

***Properties of a Biomimetic Nuclear Pore Complex. (Mentor: Ajay Gopinathan)*** Materials that are inspired by biology have the potential to take advantage of evolutionarily optimized characteristics and apply them to man-made devices. There has recently been great interest in trying to develop a biomimetic Nuclear Pore Complex (NPC) - a remarkably selective gate that regulates all transport between the nucleus and cytoplasm of cells. It is a large macromolecular complex whose main functional component is a 50-100 nanometer aqueous pore filled with polymeric disordered proteins that collectively interact with and facilitate transport of cargo carrying specific macromolecules. Our recent work has shown that the NPC disordered proteins from across the eukaryotic kingdom share some common features in the arrangements of their charges and binding sites. In this project, students will mimic those distributions of charges and binding sites in simple synthetic polymers. Using coarse-grained simulations that we have already built, they will investigate pores with grafted polymers with NPC inspired properties and look at the mesoscale structure and dynamics of the polymer complexes and the transport of cargo through them. Depending on the level of the students and their progress, they can also subsequently use the simulations to optimize desired transport properties through the pore. Simultaneously the students will be introduced to basic polymer physics theory and perform simple calculations related to the project. The students work will be of publishable quality and will result in a clear molecular level understanding of the transport process through our biomimetic pores and furthermore suggest design parameters for building synthetic NPC gates that can be used as highly selective tunable filters.