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Ferroelectric Twist–Bend Nematic Order from Competing Depolarization and Flexopolarization Energies

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The self-organization of recently discovered nematic phases is a central problem in contemporary soft-matter research [1, 2, 3, 4]. Several of these phases exhibit local or long-range ferroelectric order, in some cases accompanied by emergent structural chirality despite the chemical achirality of their constituent molecules. Prominent examples are the uniform ferroelectric nematic phase NF and the recently discovered heliconical ferroelectric nematic phase NTB,F. Closely related modulated phases, including the twist–bend nematic NTB and the splay–bend nematic NSB, provide a broader framework for understanding the spontaneous emergence of polar order and orientational modulation.

Here we investigate ferroelectric and modulated nematic phases within a generalized Landau–de Gennes framework in which the alignment tensor field $\mathbf{Q}$ is coupled to the polarization field $\mathbf{P}$ through bulk polar terms, a screened depolarization contribution, and the lowest-order flexopolarization coupling [5]. We expand both $\mathbf{Q}$ and $\mathbf{P}$ in helicity modes and perform global numerical minimization within a class of one-dimensional periodic structures. Within this variational class, the model stabilizes the experimentally observed uniform ferroelectric and heliconical ferroelectric nematic phases, together with additional polar and modulated structures not yet reported experimentally. The resulting phase diagrams map the stability regions of isotropic, uniform apolar, uniform ferroelectric, and spatially modulated nematic phases, and reveal how bulk polarity, depolarization, and flexopolarization jointly govern nematic self-organization. In particular, the NTB,F phase emerges from a balance between the screened depolarization energy associated with splay distortions of the polarization field and the energy gain arising from flexopolarization induced coupled deformations of $\mathbf{Q}$ and $\mathbf{P}$.

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