IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Understanding protein folding by studying the collapse of thermoresponsive colloidal chains**	
Project Number	**IMURA0908**	
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Research Clusters:

Highlight which of the Academy's CLUSTERS this project will address? *(Please nominate JUST **one.** For more information, see www.iitbmonash.org)*	
1	*Material Science/Engineering (including Nano, Metallurgy)*
2	*Energy, Green Chem, Chemistry, Catalysis, Reaction Eng*
3	*Math, CFD, Modelling, Manufacturing*
4	*CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control*
5	*Earth Sciences and Civil Engineering (Geo, Water, Climate)*
6	*Bio, Stem Cells, Bio Chem, Pharma, Food*
7	*Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng*
8	*HSS, Design, Management*

Research Themes:

Highlight which of the Academy's Theme(s) this project will address? *(Feel free to nominate more than one. For more information, see www.iitbmonash.org)*	
1	*Advanced computational engineering, simulation and manufacture*
2	*Infrastructure Engineering*
3	*Clean Energy*
4	*Water*
5	*Nanotechnology*
6	*Biotechnology and Stem Cell Research*
7	*Humanities and social sciences*
8	Design

The research problem

When a polymer chain is in a good solvent, it swells and occludes solvent to occupy a large volume. In a poor solvent, the chain collapses to form a dense, compact structure. The collapse of a polymer chain upon change in solvent conditions is believed to be relevant to the formation of a compact protein globule. Therefore, developing an understanding of polymer collapse transitions represents an important first step towards understanding protein folding. The study of polymer collapse transitions is a classical problem in polymer physics and considerable progress has been made in this area. However, there are several questions that remain unanswered. How does a polymer chain collapse when it is exposed to a poor solvent? What is the effect of backbone flexibility and polymer molecular weight on this collapse? How does the presence of charge along the backbone affect chain collapse? This project proposes to implement a radically new experimental route to address this problem, and couples this with simulations to obtain deeper insights into the experimental results.

Project aims

This project uses novel experiments that build on previous work in the Indian PI's group to synthesize colloidal chains. Colloidal chains are rendered thermoresponsive by coupling the particle surface with thermoresponsive molecules. Optical microscopy, including confocal microscopy, will be used to investigate the collapse transitions in these chains. The experimental results obtained at IITB will be simulated using models developed in the group of the Monash PI.

Expected outcomes

The work envisioned is fundamental in nature, and seeks to address some long standing open questions regarding the polymer physics of the chain collapse problem. Therefore the key outcomes will be in terms of manpower training, viz. to train the student so that s/he develops a high level of expertise in polymer and soft matter physics, and in terms of developing the capability to handle both experiments and simulations. A metric for this will be the publication of high quality, high impact publications on this fundamental problem.

How will the project address the Goals of the above Themes?

Describe how the project will address the goals of one or more of the 6 Themes listed above.

This colloidal model developed in this work is addressed towards understanding a fundamental problem – however, one can also view this as assembly of a stimulus sensitive nanostructure. Therefore, development of this model simultaneously advances tools in self assembly and nanotechnology and characterization tools that can track the time dependent structure of such nanostructures. This project combines experiments and simulations: advanced simulation tools, including possible modifications of specialized code developed in the group, will be employed to explain the experimental results. Thus, this project advances both the nanotechnology and engineering of novel stimulus sensitive colloidal nanostructures and the state-of-the-art in simulations.

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Be as specific or as general as you like. These capabilities will be input into the online application form and students who opt for this project will be required to show that they can demonstrate these capabilities.

We seek a student who has strong analytical training and good experimental skills. Specifically, students with a degree in chemical engineering (with exposure to materials, especially soft materials), or physics (with exposure to soft materials physics and/or polymers), or physical chemistry, or materials science/engineering (with exposure to soft materials physics) would be

suitable for this project.

Potential Collaborators

Please visit the IITB website www.iitb.ac.in OR Monash Website www.monash.edu to highlight some potential collaborators that would be best suited for the area of research you are intending to float.

Prof Arindam Chowdhury (Chemistry, IITB)

Select up to **(4)** keywords from the Academy's approved keyword list **(available at http://www.iitbmonash.org/becoming-a-research-supervisor/)** relating to this project to make it easier for the students to apply.

Nanoscience/Nanotechnology, Materials Chemistry/Science, Modeling and Simulation, Computational and Theoretical Chemistry