List of IC@N Research Projects and Supervisors

School of Physical & Mathematical Sciences (SPMS)	
Name of Supervisor	**Research Project Description**
Asst Prof Felipe Gracia fgarcia@ntu.edu.sg	**Mechanochemical Synthesis of Main Group Compounds and Complexes** Traditional chemical wisdom often cites Aristotle 'compounds do not react unless fluid or dissolved' as one of the original sources contributing to the default assumption of the need for solvents in molecular syntheses. This dogma of indispensable solvent use for chemical syntheses has existed for many centuries and has often been counterproductively deep-rooted in the minds of molecular synthetic chemists. There are distinct advantages to using solvents, primarily to promote the interaction of reagents, accelerate reaction rates, potentially alter the distribution of products, and the facile separation and purification of products. However, cleaner and more environmentally friendly synthetic technologies have become of pinnacle importance in both academia and industry, since commonly used organic solvents in laboratories and chemical industries are recognized as wasteful and environmentally unsustainable.
Assoc Prof Rei Kinjo rkinjo@ntu.edu.sg	**Development of Low-valent Boron Species and Its Metal Complexes** In this project the candidate will be synthesizing the novel low-valent boron-containing species and its transition metal complexes. The candidate will examine the reactivity of those complexes towards small molecules such as H2, CO2, CO. This project would be conducted through a joint PhD program, thus, the duration is 4 years.
Assoc Prof So Cheuk Wai cwso@ntu.edu.sg	**Synthesis of Low-valent Group 14 Compounds for Small Molecules Activation** This project aims at discovering new low-valent group 14 compounds, which can perform transition-metal like reactivity to activate small molecules into useful materials. The duration of the project is 6 months.
Prof Tan Choon Hong choonhong@ntu.edu.sg	**Mechanistic Studies of Halogen-Bonding in Bisguanidinium Phase Transfer Catalysis** In this project the candidate will be working on the mechanistic aspects of bisguanidinium phase transfer

	catalyzed enantioselective nucleophilic substitution reactions. He will be investigating on the existence of halogen bonding in one of the key intermediates. The minimum duration of the project is 3 months.
Assoc Prof Tan Howe Siang howesiang@ntu.edu.sg	**Ultrafast Spectroscopy of Photosynthetic Light Harvesting Complexes** We use the latest laser spectroscopic techniques to study the picosecond to femtosecond dynamics in the excitation energy transfer processes in the Light Harvesting complexes in plant and Marine phytoplankton photosynthetic systems. Photosynthesis is probably one of the most important complex biological process on earth. Much of this complex machinery is still not well understood. One important area is the Light Harvesting process which is the initial process where sunlight is captured and then channelled to reaction centre in the photosystems.
	Development and Applications of Ultrafast Multidimensional Optical Spectroscopy to the understanding of the ultrafast dynamics in complex molecular systems Ultrafast Multidimensional Optical Spectroscopy is an improvement on the more well know ultrafast pump-probe or transient absorption spectroscopy. It is able to provide both frequency and time resolution to ultrafast spectroscopic studies. We are currently developing and using these techniques to study the complex energy transfer, spectral diffusion and other ultrafast dynamics in systems ranging from biology (Photosynthetic light harvesting in plants) to nanomaterials (Quantum Dots and nanoplatelets). https://www3.ntu.edu.sg/home/howesiang/new/index.htm
Assoc Prof Xing Bengang bengang@ntu.edu.sg	**NIR Fluorescent Imaging Contrast Agents for Precise Manipulation Cell Functions and Localized Theranostics** We will design and prepare "smart" and unique optogenetic signal switching probe molecules which will specifically respond to the biological microenvironment stimulation for tumor localization and regulation of cell surface activities. The students will learn basic organic/peptide synthesis, bioconjugation, pharmaceutical science and imaging measurements. The project may need 6 months to complete.
	NIR optogentic regulation of cell membrane functions for mediating insulin resistance

	In this proposal, we create a unique and specific NIR optogenetic strategy to real-time regulate Akt, and precisely manipulate type 2 diabetes processing *in vitro* and in animal models. Through a photo-inducible protein interaction module (e.g. opto-Akt) of crytochrome2 (CRY2) and CIB1, our NIR light-mediated up conversion emission can real-time trigger the CRY2-CIB1 dimerization and induces the translocation of Akt to membrane, which thus optogenetically activate Akt signalling pathway to facilitate glucose uptake in living subjects. This project may need 6 months to complete.
Asst Prof Kiah Han Mao **hmkiah@ntu.edu.sg**	**Bounds on Constrained Codes for DNA Data Storage** The goal of the project is to study codes that satisfy certain run length and GC-content constraints with certain error-correcting capabilities. The candidate will apply techniques such as the generalized sphere-packing bounds to determine the optimal code size or code redundancy. The duration of the project is at least three months.
Asst Prof Tong Ping tongping@ntu.edu.sg	**Time Series Analysis with Deep Learning Techniques and Beyond** Time series analysis has wide applications in many fields such as economics, finance, computer sciences, engineering, and earth sciences, where understanding patterns and trends is important to decision making and predicting future behaviours. For example, the ground motion caused by an earthquake is recorded as a course of time. Time-series data are always noisy and high-dimensional. There features increase the difficulty of deep and precise analysis. Recent development in deep learning provides some new techniques for efficient time-series analysis. In this project, we aim to create new models of unsupervised learning of features for time series analysis and prediction. Applications into seismic data for earthquake identification & prediction and for petroleum exploration will be explored.
Asst Prof Xia Kelin xiakelin@ntu.edu.sg	**Topology Based Machine Learning for Biomolecular Data Analysis** In this project the candidate will be trained on topological data analysis and basic machine learning tools. The candidate will also apply these tools in realistic biological problems, such as drug design, chromosome structure characterization, molecular dynamics analysis, etc. The minimum for this project would be 3 months.

Asst Prof Marco Battiato marco.battiato@ntu.edu.sg	**Numerical Solution of the Boltzmann-Maxwell System for Ultrafast Out of Equilibrium Dynamics** The study of ultrafast dynamics (phenomena happening in less than 1 picosecond) triggered by ultra-short laser excitations present formidable theoretical challenges. Electrons within the material cannot be considered close to equilibrium. The characteristics of their strongly out of equilibrium distribution dictate the wide range of peculiar dynamics that can be observed in these extreme timescales. From the theoretical point of view, the necessity of fully accounting for a generic shape of the distribution function sharply rises the complexity of the problem. We are using and developing state of the art theoretical and numerical techniques ranging from Monte Carlo integration, discontinuous Galerkin discretization, and machine learning strategies to address the problem. The group is currently developing a large-scale software for the numerical solution of the coupled Boltzmann and Maxwell equations in real materials. The projects available cover one of the techniques mentioned above. The student will work in close connection with one of the members of the group.
Assoc Prof Chia Ee Min, Elbert elbertchia@ntu.edu.sg	**Ultrafast Terahertz Spectroscopy of Halide Perovskite Solar Cells** The student will use ultrafast terahertz spectroscopy to study organometallic halide perovskite solar cells, and from it to obtain the density, mobility, recombination kinetics and quantum yield of the photogenerated carriers.
	Spin-to-charge Conversion in Topological Materials The student will use terahertz emission spectroscopy to study the ultrafast spin injection and spin-to-charge processes in topological materials. We aim to elucidate the spin current density, surface versus bulk contribution, and spin to charge conversion timescale in various ferromagnetic/topological material heterostructures.
Assoc Prof Rainer Helmut Dumke RDUMKE@NTU.EDU.SG	**Development of Superconducting Quantum Circuits** In this project the candidate will be trained in the basics of superconducting quantum circuits. He will get an overview in basic fabrication processes as well in the design and simulation of superconducting quantum circuits. The minimum duration for this project would be 3 months.

Assoc Prof Fan Hongjin fanhj@ntu.edu.sg	**Development of Smart Nanomaterials for Metal Ion Storage** In this project the candidate will be trained in the selection and synthesis of nanomaterials, and their electrochemical properties in metal ion storage (such as Na and Zn and K). He will learn the recent advance in new-generation batteries, the structure, working mechanism and challenges. The minimum duration for this project would be 3 months.
Assoc Prof Lew Wen Siang wensiang@ntu.edu.sg	**Dynamics of Magnetic Skyrmion in Perpendicular Magnetic Anisotropy Structures** Magnetic skyrmions are particle-like magnetization configurations which can be found in materials with broken inversion symmetry. The study of magnetic skyrmions have been extensive due to the potential of exploiting the skyrmion as information carriers in memory devices. For one, the skyrmions' topological nature confer upon them a high degree of stability against external excitations. The particle-like configuration also grants the skyrmion an extra degree of spatial freedom to circumvent around random pinning sites or impurities as they move within the magnetic layer. These positive traits combined with the ultra-low electrical current required to drive the skyrmion has led to the conceptualization of a "Skyrmion memory" that could possess both the large data density of traditional hard disk and fast access speeds of random access memory. In this research project we propose to experimentally inject, detect and manipulate magnetic skyrmions in a perpendicular magnetic anisotropy film stack and demonstrate that it is possible to guide the movement of the skyrmion.
	Spin-Orbit Torque Devices as Synaptic Weights in an Artificial Neural Network An artificial neural network (ANN) takes inspiration from its biological counterpart to solve problems through processes that mimic the human brain, such as by acquiring knowledge through learning processes. In such ANNs, neurons are connected to each other through connections analogous to synapses, and each synapse has a strength or weight, w_{ij}, associated to it. In a bid to work towards energy-efficient brain-inspired computing, it is vital to seek out solutions to ANN beyond-CMOS. One such contender is in the emerging spin-orbit torque (SOT) device. The non-volatile and analogue-like response observed in SOT devices can be engineered to function as synaptic weights. Together with the appropriate electronic circuitry and neural network computing model, specific functions such as character recognition can be achieved.

Asst Prof Liew Chi Hin Timothy timothyliew@ntu.edu.sg	**Spin Switching Waves in Exciton-Polariton Condensates** Exciton-polaritons are hybrid states of light and matter forming in quantum wells strongly coupled to optical modes, typically inside a semiconductor microcavity. Being a mixed photonic-condensed matter system, exciton-polaritons have been shown to give rise to a number of striking fundamental effects, including room temperature Bose-Einstein condensation, ultra-low threshold lasing, and room temperature superconductivity. Exciton-polaritons are also known for their spin sensitive physics, where they are considered candidates for spin optoelectronics. In previous work, spinor multistability has been demonstrated under coherent resonant excitation leading to switching waves suitable for polariton-based circuits. In the present project, we will lift the requirement of resonant excitation and study non-resonantly induced bistability. From the practical point of view this allows to construct polariton-based circuits without an external laser source, using instead on-chip electrical injection techniques. From the theoretical point of view, we will need to make use of the interplay between nonlinearity and parity-time symmetry breaking. Having achieved non-resonantly induced bistability, we will be able to study the propagation of dynamic switching waves and solitons. This is a purely theoretical research project. It will involve becoming familiar with the theory of exciton-polaritons and using a combination of numerical and analytical techniques to solve nonlinear differential equations (the nonlinear Schrodinger equation). Positive results will have significance for our experimental collaborators. The duration of the project is 2 months.
Prof Phan Anh Tuan phantuan@ntu.edu.sg	**Structural Basis for the Design of Anticancer Drugs Targeted to Quadruplex DNA and RNA** DNA G-quadruplexes in telomeres and oncogenic promoters and RNA G-quadruplexes in the 5' untranslated regions of oncogenes have been established as promising anticancer targets. Development of small molecules that interact with and stabilize G-quadruplexes is of great interest to many academic laboratories and pharmaceutical companies. We will use Nuclear Magnetic Resonance (NMR) spectroscopy and other biophysical techniques to characterize the principle for molecular recognition of G-quadruplexes. Our structural studies will provide a platform for anticancer drug design.

	DNA and RNA Oligonucleotides with Anticancer and Anti-HIV Activity Several guanine-rich oligonucleotides have been shown to exhibit anticancer and anti-HIV activity. We will characterize the structures of various such sequences. These structural studies can be correlated with activity tests to establish structure-activity relationships. This work will involve preparation of DNA and RNA samples and characterization of their structures by using Nuclear Magnetic Resonance (NMR) spectroscopy and other biophysical techniques.
Assoc Prof Massimo Pica Ciamarra massimo@ntu.edu.sg	**Computational Study of Systems of Self-Driven Particles** Cars on a highway, school of fishes, bacteria colonies, cell sheets, crowd, etc, are just a few examples of systems of many "particles" which have a motility. That is, the particles move exerting a force on their surroundings. Computational models and theoretical approaches developed to study physical systems have been shown to be useful to investigate the behavior of these systems. During the GRI, the student will be able to familiarize with related computational model and to investigate the behavior of such systems.
Assoc Prof Piramanayagam S.N. prem@ntu.edu.sg	**Magnetic Devices for Neuromorphic Computing** Human brains compute complicated information with a power of around 20W, whereas powerful computers require several kW for doing the same. In this sense, neuromorphic computing is a goal of many researchers and the computer architecture, laid out by Von Neumann might be phased out in future. In this project, the student will work on designing circuits for neuromorphic computing. He will also work on fabricating some magnetic materials and devices to perform as the elements of neuromorphic computing. The student is expected to have a good set of computing and experimental skills.
Assoc Prof Pinaki Sengupta psengupta@ntu.edu.sg	**Chiral Spin Liquids in Quantum Magnet** The past decade has seen as explosion in the investigation of topological phases of matter following the theoretical prediction, and subsequent experimental discovery of topological insulators. We shall use large scale computer simulations to study magnetic analogues of topological phases of matter in interacting quantum spin systems. In particular, we shall explore the emergence of chiral spin liquids in geometrically frustrated quantum magnets. These unique spin states do not develop any magnetic order down to absolute zero temperature. Yet, they are not completely

	disordered. Instead, they possess topological order known as chiral spin order. Such states have been predicted (and putatively observed) in many real quantum magnets. Our results will lead to a better insight into the character and origin of these novel states of matter.
	Magnon Dynamics in Frustrated Quantum Magnets Quantum spin systems have long served as a paradigm for studying many body physics. The direct control of collective excitations (magnons) via an external magnetic field enables us to explore vast regions of parameter space which is usually much more difficult in bosonic systems. We shall explore approximate analytic approaches for studying the properties of magnons (static and dynamic) of magnons in a family of frustrated quantum magnets. In particular, we shall explore the emergence of topological phases of magnons in the presence of artificial gauge fields – an area of intense activity in present day Condensed Matter Physics research.
	Topological order in Bose Einstein Condensates in quantum magnets Quantum magnets have long served as ideal testbeds to realise complex bosonic phases. Inspired by the recent developments in topological quantum states, we develop a theoretical framework to realise the magnonic analogue of such phases in microscopic models of interacting quantum spins in different lattice geometries. In particular we have already found that the Dzyaloshinskii-Moriya interaction (DMI), that is present in many quantum magnets, induces topological character to magnon bands. In this project we shall systematically investigate the effects of topological magnon bands on the character of Bose Einstein Condensate of magnons in S=1/2 Heisenberg spins on the honeycomb lattice. We shall use a combination of analytical calculations and numerical simulations to study this system.
Asst Prof Ranjan Singh ranjans@ntu.edu.sg	**Superconductor Photonics** In this project, the student would unravel the photonic/ plasmonic properties of superconducting waveguides which offers almost a lossless platform for transportation of highly confined terahertz light.
	Phase Change Materials Based Microelectromechanical Cantilevers for Tunable Photonics In this project, we propose to exploit the structural phase change of Vanadium dioxide/ GST based mechanical cantilevers that would have movable characteristics and thus

	would provide large contrast metamaterial resonances for device applications.
	Lithography-free Thin Film Nanophotonic Sensors Here, we plan to excite singular phase behaviour in metal-dielectric stacks and strong absorption of light with close to zero reflection feature. Such sharp phase singularities could provide extremely ultrasensitive large area sensing of small biomolecules.
Assoc Prof Cesare Soci csoci@ntu.edu.sg	**Flexible Perovskite Lasers** Despite the simplicity of the original perovskite crystal structure, this family of compounds shows an enormous variety of structural modifications and variants with crystal structures related to the mineral perovskite $CaTiO_3$. Hybrid perovskites show very interesting properties in photovoltaics and optoelectronics application, thanks to the possibility to chemically-tune their characteristics and to process films entirely from solution. Within this project, we will embed hybrid perovskites yielding amplified spontaneous emission within planar polymer microcavities with large area (several square centimetres), in order to produce flexible and bendable lasers which are tunable over the visible and NIR spectrum.
	Plasmonic Metamaterials for Cell Optostimulation The use of light as a stimulation tool has emerged in the last decade as a valid alternative to traditional techniques based on extracellular electrode arrays for both electrical cell stimulation and cell recording purposes. In this project we will investigate new abiotic/biotic interfaces based on metamaterial surfaces in contact with living cells. The metamaterial surface, properly coated by a photoactive polymer, will allow light management for cell stimulation and control of cell physiology, and diagnostic of the cleft (the thin gap between the cell membrane and the substrate). The main idea is to exploit the evanescent field generated by the metamaterial in the NIR spectral range to address the cleft locally and obtain unprecedented information on the coupling mechanism between the substrate and the cell.
	Topological Insulator Plasmonics Topological insulator crystals are extremely attractive materials for realizing low-loss and reconfigurable nanophotonic devices owing to the presence of topologically protected surface states that can be modulated optically, electrically, or by external magnetic fields. Isolating and

	utilizing the plasmonic properties of metallic surface states in topological insulators, however, have proven challenging, particularly at optical frequencies. In this project we will use a combination of broadband spectroscopic techniques to study the optical response induced by surface states in exfoliated, unstructured and nanostructured films of chalcogenide crystals.
Assoc Prof Sum Tze Chien tzechien@ntu.edu.sg	**Probing the Energetics and Carrier Dynamics in novel Organic-Inorganic Perovskite Solar Cells** Halide perovskite solar cells are the most promising 3^{rd} generation solar cells with efficiencies exceeding 22%. In this project, we investigate the charge dynamics and relaxation mechanisms in novel halide perovskite materials (beyond $CH_3NH_3PbI_3$ – e.g. Pb-free systems). The student will be tasked with sample preparation and characterization of the band structure using UV/X-ray Photoelectron Spectroscopy and the carrier dynamics using ultrafast optical spectroscopy.
	Mesoscopic Physics in Low-Dimensional Halide Perovskites Halide perovskites have demonstrated outstanding optoelectronic properties. In this project, we investigate the photophysical properties of perovskite nanostructures (e.g., quantum dots, nanoplatelets or nanowires) using ultrafast optical spectroscopy. The student will be tasked with sample preparation and characterization using optical spectroscopy techniques like transient photoluminescence and pump-probe spectroscopy.
Asst Prof WANG Xiao, Renshaw renshaw@ntu.edu.sg	**Studying Electrical Devices Consisting of Ultrathin Materials** In this project, students will fabricate transistors using ultrathin materials, such as atomically think complex oxide, and characterize their electrical properties. The gating will be realized by gating the ultrathin materials using ionic liquids or ferroelectric oxides to modulate the properties of carriers inside. Taking ionic-liquid gating as an example, the ionic liquid, which is a type of liquid hosts a certain concentration of mobile ions, is sandwiched between a gating electrical lead and the ultrathin materials in a conventional field effect transistor configuration. Conductivity of the devices is the easiest properties to modulate. Most likely, a metal-insulator transition will be expected by modulating the electron. However, conductivity is not the only properties, magnetic properties may also be modulated.
	Investigating Photoconductivity of Nanomaterials

	In this project, students will characterize the conductivity changes of nanomaterials under the light irradiation. When light is shined on a material, electrons inside are excited by the energy absorbed by the material. Consequently, the conductivity of the materials may be enhanced. This optical and electrical phenomenon is photoconductivity. The photoconductivity phenomenon has a great application potential in many areas. Here, we propose using a laser with different wavelengths in the visible range, in order to provide different energy for excitation. Our laboratory will provide suitable nanomaterials, such as low dimensional complex oxide $LaMnO_3$. These materials will serve as the photoconductive materials to form a simplified photodetector. The performance of the photodetector will also be measured.
Asst Prof Yong Ee Hou eehou@ntu.edu.sg	**The Statistical Mechanics of RNA** In this project, students will understand 1) elastic models of RNA, 2) topological classification of RNA, 3) RNA folding, and 4) connection to random matrix theory.
	Network Dynamics In this project, students will use network science to look at properties of different complex networks, from neural networks, football clubs, tennis, etc. We will model the complex works using nonlinear dynamic equation and look at their emergent properties.