Supplementary Information for:

Field-induced anti-nematic and biaxial ordering in binary mixtures of discotic mesogens and spherical magnetic nanoparticles

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I. DETAILS ON THE GAY BERNE POTENTIAL

The discs interact via a modified Gay-Berne (GB) potential, that is, [1]

$$U^{\mathrm{r}}_{ij}(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\mathbf{r}_{ij}) = 4\varepsilon(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij})\left[\left(\frac{\sigma_0}{|\mathbf{r}_{ij}|-\sigma(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij})+\sigma_0}\right)^{12} - \left(\frac{\sigma_0}{|\mathbf{r}_{ij}|-\sigma(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij})+\sigma_0}\right)^{6}\right]. \quad (1)$$

The range parameter σ of two disclike particles of thickness l and diameter σ_0 is,

$$\sigma(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij}) = \sigma_0\left(1-\frac{\chi}{2}\left[\frac{(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_i+\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_j)^2}{1+\chi\hat{\mathbf{u}}_i\cdot\hat{\mathbf{u}}_j} + \frac{(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_i-\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_j)^2}{1-\chi\hat{\mathbf{u}}_i\cdot\hat{\mathbf{u}}_j}\right]\right)^{-\frac{1}{2}} \quad (2)$$

where $\chi = (l^2/\sigma_0^2-1)/(l^2/\sigma_0^2+1)$, $\hat{\mathbf{u}}_i$ is the director along the principal axis of particle i and $\mathbf{r}_{ij}$ is the connecting vector between the centre of masses of particles i and j.

The strength anisotropy parameter in Eq. (1) is given by

$$\varepsilon(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij}) = \varepsilon_0\left[\varepsilon_1(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j)\right]^{\nu}\left[\varepsilon_2(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij})\right]^{\mu} \quad (3)$$

with ε_0, $\varepsilon_1(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j) = \left[1-\chi^2(\hat{\mathbf{u}}_i\cdot\hat{\mathbf{u}}_j)^2\right]^{-\frac{1}{2}}$ and μ, ν are adjustable exponents. The $\varepsilon_2(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij})$ parameter adjusts the well depth ratio for the edge-to-edge (ε_ϵ) to face-to-face (ε_f) configuration of the disc particles [2] by introducing the parameter $\chi' = (\varepsilon_\epsilon^{1/\mu}-\varepsilon_f^{1/\mu})/(\varepsilon_\epsilon^{1/\mu}+\varepsilon_f^{1/\mu})$, that is,

$$\varepsilon_2(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij}) = 1-\frac{\chi'}{2}\left[\frac{(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_i+\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_j)^2}{1+\chi'\hat{\mathbf{u}}_i\cdot\hat{\mathbf{u}}_j} + \frac{(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_i-\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_j)^2}{1-\chi'\hat{\mathbf{u}}_i\cdot\hat{\mathbf{u}}_j}\right]. \quad (4)$$

For the interaction between pairs of discs and spheres we also use the Gay-Berne potential of Eq. (1). The σ_{ds} parameter depends only on the orientation of disc j, $\hat{\mathbf{u}}_j$, and the normalized vector $\hat{\mathbf{r}}_{ij}$ connecting to the centre-of-mass of sphere i, that is, [3]

$$\sigma_{\mathrm{ds}}(\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij}) = \sigma_0^{\mathrm{ds}}\left[1-\chi''(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_j)^2\right]^{-\frac{1}{2}} \quad (5)$$

where $\sigma_0^{\mathrm{ds}} = \frac{1}{2}(\sigma_0+\sigma_{\mathrm{s}})$ and $\chi'' = (l^2-\sigma_0^2)/(l^2+\sigma_{\mathrm{s}}^2)$. Similarly, the strength anisotropy for pairs of discs and spheres becomes

$$\varepsilon_{\mathrm{rs}}(\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij}) = \varepsilon_0\left[1-\chi'''(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_j)^2\right]^{\mu} \quad (6)$$

where the disc-sphere well-depth anisotropy is given by $\chi''' = 1 - (\varepsilon_e/\varepsilon_s)^{1/\mu}$. For our calculations we choose a set of parameters from well studied monodispersed system of disc particles [2], that is, $l/\sigma_0 = 0.345$, $\varepsilon_\epsilon/\varepsilon_f = 0.2$, $\mu = 2$ and $\nu = 1$. The values of the ratio $\varepsilon_s/\varepsilon_e$ are given and discussed in the main manuscript. In the present study the diameter of the spheres σ_s remains as an adjustable parameter with $\sigma_\mathrm{s}^* = \sigma_\mathrm{s}/\sigma_0$.

[1] D. Antypov and D. J. Cleaver, J. Chem. Phys. **120**, 10307 (2004).
[2] O. Cienega-Cacerez, J. A. Moreno-Razo, E. Díaz-Herrera, and E. J. Sambriski, Soft Matter **10**, 3171 (2014).
[3] D. J. Cleaver, C. M. Care, M. P. Allen, and M. P. Neal, Phys. Rev. E **54**, 559 (1996).