

Pomelo

Generic Set Voronoi Diagrams of Aspherical Particles of Arbitrary Shape

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Abstract.

1 Introduction

- Lipids and proteins form minimal surfaces like the Gyroid and the Diamond surface structures
- nanostructures have for example special photonic properties (color caused by structure/ butterfly)
- Lipids are amphiphilic molecules interacting with solvent and other lipids in a long range manner.
- what is the influence of particle shape (so purely entropically driven systems)
- liquid crystals and Hard spheres try to maximize entropy \Rightarrow order
- lipids described by cones
- Laurence and Doug simulated hard pear-shaped particles forming the gyroid
- want to generate the phase diagram and analyze gyroid phase geometrically

2 Gyroid Unit Cell

- 10000 particle system
- Clustering the systems show channel systems
- scattering functions (fft) reveal number of particles within one unit cell
- Consequently latticesize of the gyroid phase is determined ("width" of the gyroid phase)

3 Phase Diagram

- different degrees of tapering
- from lamella phase into lower density phases (nematic, gyroid, anisotropic)
- showing different pictures of the system

4 Geometrical Analysis

- distance between sheets (longitudinal distribution function)
- Mean square displacement
- Voronoi tessellation (POMELO)
- comparison between Gaussian curvature of gyroid and Volume/Surface of Voronoi cell and distance respectively
- maximizing the degrees of freedom in system (standard variation of Voronoi volume)

5 Conclusion

- entropy plays important role

6 Methods

- particle shape
- potential

Acknowledgements and References

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