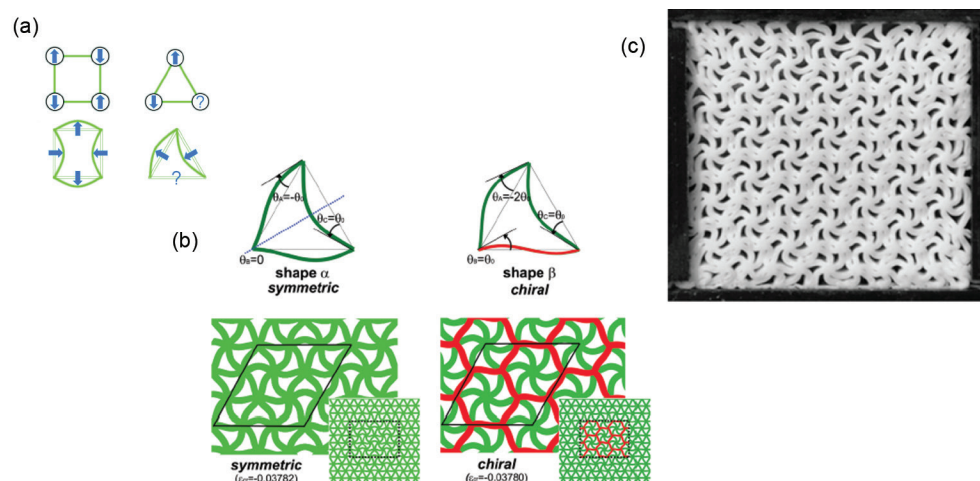


Figure 1 (a) Neighboring spins tend to align in opposite directions, which a square easily allows. Due to geometrical frustration, the same doesn't hold for triangles. Buckled beams tend to minimize deformation energy in a similar way: by minimizing angles. Again, a triangle is unable to find a single favorable arrangement. (b) Diagrams of symmetric and chiral configurations of a single triangular frame. First and second eigenmodes for a lattice structure comprised of beams with an aspect ratio of 0.2, showing the configurations in (a) on a larger scale. (c) Experimental observation of buckled triangular lattice.

LIPID MEMBRANES AS SOLVENTS FOR CARBON NANOPARTICLES

Barnoud, Jonathan, Giulia Rossi and Luca Monticelli. *Phys. Rev. Lett.* 6 Vol. 112 068102 (2014)

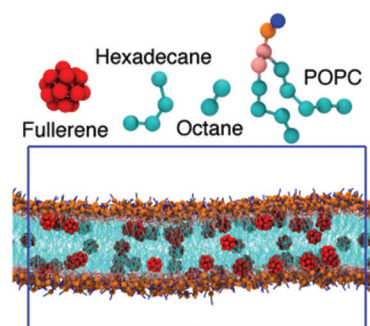
Fullerenes, specifically C₆₀, have become useful candidates as vesicles in nanomedicine. Because of their unique stability and insolubility in various polar and apolar solvents, fullerenes are very difficult to disperse. Those solvents in which they can disperse are toxic. However, it has recently been found that the C₆₀ fullerene can be incorporated and dispersed into both alkanes and lipid bilayers without sacrificing its stability making it a great option for transferring drugs. To further understand how the process works, Luca Monticelli and his team at the University of Paris Diderot simulated whether alkanes or lipid bilayers are better at dissolving the fullerene clusters.

To determine the reasons for C₆₀ solubility in alkanes and lipid bilayers, solute confinement, solvent chain alignment, solvent density and solvent chain packing were all observed individually. The authors systematically tested the effects of acyl chain alignment, the mass density differences between the two solvents, and any solvent-solvent interaction. The team used a coarse-grained computer simulation with a MARTINI force field to test the aggregation behavior of C₆₀ in homogeneous palmitoyl-oleoyl-phosphatidylcholine (POPC) membranes and the alkanes octane and hexadecane (Fig 2). To understand thermodynamic behaviors, the free energy of dimerization of the fullerene in POPC was calculated at various temperatures.

The team found that the cause of fullerene aggregation within lipid bilayers was largely enthalpic and not entropic. Confinement and chain alignment within the membrane did not affect aggregation. The effect of the bilayer on the fullerene aggregation was largely due to higher density of the membrane interior and the perturbation of chain packing by fullerene clusters. Using lipid bilayers as a solvent for fullerenes could lead to C₆₀ acting as an effective vector for therapeutic drug delivery and diagnostic contrast agents.

Read the full article [here](#) in *Physical Review Letters*

Marcus Rice



► Figure 2 - MARTINI representation of the molecules used in this paper and a snapshot of fullerenes in a POPC lipid bilayer.

EDUCATION RESOURCES ON SOFTMATTERWORLD.ORG

Have you visited the education resources pages on SoftMatterWorld.org recently? You can find lots of information on books, journals, free software and even online lectures from previous ICAMP summer schools.

Take a look at:

- ESPResSO - A free simulation package for soft matter research.

ESPResSo is a highly versatile software package for performing and analyzing scientific Molecular Dynamics many-particle simulations of coarse-grained atomistic or bead-spring models as they are used in soft-matter research in physics, chemistry and molecular biology. It can be used to simulate systems such as polymers, liquid crystals, colloids, ferrofluids and biological systems, for example DNA and lipid membranes.

- Softsimu - Free research software from the Kartunen Group.

Available through the Soft Simu website is an interesting selection of some very useful modeling software.

- Links to useful visualization software packages used in soft matter.

If you can suggest or contribute any freeware to the site please let us know - we would love to hear from you.

editor@softmatterworld.org

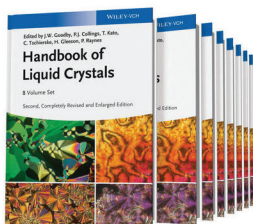


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THANKS FOR READING

LINDA HIRST, ADAM OSSOWSKI AND THE
SOFT MATTER WORLD TEAM

CONFERENCE LISTINGS DATES AND DEADLINES

GRC PRESENTS | BIOINSPIRED MATERIALS CONFERENCE AND SEMINAR

- Meeting Application - May 25, 2014

http://www.grc.org/programs.aspx?year=2014&program=grs_bioins

GRC PRESENTS | MEMBRANES: MATERIALS & PROCESSES MAKING ENGINEERING MEMBRANES ALIVE

- Meeting Application - June 8, 2014

<https://www.grc.org/programs.aspx?year=2014&program=membmat>

GRC PRESENTS | GRANULAR & GRANULAR-FLUID FLOW FUNDAMENTAL CHALLENGES AND APPLICATIONS OF PARTICULATE SYSTEMS

- Meeting Application - June 22, 2014

<https://www.grc.org/programs.aspx?year=2014&program=granular>

25TH INTERNATIONAL LIQUID CRYSTAL CONFERENCE

- Dublin - 29th June - 4th July
- Held every two years, this international meeting is the highlight of the liquid crystal conference calendar. Abstract submission is closed but you can still register to attend.

<http://www.ilcc2014.com/page/51/welcome/>

20TH INTERNATIONAL SYMPOSIUM ON SURFACTANTS IN SOLUTION (SIS 2014)

- June 22 - 27th, Coimbra, Portugal

