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We study theoretically the twist-bend nematic (Ntb) phase using Landau-de Gennes mesoscopic approach in presence of nanoparticles. The Ntb phase is commonly exhibited by curved mesogenic liquid crystalline (LC) dimers. Its basic structure is typically determined by the nematic director \vec{n} which points along a local mesoscopic uniaxial molecular order, where the states $\pm\vec{n}$ are physically equivalent. In the Ntb phase \vec{n} forms an oblique helical pattern consisting of periodic twist-bend deformation. The configuration possesses a double degenerate handedness, has a typical pitch in the order of 10 nm and \vec{n} essentially forms spatially constant conical angle with respect to the direction of helix axis. The Ntb phase is typically formed by lowering the temperature from the conventional uniaxial nematic (N) phase.

Methodology

We describe the nematic (N) and nematic twist-bend (N_{TB}) order by the mesoscopic nematic tensor order parameter \underline{Q} and dimensionless vector polarization field \vec{p} . The former is in the uniaxial approximation expressed in terms of uniaxial nematic order parameter $S \in [-1/2, 1]$ and nematic director field \hat{n} as

$$\underline{Q} = S(\hat{n}\hat{n} - \underline{I}/3)$$

The unit vector \hat{n} points along the local mesoscopic uniaxial direction.

The polarization field, fingerprinting the N_{TB} order, is given by

$$\vec{p} = p\hat{e}_p$$

where we assume $\hat{e}_p \cdot \hat{n} = 0$ (i.e., \vec{p} are locally mutually orthogonal) and $p \leq 1$. Therefore, $S = 1$ and $p = 1$ fingerprint the maximal degree of respective order.

We consider effectively homogeneous LC-NP mixture. The volume concentration of NPs is given by

$$\phi = \frac{N_{NP}v_{NP}}{V},$$

The LC free energy is expressed as the integral over the LC volume

$$F = \int (f_c^{(N)} + f_c^{(TB)} + f_e + f_f + f_i \delta(\vec{r} - \vec{r}_i)) dV$$

We use a standard Landau-type approach and expand free energy densities in terms of symmetry allowed order parameters contributions

$$f_c^{(N)} = \frac{3}{2}a_0(T - T^*)\text{Tr}\underline{Q}^2 - \frac{9}{2}b\text{Tr}\underline{Q}^3 +$$

$$\frac{9}{4}c(\text{Tr}\underline{Q}^2)^2,$$

$$f_c^{(TB)} = \alpha\vec{p} \cdot \vec{p} + 3\beta\vec{p} \cdot \underline{Q}\vec{p} + \frac{9}{2}\gamma(\vec{p} \cdot \underline{Q}\vec{p})^2,$$

$$f_e = \frac{L}{2}|\nabla\underline{Q}|^2,$$

$$f_i = -\frac{3}{4}w_1\hat{e}_i \cdot \underline{Q}\hat{e}_i + \frac{3}{4}w_2\text{Tr}\underline{Q}^2,$$

We express the total polarization of the systems

$$\text{as } \vec{P}^{(tot)} = n_{LC} \langle \vec{p}_{LC} \rangle = n_{LC}p_0 \langle \vec{p} \rangle.$$

We approximately express the effective free energy densities as

$$\overline{f_c^{(N)}} \sim a_0(T - T^*)\bar{S}^2 - b\bar{S}^3 + c\bar{S}^4,$$

$$\overline{f_c^{(TB)}} \sim \alpha\bar{p}^2 - \beta\bar{S}\bar{p}^2 + \frac{\gamma}{2}\bar{p}^4 \equiv \beta(S_c - \bar{S})\bar{p}^2 + \frac{\gamma}{2}\bar{S}\bar{p}^4, \quad \bar{f}_e \sim \frac{L\bar{S}^2}{\xi_d^2},$$

$$\bar{f}_i \sim -\frac{w_1\bar{S}}{2} + \frac{w_2\bar{S}^2}{2}.$$

In the case that NPs are homogeneously dispersed and do not form assemblies, the N-N_{TB} phase behavior is determined by

$$f = r^{(eff)}s^2 - 2s^3 + s^4 - \sigma s - A\frac{(s-s_c)^2}{s^2}$$

$$r^{(eff)} = r + \frac{\xi_{IN}^2}{\xi_d^2} + \phi \frac{\xi_{IN}^2}{d_e^{(2)}r}; \quad \sigma = \phi \frac{\xi_{IN}^2}{d_e^{(1)}r}; \quad A = \frac{\beta^2}{2\gamma a_0(T_{IN} - T^*)}$$

Results

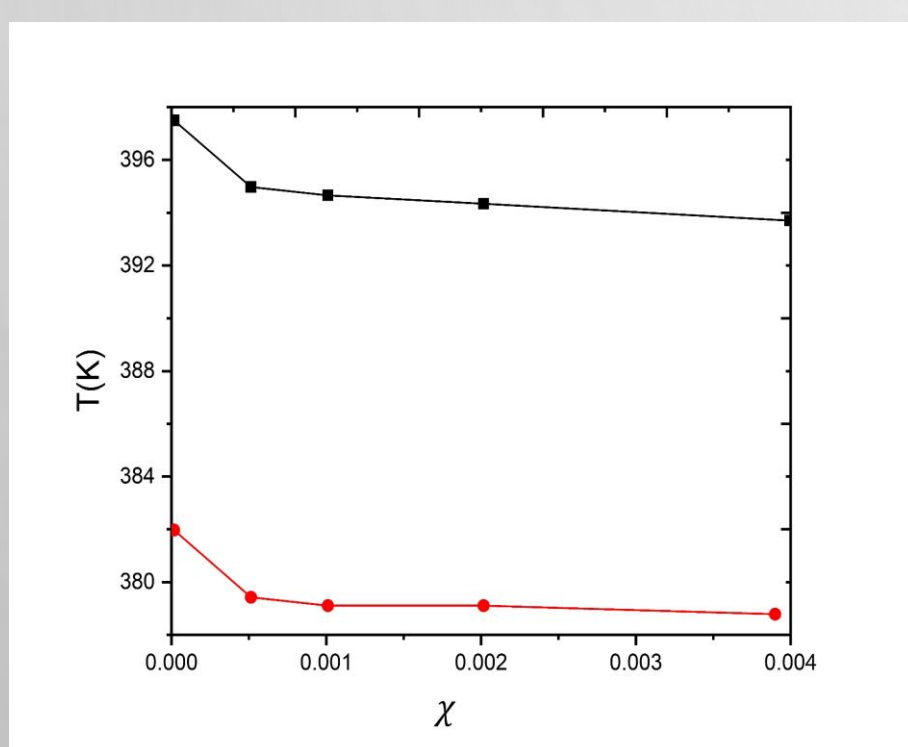


Figure1. I-N-N_{TB} phase behaviour on increasing

$\chi \sim \phi \frac{\rho_{NP}}{\rho_{LC}}$ from $\chi = 0$ (bulk LC) to 4×10^{-3} .

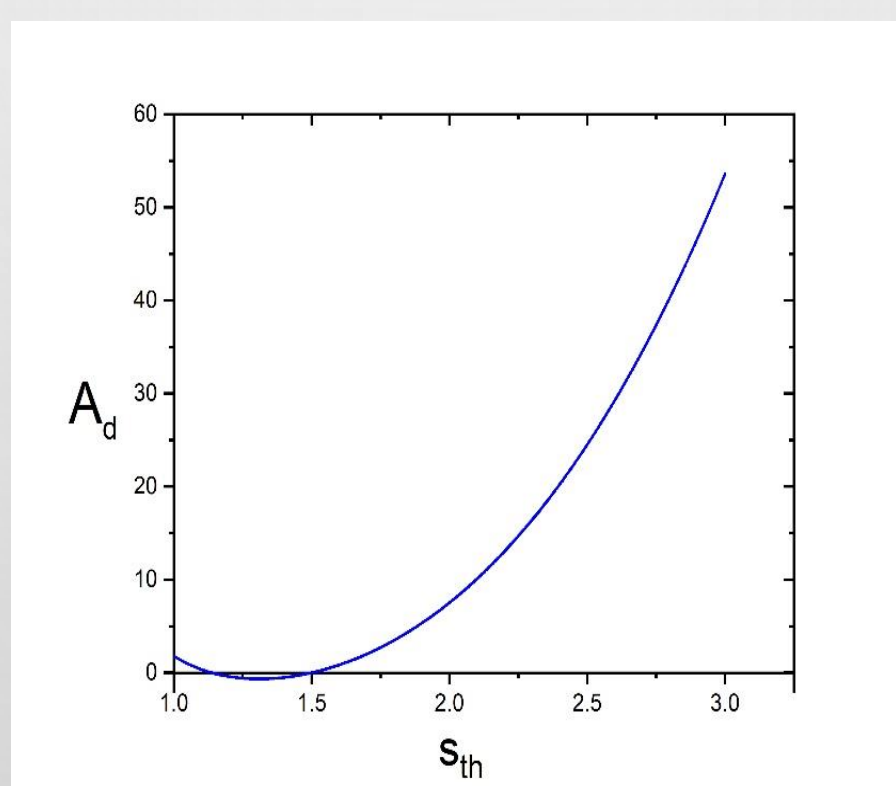


Figure2. A_c as a function of s_c . For $A \leq A_c$ and $A > A_c$ systems exhibit continuous and discontinuous N-N_{TB} phase transitions, respectively.

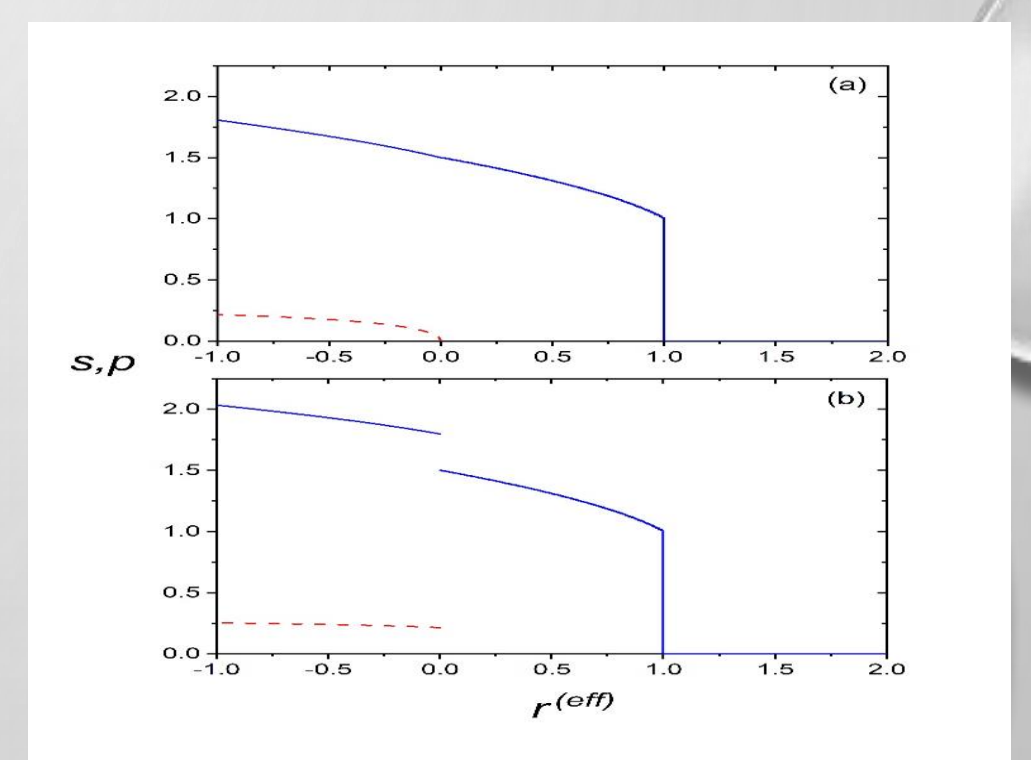


Figure3. I-N and N-N_{TB} phase behavior on varying the effective dimensionless temperature $r^{(eff)}$ where we assumed $\sigma \sim 0$ and $s_c = 1.5$. Blue lines: $s = s(r^{(eff)})$; Red dashed lines: $p = p(r^{(eff)})$. (a) $A = A_c = 20$. (b) $A = 100$.

Conclusions

Our analysis shows that nanoparticles reduce the nematic transition temperature $T_c^{(n)}$ through distortion-induced renormalization of the effective temperature, with a scaling dependence This prediction is consistent with experimental trends. In contrast, the temperature separation between the nematic and NTB transitions, $T_c^{(n)} - T_c^{(tb)}$ remains nearly independent of nanoparticle concentration, which supports the assumption that the NTB condensation parameter α is weakly temperature dependent. Furthermore, our model predicts that the N-NTB transition can be either continuous or discontinuous depending on the strength of the quartic coupling A , with a critical threshold value is given by A_c .