IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Machine-learning in self-assembly design**	
Project Number	**IMURA0950**	
MonashMainSupervisor (Name, Email, Phone)	Prof Tanja Junkers Tanja.junkers@monash.edu	*Full name,Email*
Monash Co-supervisor(s) (Name, Email, Phone)		
Monash Head of Dept/Centre(Name,Email)	Prof Phil Andrews, phil.adrews@monash.edu	*Full name, email*
Monash Department:	School of Chemistry, Faculty of Science	School of Chemistry
Monash ADGR (Name,Email)	Prof Craig White, craig.white@monash.edu	*Full name, email*
IITB Main Supervisor (Name, Email, Phone)	Prof Anil Kumar	*Full name,Email*
IITB Co-supervisor(s) (Name, Email, Phone)		*Full name,Email*
IITB Head of Dept (Name, Email, Phone)	Prof. Anindya Datta, adutta@iitb.ac.in	*Full name, email*
IITB Department:	Chemistry	

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

Define the problem

Block copolymer self assembly is a process used intensively in drug delivery and cancer treatment. Yet, while its thermodynamics is well understood, only poor knowledge and control exists over the kinetics of the process. This leads to large inconsistencies in synthesis of nanoparticles which need to be overcome. Continuous flow micromixing is a convenient tool to address these issues (demonstrated recently in publications of the Junkers group). Also, it was found that the kinetics can be used to lock in specific morphology changes otherwise inaccessible. This simplifies the synthesis enormously as in this way kinetically controlled morphologies can be accessed from one single block copolymer rather than needing a large array of polymers from a thermodynamic point of view. Morphology control is important as it predetermines cellular uptake, and thus efficacy of the drug delivery vehicles. Yet, the number of variables in the process (flow rates, composition, concentrations, choice of solvent, choice of mixer, choice of temperature) is very high, making the system highly complex. To solve this issue and to find suitable conditions for production of specific nanoparticles, we propose to use machine learning principles, such as decision tree and neural networks. The use of ML for synthesis purposes is still a young field, yet highly interesting and rewarding. This research also combines polymer science with biosciences and data science, making it exiting for new students.

Project aims

- *Synthesis of block copolymers in continuous flow, creation of product library*
- *Self-assembly of block copolymers into nanoaggregates*
- *Use of machine learning to govern design principles*
- *Loading of particles with active payloads*

Expected outcomes

Highlight the expected outcomes of the project

- application of ML to complex issue in polymer synthesis
- find new morphological control pathways to simplify drug delivery
- make drug delivery via block copolymers more reliable and predictable
- make systems ready for intense biological testing and later clinical testing

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 research is situated within the areas Material Science/Engineering (including Nano, Metallurgy) and Energy, Green Chem, Chemistry, Catalysis, Reaction Eng. Flow Chem is inherently a green methodology, whilethe synthesis target itself falls into nanoengineering of soft matter.

Within the themes, we will address
Advanced computational engineering, simulation and manufacture (data science approach) andNantotechnology (synthesis of complex nanoaggregates)

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Feel free to 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.

- Chemical synthesis
- Interest in data science/machine learning
- Block copolymer drug delivery