S/N	N	Name Faculty of PI	Department of PI	Webpage of PI	Available periods for hosting a student:	Title of Research Project	Brief Description of Project	Prerequisite & expectation for the student
1	Kokil Jaic	dka Arts and Social Sciences	Communications and New Media	https://smolproject.com/	- Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	CACTUS (Computational Analysis for Communication on Text, User-generated content, and Social networks)	This project examines the quality of online discussions across TikTok, Instagram, and Facebook using computational social-science methods. The goal is to understand what makes conversations constructive, reciprocal, or toxic in contemporary social media environments. Drawing on the CACTUS framework (Computational Analysis for Communication on Text, Usergenerated content, and Social networks), the student will analyze public comment threads to identify patterns of justification, reciprocity, conflict, misinformation, and emotional tone. The project combines automated text analysis (e.g., large language models, linguistic features, conversation networks) with theoretical constructs from deliberation, digital civility, and online behavior research. Findings will contribute toward a conference-ready abstract or paper aimed at venues such as AAAI, ICWSM, CHI, or CSCW. The student will serve as a junior investigator on the project and will participate in all stages of the research cycle. Responsibilities include conducting a targeted review of literature on online discussion quality, cleaning and organizing social-media datasets, running computational tools for text analysis (with code provided), and generating descriptive and inferential results. The student will also assist in drafting a conference-style paper, including writing sections on theory, methods, and results.	Prior coursework in NLP or linguistics, and prior experience with accessing and finetuning LLMs, cleaning social-media data, along with familiarity with Python or R, is required. The project requires attention to detail, strong communication skills, and a willingness to learn advanced analytic and writing practices.
2	Kokil Jaic	dka Arts and Social Sciences	Communications and New Media	https://smolproject.com	- Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Al and Human Cognition: Trust, Reasoning, and Dependence in the Age of Chatbots	This project explores how everyday use of AI systems—such as ChatGPT or other chatbots—shapes human cognition, judgment, and trust. It examines broad questions about when people rely on AI, how they evaluate AI-generated information, and whether frequent AI assistance affects independent thinking, critical reasoning, or tolerance for complexity. Potential directions include studying overtrust in AI (algorithmic authority), cognitive offloading and dependence, AI-assisted political or moral judgment, or the influence of AI-generated summaries on how people interpret debates. The overall goal is to better understand how human decision-making and reasoning are changing in an AI-mediated information environment. The student will help refine a research question, conduct a literature review, generate or curate AI-based stimuli, and analyzed data from surveys, experiments, or online interactions. They will work with the PI to develop a coherent research design and prepare a conference-style paper.	Prior experience working with large language models (LLMs), social-media or behavioural data, and basic Python or R is required. Curiosity about cognition, reasoning, and Al's societal impact is essential.
3	Mengze l	Li Arts and Social Sciences	Geography	https://discovery.nus.edu.sg/29567- mengze-li	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	AI modelling of wetland methane emissions	Wetlands are the largest natural source of methane, accounting for ~30% of global methane emissions. This project will integrate multiple sources of data, including physical climate models, satellite remote sensing, and ground-based observations, and apply AI algorithms to predict regional and global wetland methane emissions. Students will learn AI in climate science, climate data processing, carbon accounting, and sustainability.	Students should have taken courses related to machine learning or data science.
4	Ta-Wei H	Huang Business	Marketing	https://sites.google.com/view/taweihuang/h ome	,	Customer Value Management through Causal Inference and Machine Learning	How can firms leverage data to causally understand and enhance customer value rather than merely predict it? This project applies ideas from causal inference and machine learning to advance the science of customer value management: developing methods to quantify and optimize the true incremental impact of marketing interventions. Students will work on algorithmic and empirical approaches that integrate experimentation, modeling, and simulation to uncover how different personalization strategies affect customer retention, engagement, and long-term value under realistic constraints such as privacy and adaptivity. Depending on their interests, students may focus on (i) how privacy-preserving mechanisms such as differential privacy or machine unlearning alter firms' ability to estimate causal effects, (ii) how survival bias distorts learning in adaptive personalization frameworks like bandits and reinforcement learning, or (iii) how experimental design principles can improve the learning efficiency of large language models in marketing contexts.	Applicants should have a strong interest in data-driven research and enjoy working at the intersection of marketing, statistics, and machine learning. Proficiency in Python or R is required, while prior exposure to causal inference, reinforcement learning, or LLM fine-tuning will be considered an advantage. Successful applicants are expected to demonstrate intellectual curiosity, rigor, and ability to conduct research tasks such as data processing, simulation design, and replication of existing algorithms.
5	Kai Chi Y	Yam Business	Management and Organisation	https://scholar.google.com/citations?user= 0Ao9ImMAAAAJ&hl=en&oi=ao	- Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	The psychology of technology	Today, robots and AI help generate creative content, man hotels, and even make hiring decisions in the workplace. But how humans feel about them remains complicated. In this project, I will synthesize my past and ongoing work in an attempt to answer one question: Do humans enjoy interacting with robots and AI? The answer is that it depends — not so much on the types of robots or AI in question, but rather on what contexts we interact with them in. We generally prefer new technologies that serve us rather than those that work alongside us and are especially aversive to them in sacred and moral domains, such as religion and medicine. A final study reveals a human-AI interaction paradox: Although machines can commit wrongs and people do punish them, they cannot meaningfully receive punishment—and so justice can never feel complete.	Basic statistical analyses: ANOVA; regression; SEM; CFA/EFA Good English writing/communication skills A bachelor's degree in psychology, economics, and business is a plus
6	Haifeng \	Yu Computing	Computer Science	https://www.comp.nus.edu.sg/~yuhf/	- Sem 1: 3 Aug - 2 Oct 2026 (2 months)	Research in Distributed Systems Security (including but not limited to blockchains) and Distributed Algorithms	I am looking for students to collaborate on research in the area of Distributed Systems Security (including but not limited to blockchains, byzantine fault-tolerance, and security issues in distributed learning) and Distributed Algorithms. See https://www.comp.nus.edu.sg/~yuhf/exampleproject-html/exampleproject.html for some example research projects of mine. I can identify specific research project suitable for you, based on your interests and strengths.	The student should be in Computer-Science-related major. Students majoring in Mathematics, but with good background/interest in CS, can also apply. The student should have strong interest in doing research, and strong algorithmic background. I particularly welcome internship applicants with achievements in Mathematics/Physics/Information Olympiad at the national or international level.
7	Jingxian \	Wang Computing	Computer Science	http://wangwireless.com	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Towards Efficient Edge Computing for Al and General-Purpose Processing	This project investigates efficient computing to support AI workloads and general-purpose processing at the edge devices. It explores the design of lightweight, resource-aware computing architectures suitable for edge devices (e.g., mobile devices, IoT, phones), emphasizing energy efficiency, fault tolerance, and communication constraints. The work combines systems engineering, edge computing principles, and AI optimization for extreme environments. This is a research-oriented project suited for students with strong motivation to explore emerging technologies.	For this project, you need to have solid programming skills, background in optimization, computer systems/architecture/networks, and machine learning, and be proficient in at least one programming language.
8	Rahul Jai	nin Computing	Computer Science	https://www.comp.nus.edu.sg/~rahul/	May to July 2026	Quantum Cryptography	In this research project we will explore some recent papers in quantum cryptography, identify some questions of interest and hopefully make some progress in solving them.	Having some background in quantum computing is a plus, however not necessary.
9	Rahul Jai	nin Computing	Computer Science	https://www.comp.nus.edu.sg/~rahul/	May to July 2026	Quantum Cryptography	The project involves literature survey of recent results in quantum cryptography, identification of interesting questions and hopefully make some progress in their solution.	Some knowledge of quantum computing is helpful, however not required.

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10 Tianbai Ma	Computing	Computer Science	https://www.comp.nus.edu.sg/~tbma/	May to July 2026	Design and Implementation of Inter-Domain Peering using Software-Defined Networking		The student will need to have a strong background in computer networking.
11 Zhi Xuan Tan	Computing	Computer Science	https://ztangent.github.io/	- Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Modeling Boundedly-Rational Agents for Assistive Decision Making	People routinely make mistakes when trying to achieve our goals due to insufficient planning, limited memory, and bounded reasoning. This project will focus on how to probabilistically model such behavior in humans, allowing AI assistants to better infer human goals and provide corrective assistance when a human user makes a mistake.	The student should be familiar with the basics of probability theory (conditioning, Bayes rule, chain rule, marginalization, expected values, etc.), and comfortable with programming. Programming experience with machine learning, data analysis (pandas, R), or scientific computing (scikit learn, numpy, Julia) libraries is strongly encouraged. Familiarity with Bayesian modeling and inference, computational cognitive science, and/or probabilistic programming is beneficial but not required.
12 Ke Wei Huang	Computing	DISA		- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months)	A Large-Scale Simulation Benchmark of Feature Selection, XAI Importance, and Dimension Reduction	This project's goal is to build a large-scale simulation benchmark to "crash test" these competing methods. We will create	 Strong Python skills (e.g., scikit-learn, pandas, shap). Solid grasp of machine learning and statistics fundamentals.
Dorothy Shun Wai Tang	Design and Engineering	Architecture	https://cde.nus.edu.sg/arch/staffs/dorothy-tang/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months)	Landscapes of Extraction and Infrastructure in Asia	impacts of the electric vehicle supply chain in Thailand and Indonesia. By tracing materials and labour from sites of nickel extraction, battery manufacturing districts, to large-scale electric vehicle factories, the project aims to critically examine the	The student should be enrolled in a professional program such as architecture, landscape architecture, or urban planning. However, students in social sciences with course work in environmental or urban studies would also be welcome. The student should have working knowledge of GIS mapping processes, and Thai or Indonesian language skills would be a plus!
Frederick Chando Kim	Design and Engineering	Architecture	cdcd.ch	May to July 2026	Made in Singapore	"Made in Singapore" is an initiative to redefine Singapore as a leader in a transformative circular economy. It focuses on integrating computational design and machine learning within Singapore's architectural landscape, creating a dynamic, data driven design approach. This research aims to leverage artificial intelligence (AI) to reimagine how circular materials, cultural narratives, climate resilience, and sustainable practices can create innovative architectural forms.	
15 Rudi Stouffs	Design and Engineering	Architecture		- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months)	Predictive Modelling of Thermal Vulnerability in Ageing Urban Populations	This project integrates multimodal wearable data, mapping, environmental simulations, and machine-learning methods to examine how older adults navigate and experience urban heat. Analysis includes classifying travel modes, identifying behavioural clusters, and mapping high-strain environments. Building on these insights, the project aims to develop personalised early-warning systems by using sequence-based predictive models to determine when individuals are likely to enter a state of thermal or physiological strain based on their recent biometric signals. By delivering a user-friendly early-warning interface, the project provides a scalable, translational tool that helps older adults anticipate risk and stay safe, while informing policymakers of emerging vulnerabilities to guide heat-mitigation strategies.	The student should have skills in machine learning/data analytics
16 Rudi Stouffs	Design and Engineering	Architecture		- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months)	Spatial AI & Graph Neural Networks for Retail Valuation	taxation, aiming to develop a foundation model for spatial asset intelligence. The goal is to automate the valuation of stratatitled retail units that lack clean rental histories by learning from floor plans, tenancy data, and footfall patterns. You will contribute to an end-to-end pipeline that goes from raw architectural drawings and rental ledgers to a secure decision-support tool deployed in a production-like cloud environment. The work directly supports Singapore's Smart-Nation ambitions by reducing manual workload, improving valuation consistency, and laying the groundwork for a smarter built	We are looking for a motivated intern who ideally has: •Background in Architectural Design or a related field (senior undergraduate or Master's student preferred). •Experience with data processing. •Basic understanding of machine learning concepts. •@Bonus, not mandatory) Experience or strong interest in computer vision and graph neural networks.

17	Rudi Stouffs	Design and Engineering	Architecture		- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months)	Large Mapping Language Models for GeoAl	We are developing the Large Mapping Language Model (LMLM), an AI reasoning engine that can answer natural-language planning questions (e.g. TOD suitability, school siting) with map-ready, regulation-aware outputs. The intern will help build and test multi-layer urban knowledge graphs, connect them to large language models, and run case studies using real geospatial data from Singapore. This role sits at the intersection of AI, GIS, and urban planning, and is ideal for students interested in GeoAI, smart cities, and data-driven urban decision-making.	 ©urrently enrolled in a Bachelor's or Master's programme in Computer Science, Data Science, GIS/Geography, Urban Planning, or a related field. Strong Python skills (data processing and basic scripting; e.g. pandas, NumPy). Eamiliarity with at least one of the following: Databases / graph data (e.g. Neo4j, networkx), or Deep learning / LLMs. ©omfortable working with technical documentation and reading research-style materials.
18	Yiyuan Yang	Design and Engineering	Biomedical Engineering	https://harlonyang.wixsite.com/neurolab	- Sem 1: 3 Aug - 2 Oct 2026 (2 months)	Intelligent Multimodal Electrochemical Sensors for Real-Time Analysis of Organoid Function in High-Throughput Assays	In this project, we aim to develop an intelligent multimodal electrochemical sensing system compatible with conventional cell culture well plates for simultaneous, continuous, real-time, and label-free in situ monitoring of multiple organoids. By integrating artificial intelligence (Al)-driven analytics, this platform will interpret dynamic biosignals to assess both the physiological state of individual organoids and the condition of their microenvironments. This enables real-time adjustments to the culture media tailored to the specific needs of each organoid, ensuring optimal growth conditions and enhancing overall viability. Implementing such a scalable and adaptive system is expected to revolutionize organoid-based research and medical applications, particularly in drug screening and personalized medicine for complex diseases as this system expects to remarkably expands the accessibility of organoids by significantly reducing the costs associated with cultivation.	No prerequisite is required. Previous wet lab experiment experiences and AI analysis skills are more preferred
19	Li Shan Eliza Fong	Design and Engineering	Biomedical Engineering	www.ttelab.com	' '	Use of biomaterials for live-preservation of patient-derived tumor explants	Patient-derived tumor explants are pieces of surgically resected specimens that can be cultured ex vivo. These models are advantageous as they potentially can preserve the entire tumor architecture and composition for drug evaluation. This project will look at the use of engineered biomaterials/microfluidics for the extended culture of tumor explants ex vivo for drug testing.	biomaterials engineering, cell culture
20	Sergey Kozlov	Design and Engineering	Chemical and Biomolecular Engineering	https://blog.nus.edu.sg/compnanocat/	Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Machine Learning and Quantum Chemistry for CO2 Electroreduction Catalysts	Electrochemical reduction of carbon dioxide (CO2RR) is a promising way to transform an abundant greenhouse gas and common industrial by-product into value-added chemicals using electricity. For industrial relevance, electrocatalysts must combine high activity and stability with selectivity toward desired products. Rational development of such (electro)catalysts requires understanding the reaction mechanisms at atomic and nanometer length scales, which is where computational modeling becomes essential. In this project, we will apply machine-learning interatomic potentials and quantum-chemical software to model CO2RR on advanced catalyst materials. Python scripting will be used to automate the setup of calculations, manage and analyze simulation data, and explore new reaction pathways and catalyst compositions. The ultimate goal is to gain mechanistic insight that can guide the design of non-conventional CO2RR catalysts and provide a realistic view of how electrocatalysts are currently developed in academia and in technology companies.	Background knowledge: 1.Solid understanding of physical chemistry (thermodynamics, kinetics, basic electrochemistry). 2.Prior exposure to density functional theory (DFT) in coursework or projects is strongly preferred. Technical skills: 1.Competent Python programming (data handling, simple scripting, basic plotting). 2.Eamiliarity with Linux command line environments. 3.Basic understanding of machine learning and statistics (regression, training/validation concepts). Expectations: 1.Motivation to learn modern computational tools for catalysis and materials modeling. 2.Willingness to work with existing codes and to write simple automation scripts. 3.Ability to document results carefully and to present findings in short written and oral reports in English.
21	Lakshminarayanan Samavedham	Design and Engineering	Chemical and Biomolecular Engineering		- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Symbolic Regression for Hybrid Modeling of Dynamical Systems	Hybrid modeling that combine mathematical equations emerging from known scientific laws and model elements based on machine learning using process data are being explored by engineers and scientists. In this project, the student will explore this area with symbolic regression as the tool of choice for transparent and explainable machine learning.	MATLAB or Python coding knowledge Engineering Mathematics (ordinary differential equations)
22	Rahul Prasanna Misra	Design and Engineering	Chemical and Biomolecular Engineering	https://www.misralabnus.com/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Computational Investigation of Nanomaterials for Membrane-Based Applications	Molecular simulations and multiscale modelling are vital tools for understanding how intermolecular interactions among water molecules and salt ions translate into macroscopic observables such as water permeability and ion selectivity—key indicators of performance in membrane separations. In this project, students will be introduced to fundamental concepts of statistical mechanics and will carry out computer simulations to investigate nanomaterials such as graphene nanocapillaries and carbon nanotubes used in membrane-based applications. Students will gain hands-on experience using open-source molecular dynamics software such as LAMMPS, along with visualization and post-processing tools including Visual Molecular Dynamics (VMD) and Python. From a mechanistic standpoint, the project will elucidate how confinement, interfacial interactions, and material properties govern fluid and ion transport at the nanoscale.	Applicants should have a strong background in undergraduate-level thermodynamics, physical chemistry, or transport phenomena, with an interest in molecular-scale modeling of fluids and materials. Prior exposure to programming (e.g., Python) and basic numerical methods is highly desirable, though not mandatory. Familiarity with statistical mechanics, molecular simulations, or materials science is an advantage, but motivated students will be provided with the necessary training.
23	Peichen Zhong	Design and Engineering	Department of Materials Science and Engineering	https://zhongpc.github.io/	Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Atomistic generative modeling of reaction pathway prediction in solid-state reactions	This project aims to develop a generative model to predict the reaction pathway in solid-state materials. Given the reactant and product materials, we aim to use the foundation potential and diffusion/flow-match model to map the reaction pathway and minimize the free energy landscape. It is a highly interdisciplinary research at the intersection of AI for Science and materials chemistry.	Requirement: (1) Strong foundation in applied math, statistical mechanics, and thermodynamics. Good skills in coding. (2) Basic knowledge of the diffusion or flow matching model. (3) Basic knowledge of computational materials science or chemistry. (4) Proficiency in at least one mainstream deep learning framework (PyTorch or JAX) and MLIP-based MD simulations. (5) Expertise in geometric deep learning is a big plus.

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24	Zeyu Deng	Design and Engineering	Department of Materials Science and Engineering	https://matsci.dev/	May to July 2026	Accelerating Ion Diffusion Studies in Rechargeable Batteries using Machine Learning and Kinetic Monte Carlo	tearning interatomic Potentials (MLIPS) with Kinetic Monte Carlo (KMC) simulations. ba sc The primary workflow involves utilizing MACE (Multi-ACE), a state-of-the-art equivariant machine learning potential, to accurately and efficiently compute activation energy parriers for ion migration. These computed parriers will subsequently	essential: Proficiency in Python programming and a strong ackground in atomistic simulation/computational materials cience. esirable: Familiarity with machine learning frameworks, articularly PyTorch.
25	Jinying Xu	Design and Engineering	Department of the Built Environment	https://cognitionx-lab.github.io/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Nexus of carbon reporting and financial reporting: Gaps and future of synchronisation	Data Science, this project aims to: 1. Man the Gan: Analyze the financial statements of global carbon-intensive firms	enior Undergraduate or Master's students in Quantity Surveying, roject Management, Real Estate, Accounting, Finance, Economics, Data Science.
26	Mehul Motani	Design and Engineering	Electrical and Computer Engineering	https://cde.nus.edu.sg/ece/staff/mehul- motani/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Generative AI for Healthcare Applications	data, the chatbot provides patients and providers with personalized, accurate guidance on symptoms, treatments, and ha	cudents should be curious and ready to innovate and get their ands dirty. Prior experience with programming with AI and, in articular, generative AI will be very useful.
27	Mihindukulasooriya Sheral Crescent Tissera	Design and Engineering	Electrical and Computer Engineering	https://sheraltissera.com/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Technologies for Next Generation Autonomous Satellites	capabilities are increasingly integrated to support real-time decision-making, enabling satellites to operate semi- lindependently or cooperatively as part of a larger autonomous network.	am looking for motivated students in Electronic Engineering, echanical Engineering, Computer Engineering/Science, Physics nd Mathematics to join my team in advancing research on next- eneration autonomous satellite systems.
28	Irmandy Wicaksono	Design and Engineering	Industrial Design	https://www.irmandyw.com		XSuit: Wearable Technologies for Physiological and Physical Activity Immersion	With a unified and scalable sensing interface, the suit enables detailed mapping of full-body movements and subtle physiological activities. These signals are processed to construct responsive and personalized avatars that integrate exteroceptive, proprioceptive, and interoceptive cues. The outcome enhances immersion, improves interaction fidelity, and strengthens social presence, while enabling emerging applications in remote healthcare, rehabilitation, and XR-based	oplicants should be creative, self-motivated, and comfortable orking independently. Students with interest or experience in one more of the following: wearable/garment design, printed circuit esign, sensor networks, embedded hardware systems, machine arning, biomechanics, or AR/VR/XR development (i.e. Unity) are rongly encouraged to apply.
29	Wang Chi Cheung	Design and Engineering	Industrial Systems Engineering and Management	https://cde.nus.edu.sg/isem/staff/cheung- wang-chi/	Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Length optimization in conformal prediction	prediction is a machine learning framework that provides reliable measures of uncertainty alongside model predictions by generating prediction sets or intervals that are guaranteed to contain the true outcome with a chosen probability, such as 90% or 95%. Instead of outputting a single point prediction, it produces a range (for regression) or a set of possible labels (for classification) that reflects the model's confidence. A gentle introduction to conformal prediction can be found in this introductory article: https://arxiv.org/abs/2107.07511. In this project, we will explore the minimization of prediction set sizes for conformal prediction. Given a set of training data, we aim to produce a prediction set that approximately achieves the minimum in terms of its size. In this journey, we will explore ways to overcome the statistical challenge of generating such a set with finite-sample guarantees, and to overcome the computational challenge with solving certain integer programs. While the PI will take the lead in the theoretical development, the internee is expected to conduct numerical experiments to validate the theoretical findings.	cudents should have competent technical and coding knowledge in machine learning. In terms of technical knowledge, students hould be comfortable with basic notions in machine learning, at last to the point of understanding the introductory article in the roject description. Such an understanding will be crucial for the ternee to understand the assigned computational tasks. The core equirement is in coding knowledge. The student must be proficient Python, particularly with training machine learning algorithms mostly on classification/regression, but need to be able to handle real life data). The student must be able to code different conformal rediction algorithms in Python, and be able to write a Python ackage professionally.
30	Napat Rujeerapaiboon	Design and Engineering	Industrial Systems Engineering and Management	https://sites.google.com/view/napatrujeera paiboon/home	May to July 2026	Reliable Decision Making via Robust Data- Driven Optimization	when data or predictive models are inaccurate. The goal is to develop and test optimization frameworks that explicitly account for uncertainty in data and predictions, ensuring more reliable decisions, to be demonstrated on an application of	asic linear algebra is required for participation in this project. Reperience with scientific coding (e.g., MATLAB or Python) is helpful at not required, and students who are new to coding will receive uidance as needed.

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31 Mario Lanza Martinez	Design and Engineering	Materials Science and Engineering	lanzalab.org	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months) memristors	Help to co-design spiking neural networks for the realization of low-energy artificial intelligence applications. The fundamental building block to work with is explained in this article: https://www.nature.com/articles/s41586-025-08742-4 The main idea is to make circuits with associations of this device, first through modelling and later it will be fabricated in 130 nm node technology foundry. While that may happen after the internship ends, the student will participate in the design and in the measurement of other microchips that we already have. He/she will participate in future publications based on his/her design.	Verilog, DSA, PyTorch. Programming in FPGA using SystemVerilog to run 32-bit programs, integrating instruction execution, SRAM
32 Mario Lanza Martinez	Design and Engineering	Materials Science and Engineering	lanzalab.org	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months) synaptic random access memories (NSRAM)	opportunity of learning now we do that and contribute with some customized analyses and examples.	The student must have courses some coruses in the field of computer science Programming Skills: C++, Python, RISC-V, Verilog
Silvija Gradecak- Garaj	Design and Engineering	Materials Science and Engineering	silvija.org	- May to July 2026 - Sem 1: 3 Aug - 3 Nov 2026 (3 months) Nanostructured materials for the next generation microelectronics, photonics, and optoelectronics	This project focuses on the synthesis, characterisation, and applications of nanostructured materials for the next generation microelectronics, photonics, and optoelectronics. Due to their low dimensionality, nanostructured materials exhibit properties that are distinct from their bulk counterparts. At the same time, the role of defects and interfaces becomes more critical. This project aims to answer how these properties can be controlled through controlled synthesis methods.	Students with a background in materials science, physics, electrical
34 Yan Jing	Design and Engineering	Materials Science and Engineering	https://research.nus.edu.sg/thejinggroup/	Sem 1: 3 Aug - 2 Oct 2026 (2 months) Electrochemical carbon capture	Removing CO2 from the atmosphere for the hard-to-abate industries is indispensable to limit global warming to 1.5–2 °C above pre-industrial levels. My group is interested in utilizing electro-active materials to selectively capture CO2 from the air and release pure CO2 for further sequestration or CO2 reduction.	Students with organic chemistry and electrochemistry background are preferred.
35 Yi Wan	Design and Engineering	Materials Science and Engineering	https://research.nus.edu.sg/wan-yi/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months) Characterization of 2D Materials	This project introduces students to the growth of two-dimensional (2D) semiconductors using chemical vapor deposition (CVD) and the use of automation and machine learning to optimize synthesis. Students will carry out controlled CVD experiments, characterize the resulting materials using optical microscopy and Raman spectroscopy, and build a small dataset linking growth conditions to material quality. Simple machine-learning models will then be applied to identify trends and propose improved growth parameters. The project provides hands-on experience in both experimental 2D materials	Students should have a basic background in materials science, physics, chemistry, or a related engineering discipline. Prior experience in Python programming or data analysis is helpful. The student is expected to be motivated, responsible in following lab safety procedures, and willing to learn both experimental techniques (CVD growth, microscopy, Raman characterization) and basic machine-learning tools. Active engagement, good documentation practices, and consistent weekly updates are expected throughout the project.
Adrien Sartoretti Guillaume	Design and Engineering	Mechanical Engineering	https://marmotlab.org/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months) Research Football	This project aims to investigate the use of a hierarchical planner for multi-agent Google Research Football. The hierarchical planner consists of a centralized high-level strategy planner (Coach) running at lower frequency that will choose a strategy to execute at current moment and a decentralized low-level control planner (Player) running at a higher frequency that is responsible for generating actions for individual agents conditioned on the current strategy and their local observations. The granularity of strategies could be as simple as offence / defense with different formations (4-4-2, 4-2-4, etc.) to actual plays like "Triangular play" or "Zone defense". Since there are countless known tactics in football, we could leverage this knowledge to define reward functions (or use LLM generated reward functions) per strategy and train the low-level controller using the Centralized Training Decentralised Execution (CTDE) paradigm for Multi-Agent Reinforcement Learning (MARL). Lastly, we will investigate different methods (LLM or RL) to chain and dynamically switch these predefined set of strategies to result in a strong performance on the Google Football benchmark.	Comfortable with Python, Linux, PyTorch, Reinforcement Learning, Deep Learning Good to have some knowledge of MARL, LLM/VLM, Football!
Adrien Sartoretti Guillaume	Design and Engineering	Mechanical Engineering	https://marmotlab.org/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months) using Human Videos	Humanoid robots can now learn complex skills by imitating human demonstrations captured from everyday video. In this project, we will build an end-to-end pipeline that converts raw human videos into robot-executable motions using existing components such as video-to-SMPL pose estimation and DeepMimic-style reinforcement learning. While prior work has shown strong results for locomotion and single-agent motions, this project extends the pipeline to interactive tasks—such as moving objects, sitting on a chair, picking and placing, throwing, or even dynamic skills like skateboarding or jumping onto platforms. The workflow will be: Video → SMPL / 3D human motion using state-of-the-art pose reconstruction models. Motion retargeting from SMPL to the target humanoid robot morphology. DeepMimic-based imitation learning in simulation to acquire the skill. Interactive task extensions, incorporating object manipulation or environment contact. Sim2Sim generalization tests (e.g., transferring policies across simulators such as Isaac Gym ↔ MuJoCo). If time permits: deployment on real humanoid hardware to validate sim2real feasibility.	GitHub, Basic Python, (Optional) Reinforcement learning knowledge, (Optional) Experience with simulators (Isaac Lab / MuJoCo / MJlab)

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38 Yu Jun Tan	Design and Engineering	Mechanical Engineering (ME); Advanced Robotics Centre (ARC)	https://yujuntan.com/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months) Cellulose from Kombucha SCOBY	Idoning holymer hiending or salt incornoration while maintaining its mechanical strength and sustainability. The goal is to	1. Feels strongly for a more sustainable future 2. Prior undergraduate research experience 3. Strong interest in flexible electronics and material science
39 Yu Jun Tan	Design and Engineering	Mechanical Engineering (ME); Advanced Robotics Centre (ARC)	https://yujuntan.com/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Tone direction. Students will experiment with techniques such as controlled stretching, extrusion, or templated growth to	2. Prior undergraduate research experience 3. Strong interest in manufacturing and material science
40 Ahmet Avsar	Design and Engineering	MSE	https://sites.google.com/site/aavsar	- May to July 2026 - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	This project focuses on reconfigurable tunneling field-effect transistors (TFETs) using a low band gap 2D semiconductor. By stacking n-type and doped p-type layers, the student will fabricate and study TFET behavior. He will prepare the heterostructures and perform basic electrical measurements. Additionally, he will understand TFET operation principles.	Introduction to solid state physics & semiconductor modules & familarity with 2D materials device fabrication process.
41 Changsheng Wu	Design and Engineering	MSE	https://cde.nus.edu.sg/mse/wugroup	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months) Privacy-Preserving Speech Reconstruction via Wearable Mechano-Acoustic Sensing for Assistive Communication	Imechano-acoustic approach is inherently private as it is insensitive to ambient conversations, providing a secure and	Programming skills related to digital signal processing and machine learning are highly preferred.
42 Di Zhu	Design and Engineering	MSE	https://www.dizhulab.org/	May to July 2026 Integrated quantum light source		Students with backgrounds in optics, electronics, or programming are highly preferred.
43 Julius Fredens	Medicine	Biochemistry	https://genomeeng.org	- Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months) Adaptation of a bacteriophage to new hosts	lunderstanding of phage-host dynamics and evolutionary adaptability, with broad implications for developing diverse phage	Understanding of molecular biology. Experience cloning plasmids is beneficial
44 Qin En Cheryl Lee	Medicine	Department of Microbiology and Immunology		- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	response and how the identified allele variants affect the genes' ability to carry out their functions. We will utilize CRISPR-	Student should have basic understanding of the principles behind different molecular techniques like PCR, western blot, RT-qPCR and flow cytometry.
45 Ai Peng Tan	Medicine	Diagnostic Radiology		- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months) mental health disorders	and epigenetic mechanisms remains unclear. Research shows that ELS alters stress physiology and systemic inflammation, which in turn influence brain maturation. Epigenetic mechanisms such as DNA methylation (DNAm) mediate environmental	lindependently, student with

46	Le Thi Nguyet Minh	Medicine	Pharmacology	https://lelabnus.wordpress.com/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Development of cosmetic products based on exosomes	We will develop a line of topical skincare and haircare products powered by exosome-enriched extracellular vesicles (EVs) that deliver bioactive cargos to dermal cells and hair cells to improve barrier function, and reduce inflammation. Students will learn how to isolate, engineer EVs, and conduct basic in vitro tests.	Students should have some background in cell biology or dermatology, and interest in further collaboration with our group.
47	Antonia Alberto Fraser Monteiro	Science	Biological Sciences	https://lepdata.org/monteiro/	- Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	How do butterfly caterpillars learn new plant odors and pass these preferences to their offspring?	This project will test whether butterfly larvae learn to prefer different food odors by eating them and also whether they learn to prefer them or to avoid them, and to impart those preferences to the next generation. The project involves plant odor manipulation (by rubbing a new odor onto leaves), butterfly Y-maze testing, butterfly breeding, data collection and analysis.	biological statistics is a required course.
48	Jun Ying Lim	Science	Biological Sciences	https://peeb-lab-nus.com/	Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Biogeography and trait evolution in Dipterocarpaceae	have come to dominate lowland forests of the region is not well understood. Student will integrate species occurrence,	Student should preferably have some background in evolutionary biology, biogeography and/or phylogenetics. Student should be proficient in R or similar programming languages.
49	Jie Wu	Science	Chemistry	https://www.wujiegroupnus.com/	- May to July 2026 - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Close Loop Drug Discovery through Automated Synthesis of Molecules	In this project, we aim to apply the latest advanced automated synthesis technology to speed up design-make-test-analysis cycle for hit-to-lead optimization.	The student should have taken courses in organic synthesis. Preference will be given to student who knows how to do multistep organic synthesis.
50	Jie Wu	Science	Chemistry	https://www.wujiegroupnus.com/	- May to July 2026 - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	End-to-end synthesis of drug molecules	In this project, the student will help to develop end-to-end synthesis platform for active pharmaceutical ingredients. 100g/cycle production will be targeted.	The student needs to know how to conduct research in organic synthesis.
51	Pengfei Ou	Science	Chemistry	https://www.pengfeiou.com/	- Sem 1: 3 Aug - 2 Oct 2026 (2 months)	AI-Enabled Design of Next Generation Membranes for Energy-Efficient Seawater Desalination		Foundational knowledge of: (1) Thermodynamics and basic statistical mechanics; (2) Fluid transport and mass transfer; (3) Basic concepts of membrane processes or separations (helpful but can be learned on the project). Programming skills: (1) Comfortable with Python (or willing to ramp up quickly); (2) Experience with at least one of: NumPy/Pandas, basic ML libraries (e.g., scikit-learn, PyTorch/TensorFlow), or scientific computing tools; (3) Familiarity with Linux/command line and basic scripting is an advantage.
52	Frank Christian Stephan	Science	Mathematics	http://www.comp.nus.edu.sg/~fstephan/	- Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)		The above are three possible areas, you might choose just one of them. Automata theory studies the languages of the Chomsky hierarchy with respect to various formal aspects. A manuscript is available, http://www.comp.nus.edu.sg/~fstephan/fullautomatatheory-pstopdf.pdf Please read in it to get an idea on possible research questions. Recursion theory studies computation from a very abstract perspective not taking time bounds into account. There is more a principle question what an algorithm can do and whether algorithms can solve a problem A when they have access to a problem B, that is, reduce A to B, the nature of reductions has to be formalised, as the answer whether this can be done, depends on A, B and the framework for the reduction. See https://www.comp.nus.edu.sg/~fstephan/recursiontheory-pstopdf.pdf for more information. Exponential time algorithms are algorithms to study possibilities to solve certain NP-hard or otherwise complicated problems with algorithms are algorithms to study possibilities to solve certain NP-hard or otherwise complicated problems with algorithms taking exponential time. By the exponential time hypothesis, the might for many NP-hard problems not be better algorithms to one hand, for certain problems like 3SAT and Count2SAT, though there are NP-hard, one can have algorithms in O(c^n) where n is the number of variables and c a suitable constant strictly between 1 and 2. Finding algorithms with low such constants is part of the business in Exponential Time Algorithms; another is to compare the hardness of problems by translating algorithms from one problem to the other, for example, given an algorithm for Count2SAT (counting the number of 2SAT solutions), can it be translated into an algorithms (which exists if and only if ETH is true), can one derive a lower bound for the other constant in some way?	The student should read about the selected option from above, either by studying lecture notes or research papers and then the student can join the research group to see whether possible joint work can be developped. If participating regularly in meeting and contributing to the work, the student can be a coauthor of the resulting paper (provided that some results by the joint discussions).
53	Hung Minh Tan Nguyen	Science	Mathematics	https://tanmnguyen89.github.io/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Scientific Large Language Models	This project develops a principled, inference-time control method for large language models (LLMs) that keeps models helpful on scientific tasks while robustly enforcing safety and compliance. The core idea is Angular Steering-a rotation of hidden activations in a 2D plane aligned to a learned "behavior" direction (e.g., refusal or compliance)-which yields smooth, fine-grained behavior control without retraining or loss of general capability. Building on our prior finding that high-dimensional linear structure in LLM representations enables "activation engineering" jailbreaking and that projecting into lower-dimensional subspaces can preserve alignment while reducing exploitability, we will couple Angular Steering with lightweight representation compression to harden safety during agentic use. The application domain is scientific LLMs and agentic Al for science, where domain-specific models, multimodality, and autonomous research agents are rapidly maturing but still face reliability and evaluation challenges.	Linear Algebra, Machine Learning, Python Coding

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54 Louxin Zhang	Science	Mathematics	https://blog.nus.edu.sg/louxinzhang/	May to July 2026	Deep learning approaches for inferring phylogeny from CRISP-based single-cell lineage tracing	missing or noisy observations.	Students are expected to have a solid foundation in machine learning and strong programming skills. They should also be familiar with the processing and analysis of single-cell sequencing data.
Subhroshekhar 55 Ghosh	Science	Mathematics	https://subhro-ghosh.github.io/	May to July 2026	Clustering through the lens of statistical physics	We propose to leverage ideas and techniques from statistical physics to provide improved algorithms for clustering, especially in the setting of unbalanced clusters, substantiated with robust theoretical guarantees. This will, in particular,	The student should have taken courses in probability and real analysis. Programming skills in Python (or R or C++) would be helpful. Self study or guided reading on mathematical aspects of machine learning is a plus. Successful math olympiad experience at more formative levels would also be a positive factor.
56 Rachel Ee Pui Lai	Science	Pharmacy and Pharmaceutical Sciences	https://www.ee-research-group.com/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months)	Exploring Peptide Nanonets as a Novel Strategy to Trap and Kill Fungal Pathogens	Peptide nanofibers represent a promising strategy for controlling pathogenic infections and offer new avenues to tackle antimicrobial resistance. In our previous work, we developed a library of peptides that self-assemble into unique nanonet structures capable of trapping and killing bacteria. However, the potential of these nanonets to target fungal pathogens remains largely unexplored in both the field and in our own studies. This project aims to investigate whether our peptide nanonets can self-assemble on fungal surfaces, disrupt fungal growth, and elucidate the underlying mechanisms behind their antifungal activity. This work will contribute to understanding a novel mode of action and may open new directions in antifungal therapeutic design. Students joining this project will gain hands-on experience in microbiology techniques, peptide characterization, scanning electron microscopy, and key molecular biology assays. This project is ideal for students interested in antimicrobial research, biomaterials, or translational biomedical science.	1) Some lab experience (pipetting, sterile work) is helpful. 2) Willingness to learn new experimental techniques. 3) Able to follow safety procedures and keep good lab notes. 4) Motivated, careful, and able to work independently.
57 Alexey Berdyugin	Science	Physics	https://qtlab.pro/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Free standing moiré superlattices. Towards novel high temperature superconductors	project will also involve further detailed mechanical and electrical characterization of these devices. Such suspended structures are expected to host strongly correlated electronic states and may exhibit superconductivity with a critical	The student should have a solid background in condensed matter physics and at least a basic understanding of two-dimensional materials. Preferred duration of the internship is 3 months.
58 Slaven Garaj	Science	Physics	garaj-lab.org	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months)	Single-biomolecule nanopore sensors:		Student should be open to learn new skills and instrumentation, but no specific requirements on prior experience.
59 Yvonne Yuan Gao	Science	Physics	www.quantumcrew.org	- Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	understanding light-matter interaction using	This short, exploratory project investigates how strong, time-dependent electromagnetic fields drive non-linear responses in quantum systems, leading to phenomena beyond simple perturbative regimes. The project aims to develop potential testbeds to probe the different interaction regimes, from weak to strong, and ultra strong coupling and identify qualitative changes in the dynamics.	strong foundation in physics and/or engineering training, good communication skills in English, programming skills in python, some prior experience with hands-on work either in research or other context
60 Zhou Doudou	Science	Statistics and Data Science	e https://doudouzhou.github.io/	May to July 2026	II earning Ontimal Oliestioning Policies for Al	This project studies how AI customer service agents (e.g., LLM-based chatbots) should decide which questions to ask, in what order, and when to stop asking and make a prediction or recommendation. Real-world customer interactions often involve incomplete information because the agent only observes answers to questions it chooses to ask. This project develops statistical and machine learning methods to learn optimal questioning strategies from historical multi-turn dialogue data. The goal is to design AI agents that acquire information efficiently, improve prediction accuracy, and reduce customer effort.	Completed courses in probability, statistics, and machine learning Strong Python programming skills (e.g., NumPy, PyTorch, data processing) Experience with NLP or large-language-model APIs is a plus Familiarity with reinforcement learning is helpful but not required Good communication skills and ability to read research papers
61 Mandar Anil Chitre	Design and Engineering	ECE	https://arl.nus.edu.sg	Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Icompression for underwater communications	Ito compress the data into lesser bytes than the original data stream. In this project, the student will explore state of art	Strong programming background. Good understanding of machine learning with experience in working with machine learning models.

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62 Li Xiaoyan	Science	Chemistry	https://www.xiaoyanli-mace.com/	- Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Physics-Guided ML for Cu–Support Catalysts in CO₂RR	The catalytic activity and selectivity of Cu-based systems for electrochemical CO reduction (CORR) are strongly governed by CO adsorption energetics, which are further modulated by nanoparticle size, morphology, and substrate interactions. This project aims to develop a structure-based, physics-informed machine learning (ML) framework to predict CO adsorption energies on Cu nanoparticles supported on diverse oxide, carbon, and metal substrates. We will first perform density functional theory (DFT) calculations to generate a high-quality dataset of adsorption energetics across varied Cu cluster sizes, facets, and supports under realistic electrochemical conditions. The resulting data will train graph neural network (GNN) models capable of learning adsorption energies directly from atomic structures—without relying on electronic descriptors such as d-band centers or charge densities—thereby ensuring broader generalizability. The GNN will encode atomic connectivity, composition, and interfacial geometry to capture effects of charge transfer, strain, and metal–support coupling. Rapid screening of substrate—Cu combinations will identify systems that optimally tune the CO binding strength for enhanced CO-to-C2* conversion, while explainable Al tools, such as SHAP analysis, will reveal the dominant structural features controlling CO adsorption. This physics-guided Al–DFT workflow will accelerate the rational design of stable, high-performance Cu-based electrocatalysts for efficient CO2RR.	Students have the backgrounds of chemistry, mateials, physics, or even computer science
63 Denis Bandurin	Design and Engineering	MSE	cmxlab.org	- Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Twistronics in the quantum flatland	properties. The customizability of stacking such 2D crystals offers yet another intriguing knob to fine-tune the properties of such heterostructures by twisting the relative orientation of their constituents' crystallographic axes. Twist-controlled systems exhibit a plethora of eminent quantum effects ranging from many-body correlated states and unconventional superconductivity to orbital magnetism and states with peculiar fragile topology and keep surprising scientists with brand	The student should have basic knowledge of solid-state/condensed matter physics and semiconductor devices/electronics (or similar courses). They should be comfortable working in a lab, handling samples carefully, taking measurements, and keeping clear notes. Basic programming for data plotting and analysis (Python or MATLAB) is strongly preferred. Most advanced skills (like cleanroom work, low-noise measurements, or cryogenics) are a bonus but not required—we can teach them. The key expectation is a careful, patient, hands-on attitude and regular progress updates.
64 Li Xiaoyan	Science	Chemistry	https://www.xiaoyanli-mace.com/	- May to July 2026 - Sem 1: 3 Aug - 2 Oct 2026 (2 months) - Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Physics-Guided ML for Cu–Support Catalysts in CO₂RR	The catalytic activity and selectivity of Cu-based systems for electrochemical CO reduction (CORR) are strongly governed by CO adsorption energetics, which are further modulated by nanoparticle size, morphology, and substrate interactions. This project aims to develop a structure-based, physics-informed machine learning (ML) framework to predict CO adsorption energies on Cu nanoparticles supported on diverse oxide, carbon, and metal substrates. We will first perform density functional theory (DFT) calculations to generate a high-quality dataset of adsorption energetics across varied Cu cluster sizes, facets, and supports under realistic electrochemical conditions. The resulting data will train graph neural network (GNN) models capable of learning adsorption energies directly from atomic structures—without relying on electronic descriptors such as d-band centers or charge densities—thereby ensuring broader generalizability. The GNN will encode atomic connectivity, composition, and interfacial geometry to capture effects of charge transfer, strain, and metal–support coupling. Rapid screening of substrate—Cu combinations will identify systems that optimally tune the CO binding strength for enhanced CO-to-C2+ conversion, while explainable AI tools, such as SHAP analysis, will reveal the dominant structural features controlling CO adsorption. This physics-guided AI–DFT workflow will accelerate the rational design of stable, high-performance Cu-based electrocatalysts for efficient CO2RR.	Students should have the background in chemistry, materials, physics, or even computer science
65 Pengfei Ou	Science	Chemistry	https://www.pengfeiou.com/	May to July 2026 Sem 1: 3 Aug - 2 Oct 2026 (2 months) Sem 1: 3 Aug - 3 Nov 2026 (3 months)	Surface Roughness Enhanced Synthesis of Multicarbon Products in Electrochemical CO2/CO Reduction	The electrochemical carbon dioxide/monoxide reduction reaction (CO2/CORR) offers a sustainable approach to producing multicarbon (C2+) products, including valuable fuels and chemicals. However, achieving high selectivity for ethanol remains a significant challenge because competing pathways favor the production of products such as ethylene. This project proposes a new strategy to enhance ethanol selectivity by optimizing the H2/CO ratio in the inlet gas. Preliminary grand-canonical DFT and global minimization studies reveal that varying the H2 partial pressure alters the hydrogen chemical potential, thereby affecting the surface coverage of *OH and *CO. These variations influence the degree of surface roughness on copper, which is critical for modulating product selectivity. Using DFT calculations, we aim to investigate how surface roughness modulates the selectivity between ethanol and ethylene. More specifically, we will study how the geometric and electronic structures for different Cu*OH*CO ensemble structures from the global minimum search on the energetics of key elementary steps in C2+ production, including 2*CO-to-*OCCO and *CHCOH-to-*CHCHOH, etc.	Prior experience or strong interest in Density Functional Theory (DFT) calculations Familiarity with: Electronic structure methods Periodic boundary conditions and slab models Adsorption energy and reaction pathway calculations Experience with at least one computational package is preferred, such as: VASP, Quantum ESPRESSO, GPAW, CP2K, or similar Basic understanding of: Grand canonical DFT concepts Global optimization or structure-search methods (e.g., basin hopping, genetic algorithms) are beneficial but not mandatory

Andrew Barnabas Wong	I Design and Engineering I	https://cde.nus.edu.sg/mse/staff/wong- indrew-barnabas/	May to July 2026 Sem 1: 3 Aug - 2 Oct 2026 (2 months) Sem 1: 3 Aug - 3 Nov 2026 (3 months)	·	Iwnich materials would be effective for this transformation. In this work, students will synthesize, modify, and screen related	While experience with organic chemical synthesis, polymers, and/or electrochemistry would be helpful, they are not required.
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