Investigating the phase behavior of chiral liquid-crystal systems via Monte Carlo simulations

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Liquid crystals may form phases which occur between those of solid and liquid. There are many different types of liquid-crystal phases which vary depending upon molecular orientational and positional order. Molecules exhibiting liquid-crystal phases have an anisotropic shape, and typically have rod-like or disk-like structures. The macroscopic structure of liquid-crystal phases is strongly influenced by the collective behavior of these molecules. When these phases consist of chiral molecules with rod-like structures, the chirality sometimes causes the molecules to arrange themselves into twisted super-structures. These are called chiral liquid-crystal phases and are of particular interest because of their occurrence in the natural world, as well as for commercial applications.

To study chiral liquid-crystal systems, molecular simulations like the Monte Carlo method are useful, but it is still difficult to model them at an atomistic level because large and long-time scale simulations are required [1,2]. To date, several models to mimic chiral liquid-crystal molecules have been developed [3,4]. These are very simple models but are useful to give a general understanding of the basic behavior of liquid-crystal systems. In this research, we investigated the effect of molecular elongation and anisotropic interactions on chiral liquid-crystal phases by Monte Carlo simulations. We will report the effects on the phase behavior by free energy analysis at this seminar.

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