

Adsorption of Polymers on Membranes

Prabhakar Ranganathan

Ph.D. position available

This project is a collaboration between [Prabhakar Ranganathan](#) and [Ravi Jagadeeshan](#) (in the Dept. of Chemical Engineering), and [Burkhard Duenweg](#) at the Max Planck Institute for Polymer Research (MPIPR), Mainz, Germany. We are looking for somebody with a [H1 or equivalent](#) graduate degree in either engineering, physics or mathematics to take on the challenge of setting up computer simulations to study an important problem that has potential applications in nanotechnology, microfluidics, medicine and biology. A PhD in this multi-disciplinary project can be the stepping stone to an exciting academic or research career in a number of fields: computer simulations, nanotechnology, mechanical/ chemical/ materials engineering, microfluidics, biophysics etc.

Scholarships are available from Monash University for applicants with a [strong academic background](#). Support will be available for the student during the PhD program to travel to Mainz and spend about a year with the [Theory Group at MPIPR](#), widely recognized for their excellence in the theory and simulations of soft condensed matter physics.

Aims and background

The primary objective of this Project is to use computer simulations to study the dynamic processes leading to the adsorption of a single polymer molecule on the surface of a semi-flexible biomembrane. The simulations in this study will involve the following typical scenario (see adjoining figure). The polymer molecule of interest is a flexible chain of segments, a few of which possess an electrostatic charge. The membrane is an infinite nearly elastic, nearly two-dimensional, fluid of a much higher viscosity than the ambient fluid. Scattered in the membrane are target sites with a charge opposite to the charged segments in the polymer. The attraction between the polymer segments and the target sites is however strongly screened because of the presence of ions in the fluid. The target sites may be fixed, or alternatively, may be free to diffuse within the membrane. Thermal fluctuations in the ambient fluid give rise to randomly fluctuating forces on the polymer, membrane and the diffusing target sites. The motions of the polymer and membrane in turn drive flows through the ambient fluid, which strongly affect, and couple, their dynamics.

Freely diffusing polymer molecules in solution can be thought of as long, flexible, “stringy” objects that are in constant random motion because of the continuous thermal buffeting they receive from the surrounding solvent molecules. Further, as any segment of the polymer molecule moves in response to the noisy Brownian forces

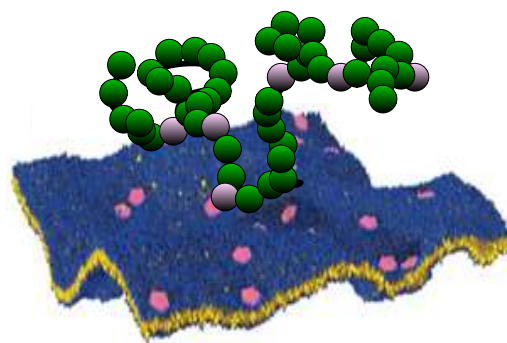


Figure 1: *Polymer adsorption on membrane: the polymer has a few sites (lighter spheres) that are attracted to sites on the membrane surface (lighter patches on membrane surface). Only a section of the membrane is shown. Both membrane and polymer are subject to thermal fluctuations, and disturb the ambient fluid as they move. Does the coupling of their motions due to the fluid flow hasten the process of adsorption in any way?*

exerted by the solvent, it experiences frictional resistance from the fluid that is proportional to its velocity relative to that of fluid in its vicinity. But the motion of the segment also perturbs the fluid. This perturbation decays slowly with distance, and thus modifies the motion of all the other polymer segments in the fluid. In recent years, computer simulations have clearly established the importance of such “hydrodynamic interactions” (HI) in determining the dynamical properties of polymer solutions.

Simulations of polymer molecules near rigid walls show that the presence of boundaries brings in additional contributions to HI that further affect how polymers move near interfaces. For instance, it is observed that the combination of the polymer’s elasticity and wall-modified HI cause it to migrate away from the wall in a shear flow. Such observations with rigid walls are fairly recent, and the dynamics of polymers near a deformable surface that is itself subject to thermal fluctuations—the central theme of the current proposal—remains to be explored.

Significance and innovation

Membranes are ubiquitous in living cells. For a long time, it was thought that cellular membranes played a largely structural role in biological processes, while genes and proteins were the kingpins in a central dogma that asserted that complicated structure is a necessary prerequisite for complicated function. However, in the last decade or so, it has become increasingly apparent that lipid bilayer membranes are not just passive compartmental walls, but in fact take an active part in the entire gamut of cellular processes, ranging from cell signalling, intracellular transport, and enzymatic regulation, to cell division, and cell death.

A common theme in several of these diverse activities that biomembranes engage in involves the adsorption of small and large molecules to multiple target sites (typically membrane proteins or sugar residues) on the membrane surface. Flows driven by the fluctuating surface may modify the motion of particles at a distance so as to increase its chances of locating specific heterogeneities on the membrane surface. The simulations proposed in this Project will examine this possibility in detail, and will lead to a deeper understanding of the dynamics of adsorption on to fluctuating surfaces.

The immediate impact of the proposed research will be a deeper understanding of the process of adsorption of polymers on membranes. More generally, this study will be a valuable contribution towards a growing body of work on the dynamics of membranes, and their role in biological processes. A knowledge of the hydrodynamics of membranes would be particularly useful in the future design of microfluidic devices and reactors. Currently, microfluidic applications are still grounded in the macroscopic paradigm that reactors and piping must be rigid, whereas solid bounding walls and sharp corners are conspicuously absent in the biological cell, the very apotheosis of a complex microfluidic device. A major bottleneck preventing our designing microreactors that mimic the cell is just this: we do not fully understand the behaviour of soft surfaces and membranes well enough.

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