**UROP Project Opportunity**

**Project Title: Bioinspired peptide nano assemblies by design**

**Term:** Fall (IAP/Spring extension available)

**Department:** Civil and Environmental Engineering (Course 1)

**MIT Faculty Supervisor:** Markus Buehler

**Project Description:** Peptide self-assembly is a spontaneous process centered around weak intermolecular interactions that can be tuned precisely for the synthesis of complex hierarchical architectures. Nature provides a myriad of example peptide sequences we can learn from, and borrow: elastin, silk, collagen, resilin, zein – to name just a few. Despite their great abundance in nature and wide range of niche functions, at their core protein polypeptides are composed of simple building block component amino acid residues. Amino acid sequence encodes the structure and function at fundamental levels, and defines the biological role of protein polypeptides. In this project, the goal is to achieve a fundamental sequence-phenomenon understanding of assembly based on a simple building block set. We aim to develop a fundamental treatment for material design beyond nature's blueprint, opening avenues for application in green technology, energy applications, sensing and biomedicine, including drug delivery and tissue engineering applications. The student will use molecular modeling approaches to automate the production of a synthetic peptide library of representative bio-inspired peptides for controlled, directed self-assembly of various nanoarchitectures, including nanospheres, nanorods, ordered arrays and reversible micellar structures.

Our lab has expertise in using molecular modeling tools for studying materials. The student will get experience in molecular visualization software, Matlab/python scripting, data analysis, molecular model development, atomistic modeling, coarse-graining approaches, molecular simulation setup and implementation on supercomputers.

**Prerequisites:** No prior experience necessary. Our field is highly interdisciplinary and welcomes students from all backgrounds. Students interested in biology, chemistry, physics, materials science and bioengineering are welcome to apply. The UROP may be taken for credit or paid. Project extension into IAP and the Spring term are possible.

**Contact:** Email Anna Tarakanova (annat@mit.edu) if you are interested to apply. Please include your resume/CV and availability to meet.

**UROP Project Opportunity**

**Project Title: SUPERmaterial – uncovering silk's secrets using modeling approaches**

**Term:** Fall (IAP/Spring extension available)

**Department:** Civil and Environmental Engineering (Course 1)

**MIT Faculty Supervisor:** Markus Buehler

**Project Description:** Spider silk is one of the strongest and toughest biological protein materials, outperforming most other natural and man-made fibers. Whereas other protein materials may swell when placed in water, at high humidity, silk is observed to shrink significantly as it absorbs water. This unique, and yet-illusive material property is called supercontraction. It renders silk a terrific candidate for designing lightweight actuators for micromachines, sensors, biomimetic muscles and green energy applications.

Our lab has used various molecular modeling tools, from the nano to the macro scale, to identify and describe the structure, biological functions and mechanics of spider silk. The student will learn molecular modeling tools to probe the mechanisms of the supercontraction phenomenon.

The student will have a chance to participate in a collaborative project with an experimental group, and if successful, contribute to a scientific publication. The student will get experience in molecular visualization software, Matlab/python scripting, data analysis, molecular model development, atomistic modeling, coarse-graining approaches, molecular simulation setup and implementation on supercomputers.

**Prerequisites:** No prior experience necessary. Our field is highly interdisciplinary and welcomes students from all backgrounds. Students interested in biology, chemistry, physics, materials science and bioengineering are welcome to apply. The UROP may be taken for credit or paid. Project extension into IAP and the Spring term are possible.

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