Spontaneous formation of chiral systems from achiral liquid-crystalline molecules

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Chirality arising from achiral molecules occurs in many liquid crystal systems. We show results from two simulation studies in which this phenomenon occurs.

1) In a DPD model of a disc-shaped chromonic molecule, containing a combination of hydrophilic and hydrophobic-lipophobic chains, self-assembly in water leads to the formation of novel complex aggregates with a three-molecule cross-section. These aggregates display a spontaneous twist to produce chiral structures (see figure), together with dynamic chirality inversion [1,2].

2) When certain achiral bent core mesogens are added to a chiral nematic liquid crystal, the chirality is seen to increase, contrary to expected behaviour [3]. We show that molecular conformations exist, which have extremely high helical twisting powers, orders of magnitude higher than those seen in conventional chiral dopants. We provide a simple simulation model that demonstrates both preferential selection of chiral conformations and chirality transfer between solvent and solute, leading to an increase in the helical twist of a chiral nematic phase.

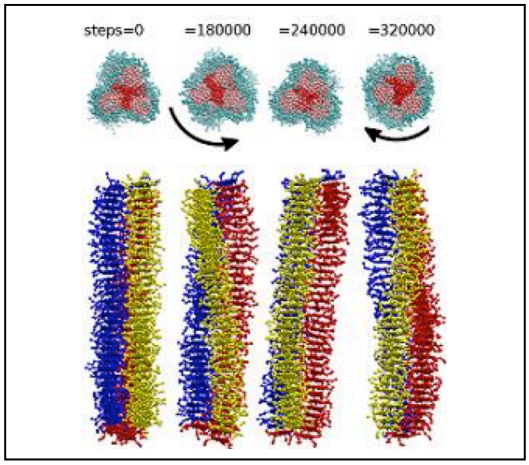

Figure. Dynamic chirality inversion in a chromonic stack formed from achiral chromonic amphiphiles

References

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