Two available PhD positions in Soft Matter Interfaces and Energy Laboratory, Department of Mechanical Engineering, University of Maryland

Two PhD positions on the MODELING AND SIMULATIONS OF FLOWS IN POLYELECTROLYTE-BRUSH-GRAFTED NANOCHANNELS are available immediately in SMIEL (Soft Matter Interfaces and Energy Laboratory) in the Department of Mechanical Engineering, University of Maryland. One of the selected students will be working with Prof. Siddhartha Das (Webpage: www.smiel.umd.edu) and the other student will work jointly with Prof. Siddhartha Das and Prof. Peter Chung (http://www.enme.umd.edu/faculty/chung).

Description of the Research Problem

Polyelectrolyte (PE) molecules form brush-like structures when they are grafted to a surface very close to one another. Such a property has been routinely utilized to functionalize nanoscale interfaces (e.g., nanoparticles or the inner walls of a nanochannel) for a plethora of applications ranging from targeted drug delivery and oil recovery to biosensing and current rectification. One of the less understood issues concerning such nanochannels with PE brush grafting is the manner in which flow occurs within such nanochannels. While there have been several papers elucidating the fluid mechanics in such nanochannels, issues that remain very poorly addressed include (a) the deformation of the pH-responsive brushes in presence of the flow field, (b) the consequent drag forces exerted by the brushes, and (c) possible nanoscale energy conversion.

This project intends to develop a combined continuum theory and atomistic (or Molecular Dynamics or MD) simulation model to provide answers to these issues. The continuum model will involve minimization of the free energies of the PE brushes with appropriate accounting of factors such as pH-responsiveness of the brushes, monomer distribution along the length of the PE brush, etc. The MD simulation model, on the other hand, will probe the atomistic details of the brush configuration and its interactions with the water molecules and the ions hydrated by these water molecules.

Desired qualifications of the candidates

The student interested to work on the continuum problem must have excellent mathematical background with exposure to (a) Euler-Lagrange minimization technique, (b) experience of solving coupled differential and possible integro-differential equations, and (c) basic understanding of Navier -Stokes equations.

The student interested to work on the MD problem must have some exposure to at least one MD simulation platform (such as LAMMPS, GROMACS, etc.).

In exceptional circumstances, however, consideration will be given to candidates who may not be familiar with some of the above topics, but consider themselves as extremely hardworking and motivated to learn and pick up the topics in very short time.

Whom to contact

Candidates who feel are qualified for one or both the positions, should apply with their detailed CV and a cover letter to Prof. Siddhartha Das (Email: sidd@umd.edu). In the cover letter, the candidate must specify how he/she meets the desired qualification for the position. Prof. Das will not respond to applications without the detailed CV or the appropriate Cover Letter.