The University of Queensland - IIT Delhi Academy of Research Joint PhD Project

Project title	**A multi-scale simulation approach for high-throughput screening of polymer blend nanocomposite formulation**
Project code	**UQIDAR 00191**
Project description	Large number of possible formulation ingredients and non-monotonic dependence of blend properties on their weight fraction makes development of polymer blend nanocomposites particularly challenging. Prior work has established that nanoscale is the key length-scale associated with several properties of these materials, e.g., water vapor permeability. The large parameter space and significant importance of the nanoscale provides an important role for computer-aided design employing molecular simulations. The proposed work will focus on development of a multi-scale simulation approach for high-throughput screening of optimal formulation compositions for polymer blend nanocomposites to meet a given set of target properties. Specifically, it will involve developing formulations for biopolymer blend films and coatings that offer product differentiation for end-user applications, e.g., in packaging materials by meeting key requirements of high gas and vapor barrier, wettability tuning, grease resistance, etc. Additive with tunable properties, such as, organically modified clay nanoparticles and ionic liquids, will be used to optimize molecular level interactions to modulate the composite morphology and, thereby, achieve the target property. Specific objectives and methodology details are as below: 1. Development of MARTINI coarse-grained force-field (MARTINI-FF) parameters for select biopolymers Slow dynamics and large length-scales in polymeric materials are two key challenges in determination of equilibrium properties from atomistic simulations. A coarse-grained force-field will be developed to provide accurate estimation of the miscibility parameters and chemical diffusivities from equilibrium molecular dynamics and Monte Carlo simulations. 2. Determination of the composite morphology A mesoscale method, such as dissipative particle dynamics, will be used wherein the system will be mapped onto a Flory-Huggins lattice model to determine the composite morphology. 3. Full-scale transport simulation Finite element method will be implemented to solve the full-scale transport model for the composite material with data on solubility, diffusivity, and composite structure obtained from molecular and mesoscale simulations.
Project outcomes	1. A multiscale approach particularly suited for computer-aided design of polymer composites. 2. Advancing the understanding of effect of additives on structure-property relationships in polymer blend composites. 3. Development of biopolymer nanocomposite formulation for niche applications as films and coatings.
Advisory team	**UQ Principal Supervisor** **Professor Suresh Bhatia** Chemical Engineering s.bhatia@uq.edu.au https://researchers.uq.edu.au/researcher/161 **IITD PrincipalSupervisor** **Associate Professor Gaurav Goel** Chemical Engineering goelg@iitd.ac.in http://web.iitd.ac.in/~goelg/

	Additional Supervisor(s) **Professor Victor Rudolph** http://researchers.uq.edu.au/researcher/126
Type of student	Applications are open to: i-students who meet eligibility criteria.
Discipline background of student	Ideally, this project requires students with a background in: Chemical Engineering, Molecular Modelling
Ideal candidate	**Essential Capabilities:** Subject knowledge, especially, Thermodynamics, Transport Phenomena Excellent background in programming and scripting languages, such as C++, Python, shell scripting. **Desirable Capabilities:** Good technical communication skills, excellent work ethic **Expected qualifications (Courses/Degrees etc.):** B. Tech. or M. Tech. (or equivalent) in Chemical Engineering B. Tech. or M. Tech. (or equivalent) in Materials Science and Engineering M.Sc. or M.S. in Chemistry / Physics
Application process	Apply online by the due date: https://www.uqidar.org/students/how-to-apply/