

Chirality Amplification and Chiral Segregation in Nematic Liquid Crystals

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Liquid crystal mesophases of achiral molecules are normally achiral, yet in some materials they spontaneously deracemise and form right- and left-handed chiral domains. One mechanism that has been suggested to drive deracemisation is that of thermally induced molecular shape fluctuations between chiral conformations where molecular interactions favour matching chirality and promote helical twist [1]. Co-operative chiral ordering may also play a role in chirality amplification, as when a tiny fraction of chiral dopant drives a nematic phase to become cholesteric. We present a model of co-operative chiral ordering in nematic liquid crystals, making use a switchable chiral Lebwohl-Lasher interaction in which each rotor is also assigned a spin that switches between two states representing right- and left-handed chiral states [2]. Mean-field theory and Monte Carlo simulations predict a phase diagram shown in Figure 1 with a deracemised cholesteric phase as well as racemic nematic and isotropic phases. We also find a non-trivial temperature dependence of the helical twisting power of dopants in the nematic phase and a softening of the nematic twist constant, which may be observed even in materials where the deracemisation transition is preempted by a transition to another phase. Finally, our simulations reveal unusual coarsening dynamics in the deracemised phase. Co-operative mirror symmetry breaking via molecular shape transitions must be a common mechanism in liquid crystals [2].

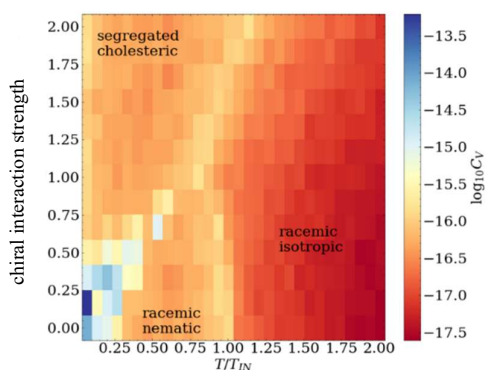


Figure 1. Heat capacity of the nematic chiral fluctuation model C_V as a function of the chiral interaction strength and temperature T scaled to the clearing temperature T_{IN} [1], showing the phase boundaries between racemic isotropic and nematic phases and the segregated left- and right-handed cholesteric phases.

References

[1] C. Tschierske, *Liq. Cryst.* **45** (2018), 2221–2252.

[2] M. J. Deutsch, R. D. Selinger and P. van der Schoot, *PNAS* **123** (2026), e2514297123.

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