Supplementary Information

for

Engineered Liquid Crystal Nano Droplets: Insights from Multi-Scale Simulations

Zeynep Sumer[1], F. Anibal Fernandez[2] and Alberto Striolo[1]

[1]Department of Chemical Engineering, University College London, London WC1E 7JE, United Kingdom
[2]Department of Electronic & Electrical Engineering, University College London, London WC1E 7JE, United Kingdom

Here we conducted Q-tensor simulations, described in main paper, by using the parameters provided in Table S1. By keeping the temperature dependent parameter, A, as A = 0, the simulations can be generalized for a wide range of LC molecules.

Table S1. Parameters for the Q-tensor calculations implemented in this study.

Calculation	Parameter	Units	Value
F_B	A	N/m^2	0
	B		-2.26×10^6
	C		1.73×10^6
F_D	K_{11}	pN	6.2
	K_{22}		3.9
	K_{33}		8.2
Fs	homeotropic	-	strong
	planar degenerate		strong

In these calculations, we took the DPD data from the main text, and we conducted the energy profile analysis and order parameter calculations based on the parameters in Table S1. Figure S1 shows the quantitative results. It is revealed that the order parameter estimation in Figure S1(a) is a better fit than the main text, particularly the low values for the droplet that have low to moderate planar degenerate anchoring on the surface. This is caused by larger defects formed, than that of droplets with $A = -1.27\times10^6$ as in the main content. These deviations also affected the energy values of the droplets. Figure S1(b) shows that the empirical model (Eq. 5) overestimates the energetics of the droplets.

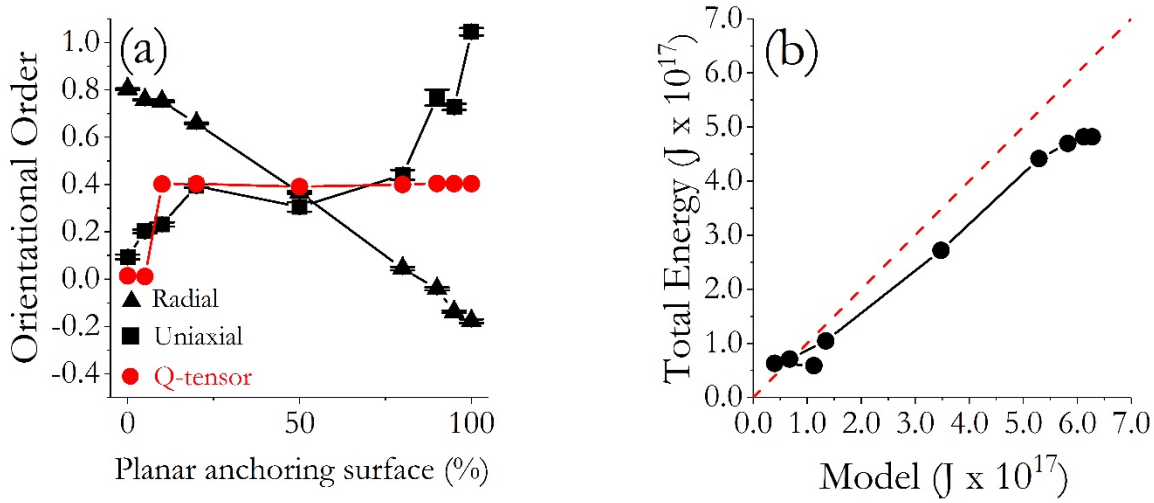

Figure S1. (a) Orientational order parameters (S) for all droplets simulated based on parameters in Table S1. (b) Relation between the proposed empirical model (Eq. (5)) and Q-tensor simulation results. The dashed red line indicates parity.

It is estimated that the generalized parameters result in larger defects, which directly affects the order parameter. In Figure S2, we mapped the defects and also corresponding local order parameter for each droplet.

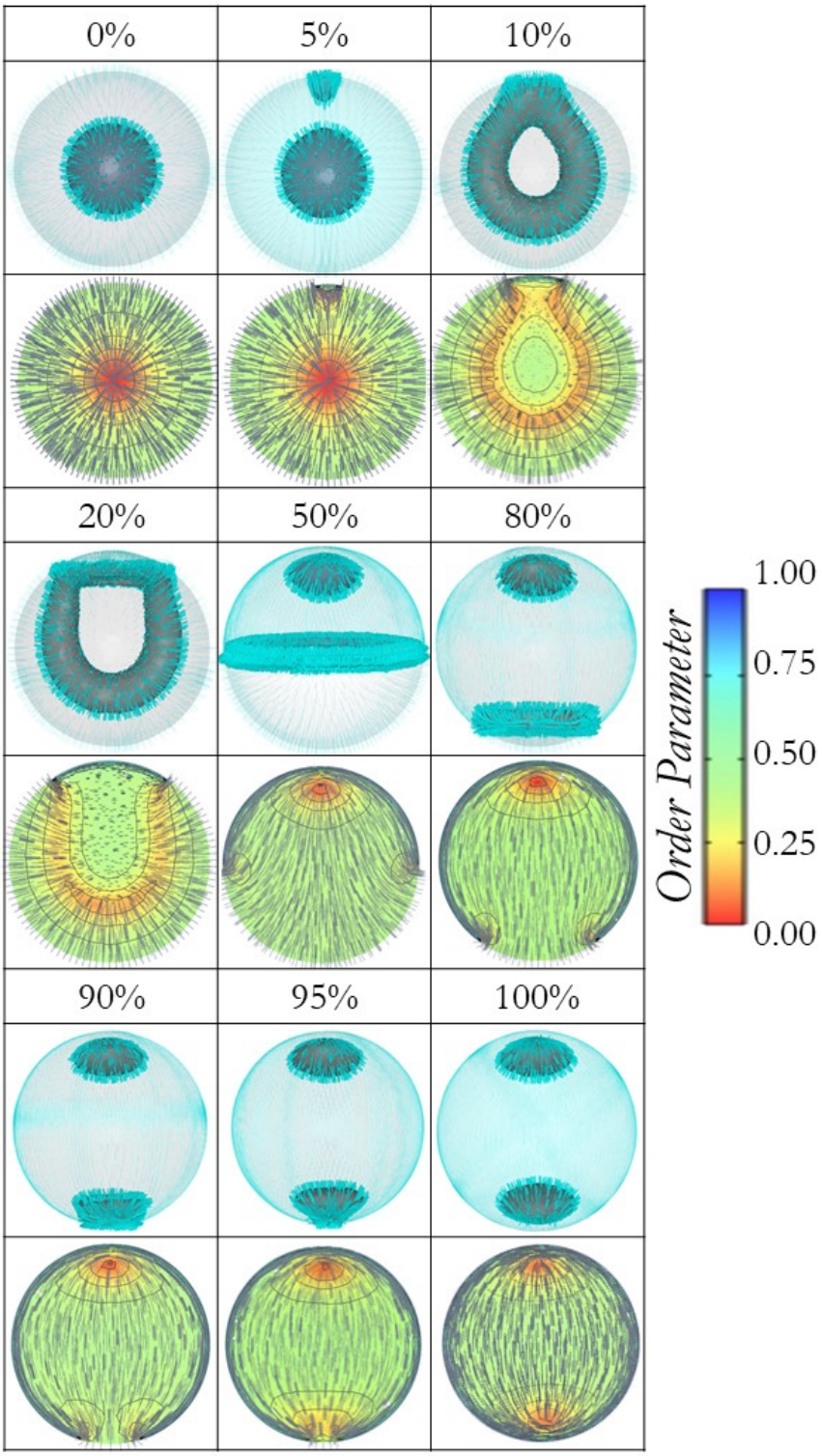

Figure S2. (Top of each panel) Snapshots of simulations by finite-element method with emphasis on defect structures, the images show surfaces of constant order for a low value of S. (Bottom of each panel) Structures observed in the simulated liquid crystal droplets as a whole. The background of each droplet is color-coded with respect to order parameters.