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

Project title	**Multiscale Modelling of the Kinetics of Transdermal Drug Delivery**
Project code	**UQIDAR 00194**
Project description	Due to its permeable nature, the skin offers an attractive route for drug delivery directly into the blood stream; this avoids metabolism in the liver and increases the drug efficacy as well as tolerability, while having greater patient acceptance compared to injectables. Understanding and modelling the kinetics of solute diffusion through the skin is therefore important to design and optimise formulations for required dosages. In addition, the skin is frequently exposed to cosmetic products, and chemicals such as sunsecreens and insect repellents, which makes the study of solute diffusion through skin of even greater interest. This project will investigate dug diffusion through the stratum corneum, the outermost barrier layer of the skin, which controls the rate of drug delivery. This layer comprises dead cells called corneocytes and lipid bilayers organised in a brick and mortar structure. Molecular dynamics simulations will be used to investigate the transport of targeted drugs and molecules used as enhancers in the lipid bilayer, and determine transport coefficients in this bilayer. The results will be combined with models of diffusion through the corneocytes in a multiscale model, to predict the drug permeability in the stratum corneum in the presence of the enhancer. The model will be supported by experimental data from the literature. The specific objectives of the project are as follows- Conduct molecular dynamics simulations in the lipid bilayer, using targeted drugs, water, and enhancer at various concentrations, and determine mixture transport coefficients.- Develop simple models of permeation through the lipid-corneocyte wall, which governs transport through corneocytes.- Develop macroscopic models of transport through the stratum corneum, using results from MD simulations in the lipid bilayers and the model for transport through the corneocytes.- Validate and refine the overall model using literature experimental data- Determine optimal compositions for required dosages of the drug into the skin.
Project outcomes	The expected outcomes of the project are as follows 1. New understanding of multicomponent solute transport in lipid bilayer, including both drug and enhancer, based on molecular dynamics simulations 2. Multiscale model of drug transport through skin in the presence of enhancer. 3. New methodology for designing formulations and optimising compositions for transdermal drug delivery, and analysing penetration of chemicals through the skin.
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 Alan Mark**

	https://scmb.uq.edu.au/profile/936/alan-mark
Type of student	Applications are open to: q-students who meet eligibility criteria.
Discipline background of student	Ideally, this project requires students with a background in: Chemical Engineering, Physics or Computational Chemistry
Ideal candidate	**Essential Capabilities:** Good 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.E. or M.E. (or equivalent) in Chemical 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/