Dear Soft Matter Colleagues,

Welcome to our May SoftMatterWorld newsletter. Its 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 its a good way to get the word out.

**Complex Ordered Patterns in Mechanical Instability Induced Geometrically Frustrated Triangular Cellular Structures**


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 chose 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 lead 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
Lipid Membranes as Solvents for Carbon Nanoparticles


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 coase-grained computer simulation with a MARTINI force field to test the aggregation behavior of C60 in homogeneous palmitoyloleoyl-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

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.

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2ND EDITION OF THE HANDBOOK OF LIQUID CRYSTALS OUT NOW

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The long awaited impressive second edition of the popular “Handbook of Liquid Crystals” is now available for purchase from Wiley. The book has been completely restructured and streamlined into 8 volumes with a new team of editors and authors from the liquid crystal community. The book series is an essential purchase for PIs working with all kinds of liquid crystal materials and should be an invaluable resource for soft matter scientists from both academia and industry.

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THANKS FOR READING

LINDA HIRST, ADAM OSSOWSKI AND THE SOFT MATTER WORLD TEAM