Project DPD I: Structural properties

Polymer adsorption on hydrophobic substrate and its application for biomedical devices

This project is designed to provide students with an understanding of phase separation driven by enthalpy. Students will use LAMMPS codes and Python scripts to generate and analyze data. In this phase, they will explore the structural properties of mesoscopic phases, learn various computational methods to characterize them, and find their relevance within the context of experimental data.

Introduction

Adsorption of polymers on surfaces is a fundamental phenomenon in material science, impacting various applications such as coatings, drug delivery, and nanotechnology. One of the key driving forces behind polymer adsorption is hydrophobicity, which governs the interaction between polymer segments and the substrate.Understanding polymer adsorption driven by hydrophobicity is crucial for designing advanced materials. Applications include, biomedical Coatings, where hydrophobic polymer coatings can enhance biocompatibility or prevent biofouling. In thin-Film technologies adsorbed polymer layers are used in nanolithography and electronics. In drug Delivery Systems hydrophobic polymer adsorption can be tailored for controlled drug release.

There have been numerous theoretical approaches developed and applied to study the colloidal system. For example, the colloidal system of polymers has been studied theoretically and through simulations by treating them as ideal gas particles within the framework of the celebrated Asakura-Oosawa model. These systems have a well-formulated and structured theory that effectively explains their properties and provides guidance to experimentalists. Various simulation methods have been developed and refined for studying such systems e.g, atomistic simulation, coarse grained Brownian dynamics simulation, dissipative particle dynamics.

In the proposed project, students will apply dissipative particle dynamics to simulate a simple system of diblock and brush polymers in the presence of a hydrophobic substrate.

The aim of the project is to investigate the system within the context of a few of the following problems,

- What are the effect of system size on the adsorption of polymers over hydrophobic surface (a preliminary preparation)?
- What is the effect of segment ratio on the adsorption properties?

- What is the effect of total polymer length on the adsorption properties?
- What is the effect of polymer morphology on the adsorption properties?
- What is the effect of substrate area to volume ratio on the adsorption properties?
- What is the effect of polymer density on the adsorption properties?

There are a number of studies done in the past. For example, study of amphiphilic polymers over the hydrophobic surface. However, these studies have been done with good parametrization, which requires a rigorous investigation which is not expected within the given time limit of the project. Therefore students are presumed to apply a very crude model to study the adsorption phenomenon.

Project tasks

In the given project, students will be provided all the templates including LAMMPS code, polymer molecule template and the relevant python codes. Where students are supposed to customize all the templates according to their need. Following are the lists of tasks.

Symbols: Before further going with the simulation details, here students are being introduced with various symbols to make things easier to perceive.

Symbols	Meaning	Definition
V	total volume of the box	$length \cdot width \cdot height$
a	area of substrate including both sides	$2.0 \cdot length \cdot width$
N	number of polymers	
n_p	total number of polymer beads	
n_w	total number of water beads	
n_{ad}	total number of adsorbed beads	
ρ_p	polymer density	total number of polymer beads/total volume
ρ_w	solvent (water) density	total number of water beads/total volume
ρ_t	total density	total number of beads/total volume
s_p	total polymer length	total number of beads ina single polymer
s_b	size of hydrophobic segment	number of hydrophobic beads
s_l	size of hydrophilic segment	number of hydrophilic beads
a_r	fraction of hydrophobic segment	s_b/s_p
Γ	ratio of area and volume	a/V
λ	fraction of adsorbed polymer beads	n_{ad}/n_p

Table 1: List of symbols and their definition.

These are some general information within the context of project tasks:

- Create a $2D$ barrier using the given python script, which is a hexagonal flat structure with its plane-normal parallel to x-axis (see tables for the specification).
- Edit the given LAMMPS input script following the given table and run the simulations.
- For each output, analyze the binned particle distribution data and compute the average number of polymer beads within the volume of simulation box lying close to the substrate (n_{ad}). Division of the quantity with the number of beads within a single polymer molecule, is your desired number of polymers adsorbed on the surface.

Simulate the system for the following tables, where students are required to produce a single plot for each table.

Study 1 ($V^{1/3}$ vs λ)

To study the effect of system size, one needs to change the extension of the box while keeping all other parameters the same. This adjustment can be made using the following set of parameters:

#	N	n_w	X	Y	Z
1	20	5680	20	10	10
2	80	22720	20	20	20
3	180	51120	20	30	30

Table 2: Simulation parameters for different systems corresponding to plot 1. The independent variables that remain constant are fixed as follows: $\Gamma = 0.1$, $\rho_t = 3.0$, $\rho_p = 0.16$, $s_p = 16$, $a_r = 0.3175$.

Study 2 (a_r vs λ)

To study the effect of the segment ratio, students are required to change the number of hydrophobic beads from a low to a high value while keeping the total polymer size constant:

#	s_b
1	4
2	8
3	12

Table 3: Simulation parameters for different systems corresponding to plot 2. The independent variables that remain constant are fixed as follows: $\Gamma = 0.1$, $\rho_t = 3.0$, $\rho_p = 0.16$, $s_p = 16$, $N = 80$, $n_w = 22720$, and $x = 20$, $y = 20$, $z = 20$.

Study 3 (s_p vs λ)

To study the effect of polymer length, increase the total number of polymers without altering any other parameters. Three different curves can be obtained for the same plot with different values of a_r:

Curve 1:

#	s_p	N
1	8	160
2	16	80
3	24	54

Table 4: Simulation parameters for different systems corresponding to plot 3. Constants: $\Gamma = 0.1$, $\rho_t = 3.0$, $\rho_p = 0.16$, $a_r = 0.5$, $n_w = 22720$, $x = 20$, $y = 20$, $z = 20$.

Curve 2:

#	s_p	N
1	8	160
2	16	80
3	24	54

Table 5: Simulation parameters for different systems corresponding to plot 3. Constants: $\Gamma = 0.1$, $\rho_t = 3.0$, $\rho_p = 0.16$, $a_r = 0.75$, $n_w = 22720$, $x = 20$, $y = 20$, $z = 20$.

Curve 3:

#	s_p	N
1	8	160
2	16	80
3	24	54

Table 6: Simulation parameters for different systems corresponding to plot 3. Constants: $\Gamma = 0.1$, $\rho_t = 3.0$, $\rho_p = 0.16$, $a_r = 0.25$, $n_w = 22720$, $x = 20$, $y = 20$, $z = 20$.

Study 4 (Γ vs λ)

To study the effect of Γ on polymer adsorption:

#	Γ	N	n_w	x	y	z
1	0.1	80	22720	20	20	20
2	0.15	54	15150	13.33	20	20
3	0.2	40	11360	10	20	20
4	0.25	38	9088	8	20	20
5	0.3	26	7573	6.666	20	20

Table 7: Simulation parameters for different systems corresponding to plot 4. Constants: $\rho_t = 3.0$, $\rho_p = 0.16$, $a_r = 0.32$, $s_p = 16$.

Study 5 (ρ_p vs. λ)

To study the effect of ρ_p on the adsorption of polymers, we consider the parameters given in the table below:

#	ρ_p	N	n_w
1	0.16	80	$22,720$
2	0.32	160	$21,440$
3	0.48	240	$20,106$
4	0.64	320	$18,880$
5	1.00	500	$16,000$

Table 8: Simulation parameters for different systems corresponding to Plot 4. The independent variables, which remain constant, are fixed as follows: $\rho_t = 3.0$, $a_r = 0.32$, $s_p = 16$, $x = 20$, $y = 20$, and $z = 20$.

Project Reports

Students are required to submit a report on their projects, which should include:

- **Introduction to the Problem**
  This section should be approximately one page long (or slightly more) and must include around five scientific references. It should discuss the significance of the project, particularly in the context of biomedical device applications. Students may also explore the chemistry of organic-inorganic interfaces, which could hold key insights into the origin of life on Earth.

- **Technical Description**
  This section should provide a clear description of the theory and model, where in model part student should discuss about the DPD simulation method, where it can be mentioned about the pros and cons of the method along with basic equations and conservation laws being followed in the simulation box e.g, momentum, angular momentum, energy etc. It must also include at least one reference and be approximately half a page to one page in length.

- **Main Findings**
  This section, forming the core of the report, should provide a thorough explanation of the results and how they were obtained. It should be between 5 to 10 pages long.

- **Conclusion**
  Summarize the key findings and their implications. This section should be about half a page to one page in length.

Although students are encouraged to collaborate and divide tasks as needed, each student must submit a complete, individual report for evaluation. Data can be shared among students, but writing and other technical components must be completed independently.

Future Aspects

The project is designed to introduce students to the adsorption phenomenon using the Dissipative Particle Dynamics (DPD) simulation approach. However, the study can be extended to explore:
The effect of substrate features on the absorptivity of the materials, such as patches on the substrate and different geometries like convex or concave surfaces.
The trapping of particles using micelles and substrates.
The influence of undulation on biological interfaces. While the substrate in this project is kept free of undulation, most tissues and protein interfaces exhibit undulations that play a crucial role. Extending the project to study interface undulations holds great potential for understanding complex biological systems.
