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On the role of entropy in the emergence of chirality in systems of achiral particles.

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Spontaneous symmetry breaking is a fundamental concept that represents an underlying mechanism for a number of physical phenomena including the emergence of spontaneous self-organization in soft and condensed matter as well as in colloidal suspensions. When the constituent particles are chiral the self-organized ordered structures exhibits macroscopic chirality which, in soft matter liquid crystalline systems, expressed in the form of spontaneously twisted orientationaly ordered states, known as cholesteric liquid crystals, or, in other cases in the form of helical nanofilaments. In this work we focus on the intriguing phenomenon of the emergence of macroscopic chirality in systems composed of achiral particles. We study, using molecular theory and computational experiments, the basic question: is it possible a spontaneous chiral symmetry breaking in systems of rigid, sterically interacting achiral particles?

Motivated by recent experimental studies on the self-organization of micron-sized equilateral triangular particles confined in two dimensions [1] we have performed large scale Monte Carlo simulations to study the order-disorder transitions of sterically interacting equilateral triangles [2]. This system, despite its simplicity exhibits a rich phase polymorphism. Besides the isotropic state the system upon compression exhibits a liquid crystalline phase that has quasi-long-range six-fold orientational order yet only short-range positional order. Upon further compression the liquid crystal phase continuously transform to a hexagonal close-packed crystal structure. Surprisingly, further compression leads, through a second order phase transition, to a novel crystalline phase where the triangles rotate collectively either in clockwise or anti-clockwise direction with respect to a fixed lattice vector. To analyze the structure of the various phases of the system we have introduced a number of appropriate multi-particle orientational/positional correlation functions that allow the study of the various phases both locally and on the macroscopic level. We discuss the entropic origins of the chiral symmetry breaking in this system and propose appropriate order parameters for the quantification of the degree of chiral ordering. Finally we discuss the role of the molecular shape in the ectopically driven self-sorting of the particles into chiral superstructures.

[1] K. Zhao, R. Bruinsma, and T. G. Mason, *Nature Communications.* 3, 801 (2012).
[2] F. Priftis, MSc Thesis (http://hdl.handle.net/10889/9199), Department of Materials Science, University of Patras, (2015).