Statistical Mechanics of Lipid-Liquid Crystal Systems: From Fundamentals to Sensing Applications

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Abstract

Attempts at understanding the thermodynamics of small systems have a well-established history due to the highly non-intuitive behavior of many properties of these systems. In particular, the intensive properties of small systems comprised of less than a few hundred particles have important implications in many areas of engineering and materials science. Nevertheless, many open questions about the thermophysical properties of systems that are not in the thermodynamic limit remain unanswered. In the first part of this study, we explore the consequences of the coupling of two small subsystems that together make up a larger isolated system through the use of statistical mechanics and molecular dynamics simulations of Lennard-Jones particles in two dimensions. The results from this study show that the average thermodynamic temperature and the average thermodynamic pressure of both subsystems can be different, with the relative difference being based on the number of particles making up the two subsystems. We also provide theoretical and simulation proof that the chemical potential of the two subsystems do not need to be the same if the temperature and pressure of the two subsystems are the same, as would be the case in the macroscopic limit.

Molecular recognition through ligand-receptor binding has traditionally been monitored by techniques that either requires a label to be attached to the analyte or complex optical methods to be detected. This has motivated the research for label-free assays to detect interfacial biological interactions without the use of special optical devices under controlled conditions. Phospholipid monolayers coupled with thermotropic liquid crystals as a responsive support can be used as a label-free biosensor. The hydrophobic acyl chains of the lipids contact the hydrophobic liquid crystal surface and the polar lipid head groups are presented to specific binding events involving proteins, enzymatic reactions, viruses, bacteria, etc. The mechanism by which lipid anchoring effects the liquid crystal surface remains to be elucidated. Therefore, a molecular study of the phospholipid/liquid crystal interface to determine the mechanisms by which binding events are transmitted from the analytes to the liquid crystal layer is crucial for the design of novel sensors. In the second part of this study, through a molecular model, we mimic the experimental systems by specifying interaction energies and their positional and angular dependencies. Our model allows us to fully characterize the organizations of phospholipids within the monolayer and also the orientations of liquid crystals in the bulk.

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