Electronic Supplementary Material (ESI) for Soft Matter.

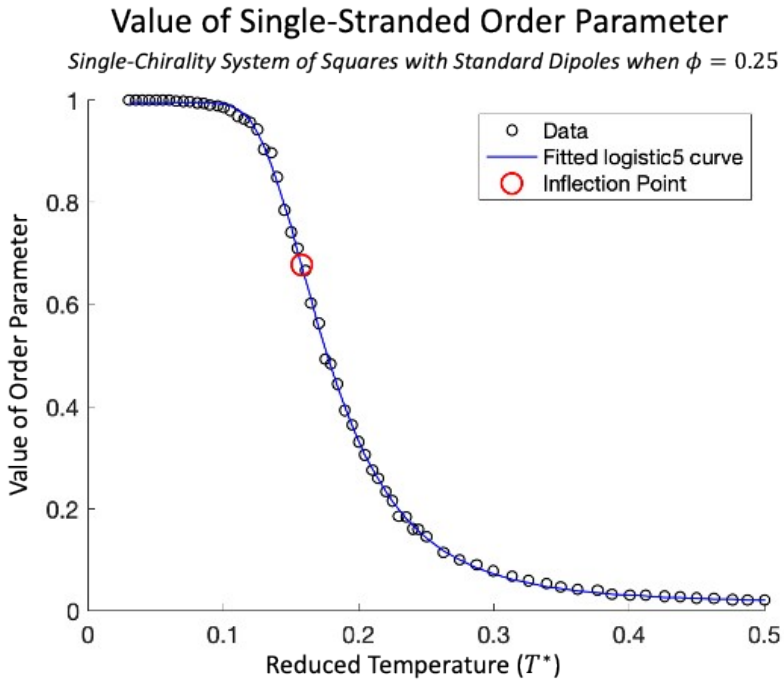
Computational Investigation of the Phase Behavior of Colloidal Squares with Offset Magnet Dipoles

Matthew A. Dorsey [a], Orlin D. Velev [a], and Carol K. Hall [*a]

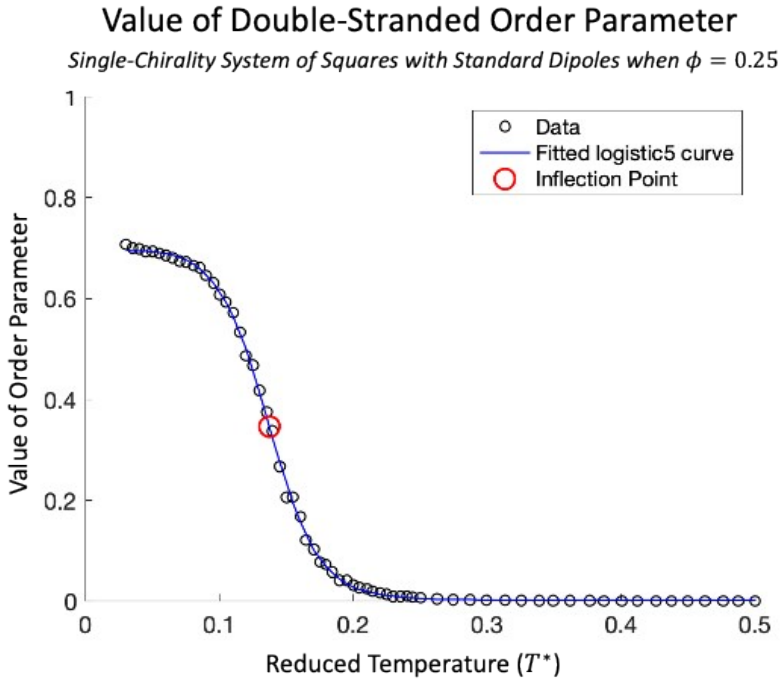
[a] *Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC 27606*

ELECTRONIC SUPPLEMENTARY MATERIAL

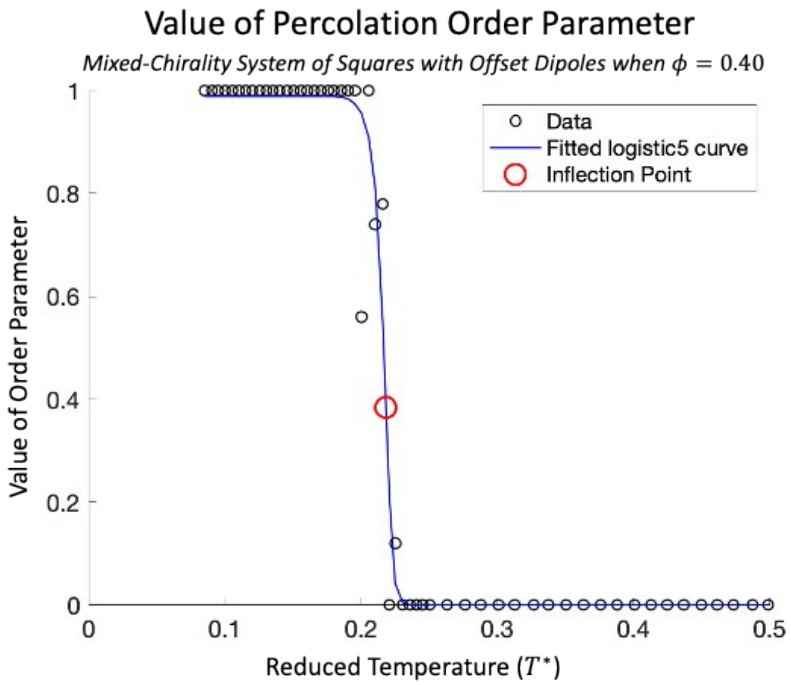
Examples of logstic5 Curve Fit to Selected Order Parameter Data



ESI Figure 1 – Logistic5 curve fit to single-stranded order parameter data collected from simulations preformed for systems of squares with embedded standard dipoles at an area fraction of ϕ = 0.25.



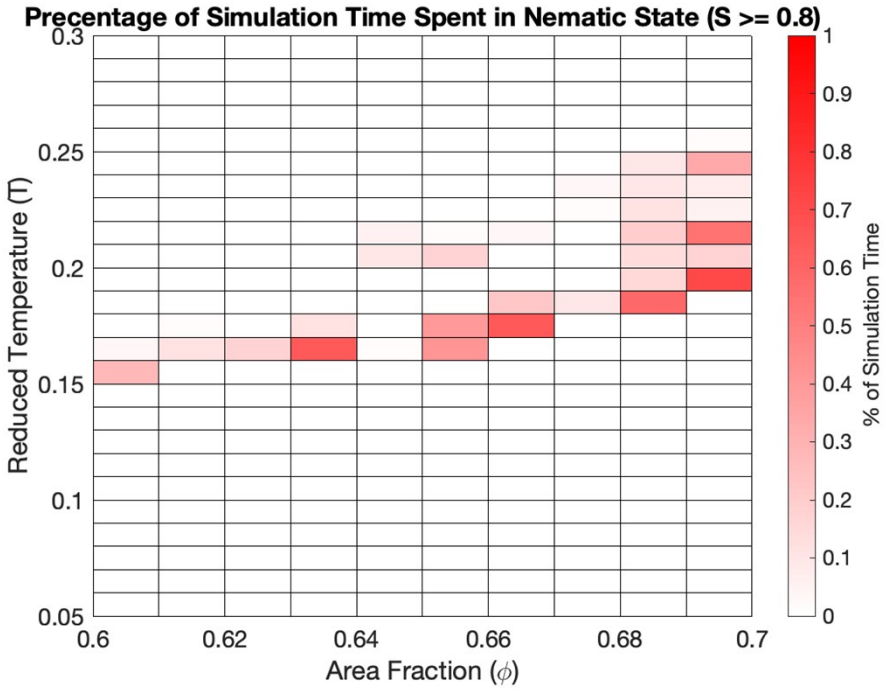
ESI Figure 2 – Logistic5 curve fit to double-stranded order parameter data collected from simulations preformed for systems of squares with embedded standard dipoles at an area fraction of ϕ = 0.25.



ESI Figure 3 – Logistic5 curve fit to percolation order parameter data collected from simulations preformed for systems of squares with embedded offset dipoles at an area fraction of $\phi = 0.40$.

Frequency of the Occurrence of a Nematic State for Single-Chirality Systems of Squares with Standard Dipoles at High Densities

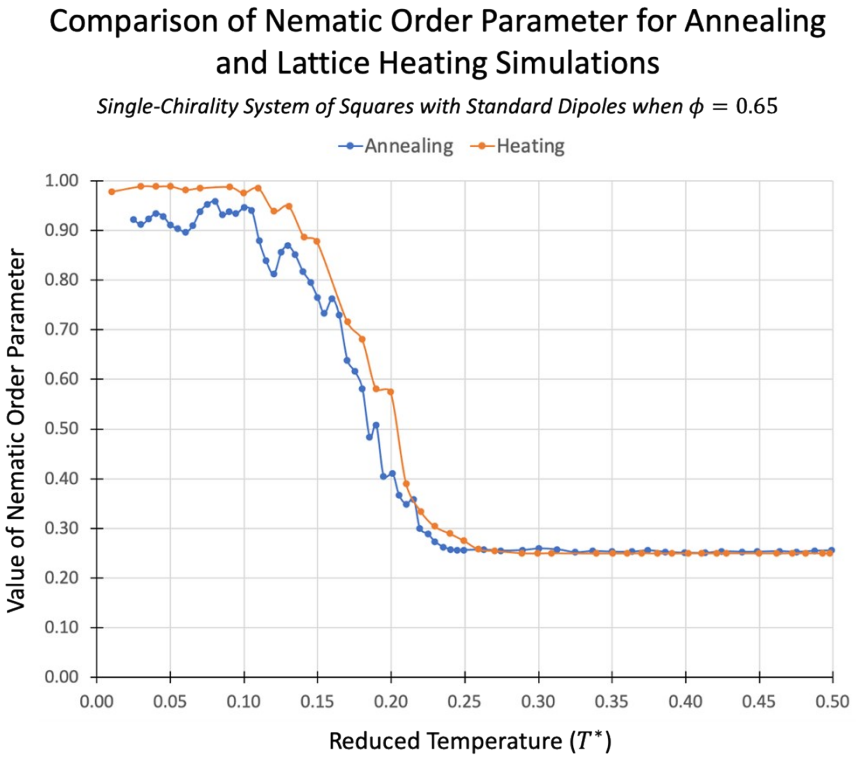
We performed constant temperature simulations of single-chirality systems of 256 squares with standard dipoles that varied in the temperature set point $T^* = \{0.01{:}0.01{:}0.50\}$ and area fraction $\phi = \{0.60{:}0.01{:}0.70\}$. Each simulation started in a random configuration and was run for 100 billion events. At the end of the simulation, the fraction of time that the simulation spent in the nematic state was calculated, shown in ESI Figure 1. We find that for each density, there exists a unique temperature range where the system might enter a nematic state. However, outside of the temperature range, the system will not enter a nematic state. Additionally, we notice that as the density increases, the temperature range in which the system might enter a nematic state grows.



ESI Figure 4 – Amount of simulation time spent in a nematic state for constant temperature simulations of single-chirality systems of squares with standard dipoles at various temperatures and densities. The percentage of time spent in the nematic state is calculate by the time the simulation spends in a nematic state normalized by the total amount of simulation time.

Heating of a Nematic Lattice

At a constant density of $\phi = 0.65$, we performed simulations for single-chirality systems of squares with standard dipoles where the system was start in a nematic, lattice configuration at a temperature of $T^* = 0.01$ and then heated to a temperature set point. The nematic order parameter is calculated once the system has equilibrated to the temperature set point. ESI Figure 2 compares the nematic order parameter for both annealing (blue) and heating (orange) simulations. We find that the equilibrium values of the nematic order parameter are similar for both the heating and annealing curves at each temperature, which is to say that the transition occurs at approximately the same temperature. There is a slight lag between the annealing and heating simulations, which could be explained by the fact that the annealing simulation starts from a completely random state, where as the heating simulations starts from a nematic lattice state.



ESI Figure 5 – Comparison of nematic order parameter values for annealing simulation started in a random configuration, and heating simulations started in a nematic, lattice configuration.