Electronic Supplementary Material (ESI) for Soft Matter.
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Self-assembly and mesophase formation in a non-ionic chromonic liquid crystal: insights from bottom-up and top-down coarse-grained simulation model

Electronic supplementary information.

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1 Intramolecular components of the coarse-grained force field

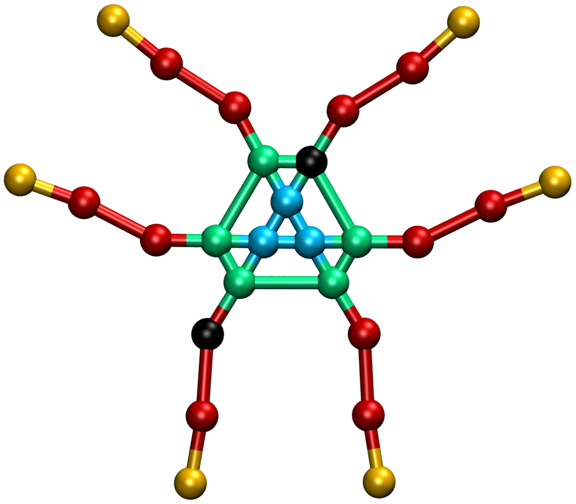

Fig. 1 Connectivity of the coarse-grained TP6EO2M model. All 1-3 and 1-4 interactions, as well as the 1-5 interactions of the type indicated by the black beads, were excluded from the reference trajectory in the final HFM models developed.

Table 1 TP6EO2M bond parameters.

Bond	r_0 / nm	k_{bond} / kJ mol^{-1} nm^{-2}
CC–CC	0.212	15000
CC–CO	0.212	15000
CO–CO	0.212	15000
CO–CO^a	0.424	15000
CO–AI	0.276	10000
AI–AI	0.328	10000
AI–AO	0.282	10000

^{a}The CO–CO* bond is along the long edge of the aromatic core.

Table 2 TP6EO2M angle parameters.

Angle	θ_0 / deg	k_{angle} / kJ mol^{-1} deg^{-2}
CC–CO–AI	180	85.0
CO–AI–AI	130	85.0
AI–AI–AO	130	85.0

Table 3 TP6EO2M improper dihedral parameters.

Dihedral	ϕ_8 / deg	k_ϕ / kJ mol^{-1}
CO–CC–CC–CC	0	30.0

2 Hybrid force matching intermolecular potentials (C-C interaction)

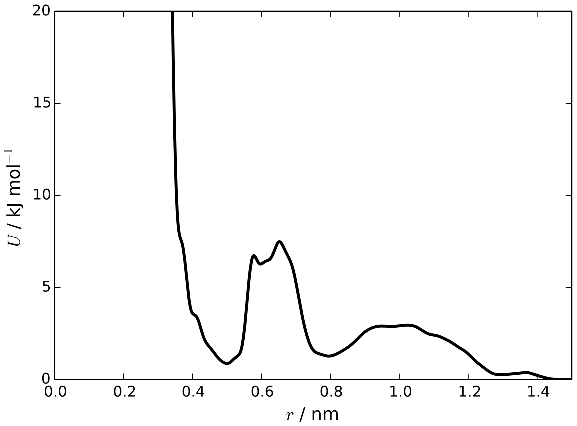

Fig. 2 C-C interaction potential calculated using HFM, after excluding only coarse-grained bonds and angles from the reference trajectory. The sharp peaks in this are due to 1–4 C-C interactions, and disappear when these pairs are excluded.

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3 Snapshot configurations showing self-assembly in solution

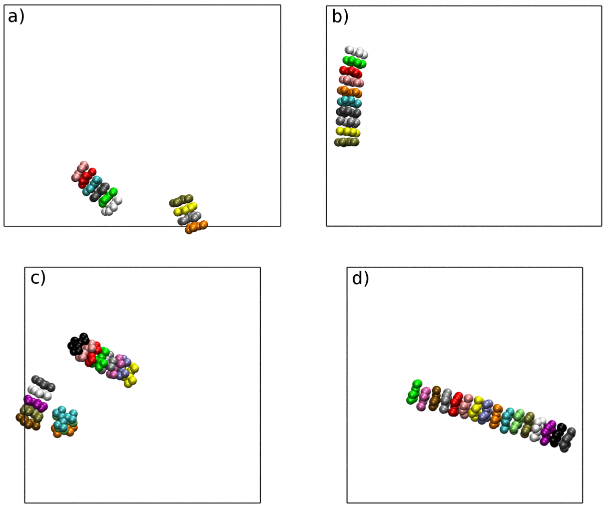

Fig. 3 Snapshots taken from simulations of 10 (a and b) and 16 (c and d) TP6EO2M molecules, from dispersed starting configurations, using the FM-N (a and c) and FM-Q (b and d) models. (For clarity central cores are shown, water and EO arms are hidden.)

4 Structural data for chromonic stacks

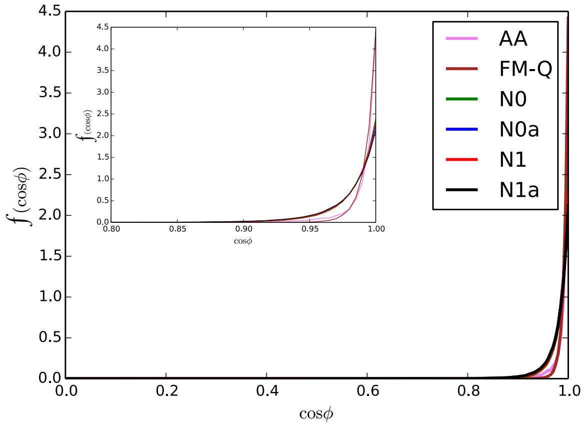

Fig. 4 Distribution function, $f(\cos(\phi_{ij})$, for angles ϕ_{ij} measured between the short axes of neighbouring molecules i and j within TP6EO2M stacks in the isotropic phase. $f(\cos(\phi_{ij})$ indicates that tilt angles are strongly peaked around zero for each model. The HFM model almost exactly follows the atomistic distribution function. MARTINI 3 models show a small degree of additional orientational disorder.

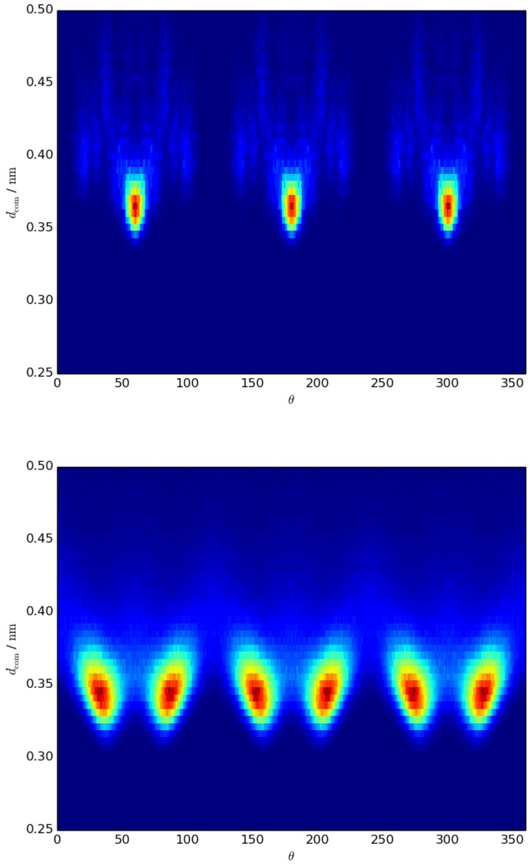

Fig. 5 2d distribution function, $f(d_{\mathrm{com}}, \theta_{ij})$, for azimuthal angles θ_{ij} measured between a reference vector in the plane of the aromatic rings for pairs of adjacent molecules i and j for TP6EO2M stacks. Top: atomistic model. Bottom: MARTINI N1a model. The atomistic model shows three peaks at 60, 180 and 300 degrees corresponding to staggered conformations of adjacent molecular cores. These peaks are split into two in the coarse-grained MARTINI model due to the presence of the CO beads.

5 PMFs for TP6EO2M dimers

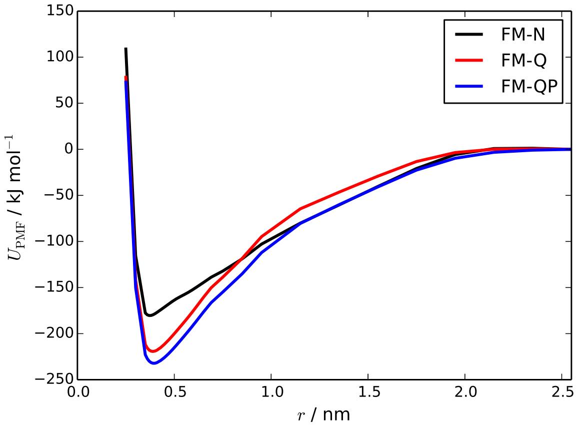

Fig. 6 PMFs for the formation of a TP6EO2M dimer, calculated using the FM-N and FM-Q models. Also shown are PMF results from a variant of the FM-Q model, FM-QP, where pressure corrections have been applied in fitting the atomistic configurations.

6 Snapshots from liquid crystal phases

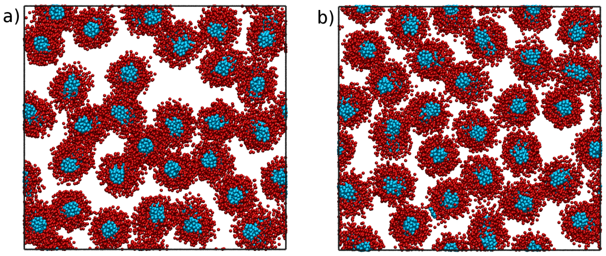

Fig. 7 Configurations taken after 200 ns of simulations of the 55.8 wt% TP6EO2M/water system. a) The N1 model results in clustering of the columns, while b) the N1a shows the C_H phase. simulations show only cores (cyan) and arms (red).