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Lecture Title:
Modeling membrane self-assembly of rigid elongated molecules

Abstract:
Using a rigid and geometrically simple molecular model for elongated molecular chains, we investigate numerically the process of membrane self-assembly in a couple of different systems of physical relevance.

One model investigation [1-3] is the self-assembly of molecular monolayers of alkane-thiol on gold(111); a system that has been studied extensively, both experimentally and theoretically, for two decades due to its conceptual simplicity. This system therefore provides a rich source of experiences that can guide theoretical model reductions necessary for large scale, long time simulations that can provide direct comparisons with experimental observations. We demonstrate an integrated modeling approach that involves various empirical surface interactions developed from electronic structure calculations, and mechanical structural reductions parameterized from atomistic considerations. The approach produces simulation data of relevant scales, and we make direct connections to the interpretations of, e.g., self-assembly, domain formation, spontaneous defect production, as well as many other features that can be (and has been) observed experimentally.

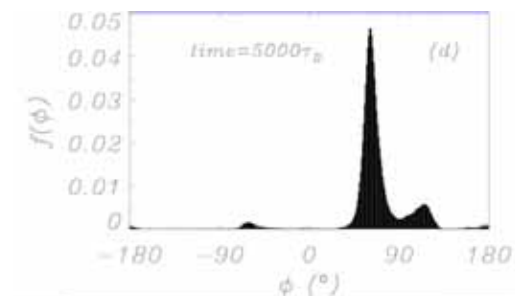
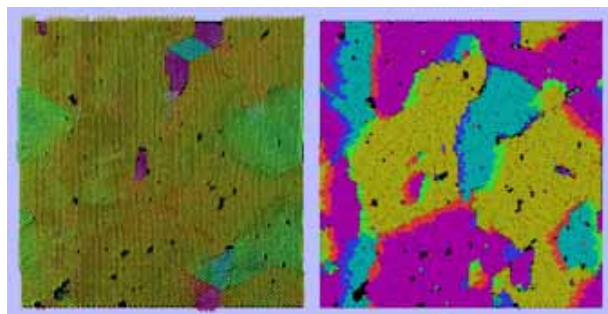


Figure 1. Left: Top view of large scale self-assembled monolayer of alkane-thiol on gold(111). Different colors represent molecular orientations and head-group positions. Right: Composition density of the molecular azimuthal angle in the sample.

Another model investigation [4-5] is the self-assembly of bilayer lipid membranes with DNA segments into lamellar complexes in aqueous media. This system has a solid body of experimental characterization produced over the past decade, but, as with the example above, direct numerical studies of the macroscopic self-assembly are largely prohibited by the vast spatial and temporal scale involved; unless

consistent model reductions are completed. We present a modeling approach that is structurally similar to the one we described above for alkane, but where the inter-molecular force fields now mimic the aqueous environment and the electrostatic complexity of the system. We demonstrate the self-assembly of the lamellar lipid-DNA complex from disordered initial conditions, and we further investigate the model for some of the detailed properties that are observed experimentally in the real complex.

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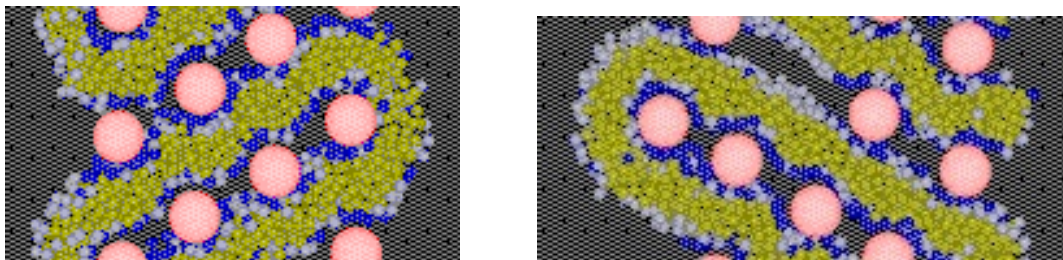


Figure 2. Snapshots of two simulations of charged (blue/green) and neutral (cyan/green) lipids with DNA (yellow) after lamellar structure has self-assembled from random initial condition.

The presentation will discuss modeling approaches, numerical methods, and how we integrate the modeling strategy with experimental and computational realities.

The following references, which cite relevant literature, serve as a link to parts of the material in the presentation.

(References ;)

- [1] *Determination of the headgroup-gold(111) potential surface for alkanethiol self-assembled monolayers by ab initio calculations*, Keith M. Beardmore, Joel D. Kress, Niels Gronbech-Jensen, and A. R. Bishop, *Chemical Physics Letters* **286**, 40 (1998).
- [2] *Rigid Molecular Model for the Assembly Characteristics and Optimal Structure in Molecular Monolayers of Alkanethiols on Au(111)*, Niels Gronbech-Jensen, Atul. N. Parikh, K. M. Beardmore, and Rashmi C. Desai, *LANGMUIR* **19**, 1474 (2003).
- [3] *Density dependent empirical potential for methyl-thiol on a gold(111) surface*, Byoungseon Jeon, Joel D. Kress, and Niels Gronbech-Jensen, submitted for publication (2006).
- [4] *Meso-scale computer modeling of lipid-DNA complexes for gene therapy*, Oded Farago, Niels Gronbech-Jensen, and Philip Pincus, *Physical Review Letters* **96**, 018102 (2006).
- [5] *Computational and analytical modeling of cationic lipid-DNA complexes*, Oded Farago, Niels Gronbech-Jensen, submitted for publication (2006).