List of IC@N Research Projects and Supervisors

School of Chemical and Biomedical Engineering (SCBE)

Name of Supervisor	Research Project Description
Asst Prof Ni Ran **R.NI@ntu.edu.sg**	**Dynamic assembly of active colloids** Active matter consists of objects or particles continuously converting the biological/chemical energy to drive their motion. The interest in studying active matter originates from the wish to understand the intriguing self- organization phenomena in nature, e.g. bird flocks, bacteria colonies, tissue repair, and cell cytoskeleton. Very recently, breakthroughs in particle synthesis enabled the fabrication of active colloidal micro swimmers, which have quickly shown promise in applications such as biosensing, drug delivery, etc. In this project, we will use computer simulations to investigate the dynamic pattern formation in systems of active colloids.
	Computational design of polyelectrolyte for drug delivery Hierarchical progress in modern drug delivery starts with the use of polymer carriers to elicit spatiotemporal release of therapeutics in both pulsatile dose delivery products and implanted reservoir systems. Recent advances in polymer science have offered great opportunities for developing a new nano-medicine platform for drug delivery. In this project, we will use computer simulation to study the complexation of drug molecules with oppositely charged polyelectrolytes of different topological structures to realise a rational design of polyelectrolyte systems for drug delivery.
	Self-assembly of photonic crystals using anisotropic colloids Colloidal crystals with complete photonic bandgaps (PBGs) in the visible region provide a versatile platform for fabricating photonic semiconductors with many applications for optical communications, information technology, solar energy harvesting, and medical diagnostics, etc. To fabricate 3D photonic crystals various techniques have been used, including photolithography and etching techniques, which require complicated processes and clean room environment and the efficiency is very low. In this project, we will use computer simulation to study systems of anisotropic colloids self-assembling into photonic crystals, which may open new possibilities for guiding the large scale fabrication of photonic materials in experiments.

Asst Prof Tan Meng How **MH.TAN@ntu.edu.sg**	**Development of novel CRISPR-Cas technologies for genome engineering** In recent years, the CRISPR-Cas system has emerged as a powerful tool for engineering complex genomes. Besides DNA editing, it can be adapted to perform a suite of other functions, including gene regulation, epigenome editing, 3D chromosome re-organization, and genomic imaging. However, existing CRISPR-Cas technologies still suffer from several shortcomings that preclude their widespread adoption in the clinic. The student will be involved in our lab's efforts to alleviate some of these shortcomings, so that we can bring CRISPR-based therapeutics closer to reality. Project Duration: 6 months
Assoc Prof Chew Sing Yian **SYCHEW@ntu.edu.sg**	**Scaffold-mediated delivery of non-coding RNAs to direct cell fate** We hypothesize that substrate topography plays a significant role in dictating cell fate. Combined with biochemical signalling in the form of non-coding RNAs, synergistic cues may be presented to enhance stem cell commitment. The objective of this project is to understand the effects of substrate topography in directing cell differentiation and uptake/silencing of genes by siRNA/miRNA-mediated pathways.
Assoc Prof Lee Jong-Min **JMLEE@ntu.edu.sg**	**Noble nanomaterials** Fuel cells are recognized as efficient, green energy conversion technology, and can directly convert chemical energy to electrical energy, which has high energy conversion efficiency, low pollution, and fuel diversification. Low-temperature polymer electrolyte fuel cells (LPEFCs), such as proton-exchange membrane fuel cells, direct alcohol fuel cells, and direct formic acid fuel cells are regarded as promising power sources for automotive, portable and stationary systems. Platinum-electrocatalytic oxygen reduction reaction (ORR) is one of the key reactions in LPEFCs.
Asst Prof Paul Liu Wen **WENLIU@ntu.edu.sg**	**Hypothesis-driven synthesis of selective hydrogenation catalysts** Hydrogenation is a class of important feedstock upgrading processes in the chemical industry. In particular, the selective hydrogenation of chemically stable double bonds over chemically unstable ones and the partial hydrogenation of C=C to C=C bonds have been long standing challenges in

	heterogeneous catalysis. This project aims to design, synthesise, test and characterise novel supported metal catalysts for selective hydrogenation reactions. This will be achieved through tuning the activity and selectivity of the active sites by means such as alloying, support doping, defect engineering and nanostructure engineering. Project Duration: 5 months
	Ruddlesden-Popper phase oxides as catalysts supports Ruddlesden-Popper (RP) phases are a type of perovskite structure that consists of two-dimensional perovskite-like octahedra interlayered with large cations. Owing to the stable layered structure, RP phases can accommodate high degrees of oxygen non-stoichiometry, as well as highly redox active metal centres. The aim of this project is exploit the high oxygen conductivities of RP phases as heterogeneous catalysts supports for oxidative reactions. The research will involve hypothesising and designing new formulations of RP materials to simultaneously achieve (i) high catalytic activity and (ii) long-term stability. Project Duration: 5 months
Asst Prof Tej Salil Choksi tej.choksi@ntu.edu.sg	**Designing catalytic nanoparticles for converting CO2 into fuels** Decarbonising the chemical industry is a critical step towards mitigating runaway climate change. One decarbonisation strategy employs captured CO_2 as a feedstock for synthesizing chemicals and fuels. Using hydrogen obtained from renewables, this CO_2 is reduced to generate valuable building blocks like methane, methanol, and ethanol. Such manufacturing processes essentially reverse combustion. The industrial scale deployment of such technologies is primarily limited by the lack of catalysts that selectively convert CO_2 into methane, methanol, or ethanol. It is possible to control selectivity by tailoring the molecular structure and composition of catalytic active sites. Using state of the art computational modelling, we will design active site ensembles that selectively convert CO_2 into methane and ethanol. Both methane and ethanol are considered as alternative gas and liquid fuels that will replace petroleum-based fuels. The computational models for catalyst design are based on quantum mechanical methods like Density Functional Theory (DFT). These models help form relationships between the reaction selectivity (e.g. CO_2 to ethanol) and the structure and composition of active sites at the nanoscale. Using this modelling framework, we will select the shape, size, and composition of metallic nanoparticles such that these nanoparticles contain active sites that selectively generate methane or ethanol during CO_2 hydrogenation. This is a

	computational project with no laboratory work. No pre-requisites are necessary. The student should have a general interest in computational modelling but does not need to have any prior knowledge in this field. The student will be taught elementary Python, how to use existing computational modelling packages, and how to determine selectivity of CO_2 hydrogenation to methane or ethanol. Project Duration: 5 months
	Engineering Catalytic Nanoparticles by Mining Materials Databases Our transitions towards sustainable energy will entail the development of new manufacturing processes for chemicals and fuels. Examples of these manufacturing processes include synthesizing chemicals using CO_2, transforming existing carbon sources (plastics, waste) into value, and producing renewable hydrogen using electricity, water, and sunlight. There is an urgent need to discover catalytic materials that facilitate such chemical transformations. Atomistic modelling techniques have revolutionized the way we search for new materials, and ultimately design the best performing materials. In recent years, results from thousands of such calculations have been curated into publicly available databases like the Materials Project (Berkeley), Open Quantum Materials Database (Northwestern University), and Catalysis-Hub (Stanford University, maintained by the group where I did my postdoc). These databases are readily searchable using graphical user interfaces and simple python-based scripting. The main objective of this project is to design new catalytic materials by mining such materials databases. We will specifically identify the nanoparticle shape, structure, composition, which yield optimal catalytic performance for the reactions listed above. This is a computational project with no laboratory work. No pre-requisites are necessary. The student should have a general interest in computational modelling but does not need to have any prior knowledge in this field. The student will be taught elementary Python, how to use existing computational modelling packages, and how to mine the databases to ultimately design catalytic nanoparticles. Project Duration: 5 months