List of IC@N Research Projects and Supervisors

School of Physical & Mathematical Sciences (SPMS)	
Name of Supervisor	**Research Project Description**
Ariel David Neufeld **ariel.neufeld@ntu.edu.sg**	**Deep Learning approach to solve portfolio optimization problems in financial markets** The goal of this project is to implement and analyze the effectiveness of different machine learning techniques such as for example deep neural networks (DNN) to optimize portfolios in real financial markets. The duration of the project is about 5 months.
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 centimeters), 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 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.
Chia Ee Min, Elbert elbertchia@ntu.edu.sg	**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.
	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.
David Paul Maxime Wilkowski david.wilkowski@ntu.edu.sg	**An optical lift for ultracold gas** The objective of this internship will be to design and realize an optical lift for an ultracold atomic gas. The gas is initially trapped into an optical standing wave, made of two counter propagating laser fields at the same optical frequency. Then, one or both optical frequencies are changed such that their difference is none zero. In this situation, the standing wave is moving at a velocity c/2 and could drag the atoms at the same speed. The change of the laser frequency must be smooth enough such that the atoms are following adiabatically the moving standing wave. The condition of this adiabatic following will be derived during the internship. Moreover, the total displacement of the atoms must be known at an interferometric level, i.e., better than the laser wavelength. To do so, a Michelson-like interferometer will be inserted into the setup to keep track of the relative phase variation of the counter propagating laser. https://ultracold.quantumlah.org/

	Dynamic of an Ultracold Atomic Wavepacket in Synthetic Gauge Potentials
Kiah Han Mao HMKiah@ntu.edu.sg	**Bee Identification for Multidraw Channels** Motivated by DNA-based applications, we study a generalization of the bee identification problem proposed by Tandon et al. (2019). Specifically, in this setup, we transmit all M codewords from a codebook over some channel and each codeword results in N noisy outputs. Our task then is to identify each codeword from the MN noisy outputs. In this project, we analyze algorithms related to this task.
	Bounds on Constrained Codes for DNA Data Storage The goal of the project is to study codes that satisfy certain runlength 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.
	Secure Multiplication using Regenerating Codes In 2016, Guruswami and Wootters showed that for the famous Reed-Solomon codes, a single node failure can be repaired with low bandwidth (arXiv:1509.04764v2). In 2021, Abspoel et al. applied this scheme to reduce the number of communication rounds in a multiparty secure computation - MPC ([ia.cr/2021/253)](ia.cr/2021/253). In this project, we study this MPC scheme in detail and look at possible extensions. personal.ntu.edu.sg/hmkiah
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, wij, 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.
Marco Battiato marco.battiato@ntu.edu.sg	**Numerical approach to multi timescale stiff differential problems** The full Boltzmann equation describes the motion of excited electrons in a material, subject to scatterings and electric fields. The equation is composed by two components: a transport operator and a scattering operator. The scattering operator is by far the most expensive to treat numerically, yet its dynamics evolves over shorter timescales compared to the transport part. Typical numerical approaches (for instance Runge-Kutta methods) must use the same time step for both operators. To avoid instability of the numerical solution caused by the transport part, a short timestep is required. That however leads to unnecessarily high numerical costs for the scattering part. The project requires the implementation in C++ of a newly developed numerical algorithm to address the problem above and its comparison with alternative approaches. The applicant is required to have some experience in programming in C or C++ (and be willing to learn more advanced programming techniques) and be mathematically inclined.

	Numerical Solution of the Boltzmann-Maxwell System for Ultrafast Out of Equilibrium Dynamics The full Boltzmann equation describes the motion of excited electrons in a material, subject to scatterings and electric fields. When coupled to the Maxwell's equations, it can describe a vast array of strongly out of equilibrium behaviors in solids. The project will focus on the implementation of a Poisson equation solver within the C++ software TORTOISE. It will be integrated with the solver for the Boltzmann equation. This will then be used to describe the propagation of excited electrons in carbon nanotubes and graphene. The applicant is required to have some experience in programming in C or C++ (and be willing to learn more advanced programming techniques) and be mathematically inclined.
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.
Peyrin Thomas thomas.peyrin@ntu.edu.sg	**Fast software implementations of new cryptographic primitives** The goal of this project is to provide optimized software implementations of two high-profile ciphers developed at NTU: Deoxys (winner of the CAESAR competition)[1] and Skinny (ISO/IEC standard 18033-7)[2]. Three platforms can be considered for the project (one or two can be selected, up to the student's choice): -high-end processors (like Intel processors from the past years), using SIMD or hardware cryptographic instructions such as AES-NI - midrange ARM processors, such as ARM-A7, using NEON instructions - constrained microcontrollers, such as ARM Cortex-M3 The candidate is expected to have some experience with optimized software programming. References: 1. https://sites.google.com/view/deoxyscipher 2. https://sites.google.com/site/skinnycipher/home

	Machine Learning for Attacking Gesture-Based Phone Unlocking Nowadays, a smartphone contains numerous instruments, such as the accelerometer, gyroscope and proximity sensors, or the classical microphone or camera. While these instruments are the basis of the smartphone functionalities, they represent a potential security vulnerability if an attacker can have access to the data produced by them when the user is entering his PIN code or some password. Indeed, much research have shown how one can recover such secret information with good accuracy using state-of-the-art machine learning and deep learning algorithms when having access to these side-channel data. For example, the orientation of the phone, the variation of light, the sound acquired when typing the password, are all slightly leaking some information about your secret data. This represents a serious threat as some applications may have access to these sensors and users sometimes do not necessarily understand the consequences of a too-permissive restriction policy. We have developed in our research team some preliminary models that allow inferring some of the digits of a PIN typed, thanks to the data leaked by these sensors. The goal of this project is to further improve our models and improve the PIN recovery phase thanks to the models' outputs. The candidate is expected to have some experience with machine learning.
	New model architectures for machine learning interpretability We have developed in NTU a very new neural network architecture so-called "Truth Table Deep Convolutional Neural Networks" or TT-DCNNs, which seems to be very promising for many real-life scenarios. They can be seen as compressed neural networks based on small lookup tables and they allow the transformation of the inference into a small system of SAT equations after learning. Thus, they are very well suited for example in constrained environments such as embedded systems, mobile phones, etc., and present other interesting properties for verifiability and interpretability. Preliminary studies show that TT-DCNNs are very simple NNs (easier to interpret and work with), while still providing a good accuracy. The goal of this project is to explore the rules-based extraction interpretability aspect of TT-DCNNs. The student will apply models based on the TT-DCNN architecture to small real-life datasets that are well suited for interpretability measures. We expect TT-DCNNs to perform better than state of the art on interpretability: https://papers.nips.cc/paper/2021/file/eaa32c96f620053cf442ad32258076b9-Paper.pdf

	Experience in machine learning is required.
Phan Anh Tuan phantuan@ntu.edu.sg	**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.
	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.
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. 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. 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 realize complex bosonic phases. Inspired by the recent developments in topological quantum states, we develop a theoretical framework to realize the magnonic analogue of such phases in microscopic models of interacting quantum spins in different lattice geometries. 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.
Rainer Helmut Dumke	**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.
Ranjan Singh ranjans@ntu.edu.sg	**Lithography-free Thin Film Nanophotonic Sensors** Here, we plan to excite singular phase behavior 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.
	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.

	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.
Roderick Wayland Bates Roderick@ntu.edu.sg	**Synthesis of Natural and Unnatural Products** The project will involve the synthesis of "small" natural products or unnatural molecules as part of ongoing projects in this lab. Examples include using the [2 + 2 + 2] cyclotrimerization of alkynes to form natural products, exploration of novel Diels-Alder reactivity, hydroformylation chemistry and cationic cyclisation. Where possible, successful synthesis of the target molecules will lead to biological studies.
S.N. Piramanayagam 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.
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.
Soo Han Sen hansen@ntu.edu.sg	**Photocatalytic Carbon-Carbon Bond Activation of Natural Products** First row transition metal complexes are cheap and abundant compounds that have applications such as catalysis for organic transformations and the photodegradation of plastics. The use of molecular compounds for the photocatalytic oxidation of plastics and non-food biomass is an underdeveloped area that is critical in Singapore since we can exploit this technology to manage our plastic waste and woody waste from neighboring countries. In this project,

	new vanadium-based molecular catalysts will be developed for light driven oxidation processes. Some recent references from our team are these: https://onlinelibrary.wiley.com/doi/full/10.1002/advs.201902020 http://pubs.rsc.org/en/content/articlehtml/2015/sc/c5sc02923f The tasks include: (1) synthesis of the new molecular vanadium catalysts; (2) preparation of suitable substrates in C-C activation reactions; (3) screening substrates for chemical reactivity. Students should be curious and adventurous. https://personal.ntu.edu.sg/hansen/webpage/public/main.htm
Sum Tze Chien **tzechien@ntu.edu.sg**	**Interfacial Band Alignment engineering of 2D-CsPbBr3 Perovskite solar cells using Ultrafast and Photoelectron spectroscopies** In this proposal, semiconductor heterostructures resulting into multiple-well quantum (MWQ) type structure will be fabricated and subsequent mechanism related to energy level alignment at the interface will be investigated. Here, organic semiconductors with varying energy levels will be interfaced along with 2D-halide perovskite layer for its application in optoelectronic devices. This project will explore the possibilities of interfacial dipoles, pinning or band bending, charge transfer or surface photovoltage effect using photoelectron spectroscopy. Furthermore state-of-the art measurement technique such as ultrafast surface second harmonic generation (SSHG) will be employed to investigate the interfacial mechanism with sandwiched 2D-haide perovskite and organic semiconductor layers. https://dr.ntu.edu.sg/cris/rp/rp00384 **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. https://dr.ntu.edu.sg/cris/rp/rp00384

	Probing the Carrier Multiplication in 2D-perovskite nanocrystals Ultrafast spectroscopy will be employed to investigate the carrier dynamics of 2D-perovskite nanocrystals. In particular, the focus will be to explore the possibility of Carrier multiplication or multiple exciton generation in these nanocrystals. Time-resolved measurements techniques dealing either with doped or undoped systems will also be considered. Typically, carrier multiplication or impact ionization is a process where valence band electron is promoted across a band gap due to its impact with other charge carrier. Therefore, final goal will be to measure the external quantum efficiency (EQE) where carrier multiplication is characterized with an increment of photon energy by band gap resulting in a new electron-hole pair thus showing an increase in EQE by 100%. https://dr.ntu.edu.sg/cris/rp/rp00384
	Probing the Energetics and Carrier Dynamics in novel Organic-Inorganic Perovskite Solar Cells Halide perovskite solar cells are the most promising 3rd 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 etc). 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. https://dr.ntu.edu.sg/cris/rp/rp00384
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.
Tan Howe Siang **howesiang@ntu.edu.sg**	**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 can 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
	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 processes 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 channeled to reaction centre in the photosystems.
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 optogenetic 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 signaling pathway to facilitate glucose uptake in living subjects. This project may need 6 months to complete.

Yong Ee Hou eehou@ntu.edu.sg	**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.
	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.
Zhang Baile blzhang@ntu.edu.sg	**Topological phases in classical wave systems** Classical waves, such as electromagnetic waves and sound waves, provide a very useful platform to explore exotic topological phases of materials. In this project, we will design a one-dimensional topological insulator using classical waves and study its unique properties.

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