Research project and supervisory team

Supervisory Team	Dr. Ibrahim Khan (PhD, Postdoc) (UNNC)
Short introduction & description of research project	Carbon Neutrality and energy generation are the key research paradigms in modern research. One of the strategies is to replace the existing fossil fuel technologies with green alternatives. Photoelectrochemical water splitting (PEC-WS) technology offers a great choice to produce green or yellow hydrogen (H2) energy from water, which is considered a zero-emission energy with great fuel value and hence contributes to carbon neutrality. Many state-of-the-art materials such as TiO2, WO3, ZnO, BiVO4, Fe2O3, CuO/Cu2O, etc. have been exploited for a long time without any industrial success. Recently, single-crystal Si-based architectures have demonstrated outstanding performance in PEC applications. However, their high cost and poor yield due to metastable nature and crystal faults pose challenges. Moreover, their experimental quantum efficiencies fall short of expectations. Group III-V semiconductors have been considered viable substitutes for Si due to their high light absorption and excellent charge transport properties in photocatalytic applications. Challenges such as low photostability and wettability modulation significantly hinder the performance of III-V photoactive materials in PEC-WS applications. Therefore, in this project, we will be dealing with two main strategies to overcome these challenges i.e., (i) optimally controlling the hydrophilicity/hydrophobicity to facilitate the adsorption of water molecules and thus facilitating H2 generation, (ii) surface protection engineering to promote the photostability of PEC devices, especially at high pH and under anodic conditions. To achieve this goal, we will use morphologically and interfacially controlled phosphorous-rich InP and GaAsP p-type photocathodes (Group III-V materials). The optimal III-V photosystem will be supported by a hydrogen evolution cocatalyst for long-term hydrogen evolution. The underlying mechanisms that control the hydrogen evolution reaction (HER) rate will be studied in detail. Due to the multi-faceted nature of the proposed challenges, the solution strategies offered by this study can be extended to other applications such as PEC CO2 conversion to fuel.
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Supervisory Team	Dr. Di Hu (UNNC), Dr. Bo Li (UNNC) and Dr. George Z. Chen (UNUK)
Short introduction & description of research project	**Green Upcycling of Titanium and Alloying Elements with Valorisation of Metallurgical Slags via High-Temperature Molten Salt Solid-State Deoxidation Process** **Project Overview:** This cutting-edge project aims to develop a novel, sustainable process for the extraction and refinement of high-end titanium and its alloys from metallurgical slags, while valorising the post-treated slags. The research focuses on combining high-temperature molten salt electro-deoxidation and electrorefining processes to not only achieve titanium recovery but also enable the in-situ fabrication of titanium alloys through controlled incorporation of beneficial alloying elements (*e.g.,* aluminum and vanadium). Additionally, the project explores the eco-friendly reuse of post-treated metallurgical slag in construction materials, contributing to a circular economy. **Research Direction:** • **Molten Salt Electrochemistry:** Optimise deoxidation and refining processes using advanced electrochemical techniques. • **In-Situ Alloy Fabrication:** Innovate a dual strategy for managing window elements to promote alloy formation. • **Sustainable Valorisation:** Implement waste recycling methods that transform post-treated metallurgical slags into high-performance, eco-friendly construction materials. **Supervisory Team:** • **Dr. Di Hu (Lead Supervisor, UNNC):** Associate Professor in Chemical Engineering, expert in molten salt electrochemistry and green metal extraction. • **Dr. Bo Li (Co-Supervisor, UNNC):** Professor in Sustainable Construction Materials, specialist in waste recycling and eco-friendly composite materials. • **Dr. George Z. Chen (Co-Supervisor, UNUK):** Professor of Electrochemical Technologies, expert in molten salts innovation for materials, energy, and environment. **Application:** Enthusiastic candidates with a strong background in chemical engineering, materials science, or related fields are invited to apply. Join us in advancing green extraction technologies that promise significant environmental and industrial impact.
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Supervisory Team	Prof. Jun He (UNNC)
Short introduction & description of research project	**Available PhD research projects** The above scholarship is to support research projects outlined under the following themes: Theme: Low-carbon energy **Reductant-free low-temperature SCR process development** Project brief: This project is to develop a novel reductant-free, low-temperature Selective Catalytic Reduction (SCR) technology using photothermal synergistic catalysis to address high-temperature, energy-intensive traditional SCR systems relying on ammonia or urea. The technology enables efficient NO_x reduction at lower temperature without external reducing agents, enhancing energy efficiency and environmental friendliness. Key innovations should include catalysts designed for enhanced NO adsorption and reactive radical generation, as well as composites that facilitate efficient electron-hole separation. This technology offers a sustainable solution for industrial NO_x control in coal-fired power plants and steel manufacturing, aligning with stringent environmental regulations. The work is expected to advance photothermal catalysis theory, catalyst design, and practical applications, promising reduced energy consumption, lower costs, and mitigated secondary pollution.
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Supervisory Team	Shu Liu (UNNC) Mengxia Xu (UNNC) Anand Sreeram (UNUK) Nicholas Musyoka (UNNC)
Short introduction & description of research project	Development of Photocatalytic Asphalt Mixtures with Biomass Fly Ash-supported TiO_2 for Self-cleaning Pavements Nitrogen oxides (NOx) and volatile organic compounds (VOCs) from vehicle emissions are major sources of urban air pollution. To address this issue, researchers are developing novel materials and technologies to mitigate their environmental impact. Titanium dioxide (TiO_2), a widely used photocatalyst, can effectively degrade airborne pollutants under ultraviolet light. Current studies demonstrate that supporting TiO_2 on carbon-based materials or metal oxides can significantly enhance its dispersion and photocatalytic efficiency. However, these modifications are relatively costly, limiting their large-scale application in pavement engineering. Therefore, recent research has focused on utilising solid waste as TiO_2 carriers. This study explores the feasibility of using biomass fly ash as a TiO_2 carrier to develop self-cleaning asphalt mixtures. Biomass fly ash, a solid waste from clean energy production, possesses characteristics such as high alkalinity, a large specific surface area, and chemical stability. Meanwhile, its stronger alkalinity may further improve surface activity and dispersion during TiO_2 loading, as well as enhance the adhesion between bitumen and aggregate, compensating for the weakened surface adhesion of the aggregate-bitumen system. Additionally, environmental and economic assessments will be conducted

	to evaluate the sustainability benefits of the developed material when applied in self-cleaning pavement systems. This research could provide an innovative, cost-effective solution for improving air quality while promoting sustainable development in the construction of urban pavements.
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Supervisory Team	Dr. Mengxia Xu (UNNC) Prof. Tao Wu (UNNC) Prof. Xiaolei Fan (UNNC)
Short introduction & description of research project	**Title:** Development of High-Performance Catalysts for Electrochemical CO_2 Reduction Reaction to Liquid Fuels **Description:** This PhD project focuses on the developing advanced catalysts for the electrochemical reduction of CO_2 (CO_2RR) into liquid fuels such as formic acid and ethanol. State-of-the-art *in situ* spectroscopic techniques (e.g., FTIR, XPS, XAFS) combined with density functional theory (DFT) calculations will be applied to unravel the reaction mechanisms and guide the rational design of next-generation electrocatalysts with improved selectivity, activity, and stability. By harnessing renewable electricity in the CO_2 reduction process, this study provides a sustainable solution for reducing CO_2 emissions while producing valuable chemical feedstocks. The research aligns with global efforts to advance CO_2 utilization technologies, and supports the transition to a circular carbon economy.
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Supervisory Team	Prof. Philip Hall (UNNC) Dr. Zheng Wang (UNNC) Dr. Jason Li (UNNC)
Short introduction & description of research project	**Integrated Crystallization and Separation via Novel Equipment Design** Crystallization is a critical purification process in industries such as pharmaceuticals, chemicals, and environmental engineering. However, traditional methods often face challenges related to temperature control, crystal purity, and the inefficiency of downstream separation steps. This project aims to address these issues by developing a novel crystallizer that integrates separation mechanisms directly into the crystallization process. By introducing innovative design features—such as centrifugal force generation—the goal is to pre-concentrate or separate crystals during crystallization, reducing reliance on downstream filtration and eliminating temperature-related challenges. The project will combine computational modeling and experimental validation to achieve its objectives. The candidate will use computational fluid dynamics (CFD) to simulate and optimize the crystallizer design, focusing on fluid dynamics, crystal behavior, and separation efficiency. A prototype will then be developed and tested in the laboratory to validate its performance under real-world conditions. Key outcomes include improved crystal quality, reduced energy consumption, and a more streamlined process workflow, contributing to sustainable and cost-effective manufacturing practices. We are seeking a motivated PhD candidate with a background in chemical engineering, mechanical engineering, or a related field. The ideal candidate will have experience or interest in CFD, experimental design, and process optimization. This project offers an exciting opportunity to pioneer innovative crystallization technology and make a tangible impact on industrial processes.
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Supervisory Team	Kam Loon Fow (UNNC) Lionel O'Young (UNNC) Zeping Wang (UNNC)
Short introduction & description of research project	**Optimization of Green Polycondensation Process and Property Enhancement of PBT for High-Value Medical and Textile Applications** **Area of work** Polybutylene terephthalate (PBT) is a high-performance engineering thermoplastic widely used in the industries due to its excellent mechanical, thermal, and chemical properties. It is foreseeable that there is a growing demand for PBT with enhanced properties to meet the needs of advanced applications, particularly in the medical and textile industries. PBT is typically fabricated from the polycondensation of oligomers of terephthalic acid (TPA) and 1,4-butane diol (BDO) and the polycondensation process conditions can be tuned to obtain PBT with the desired properties. However, the existing polycondensation process suffers from several major drawbacks, such as the use of non-removable homogeneous catalysts and non-sustainable petrochemical-based reactants. This project aims to develop a greener polycondensation process for making PBT and/or explore innovative methods to enhance the properties of PBT, making it suitable for high-value applications such as biocompatible medical devices and functionalized textiles. **Research objectives** This proposed research project will focus on several key themes as exemplified below: 1. *Optimization of a greener polycondensation process* • Develop and evaluate the performance of heterogenous catalysts in the polycondensation process. • Investigate the role of various design parameters in improving the efficiency and sustainability of the polycondensation process. • Develop a reaction model to predict and optimize the properties of PBT, such as polymer molecular weight distribution and thermal stability. 2. *Property enhancement for medical and textile applications* • Incorporate green additives (e.g., nanofillers, chain extenders, antimicrobial agents) to tailor properties of PBT for specific applications. • Evaluate the mechanical, thermal, and chemical properties of enhanced PBT. • Test the biocompatibility of PBT for medical applications and the durability of PBT fibers for textile applications. • Assess biodegradability and recyclability of modified PBT, supporting green chemical principles.
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Supervisory Team	Yong SUN
Short introduction & description of research project **<300 words**	The objective of this research is to address the knowledge gaps by elucidating the fundamental mechanisms governing the diffusion of solid-phase reagents in molten salt systems. This will involve an in-depth exploration of how the coupled-vacancy diffusion (CVD) mechanism triggers chemical bond rearrangements between PG and carbon, ultimately enhancing the thermal reduction process. By examining the interactions between solid reagents and molten salt molecules, we aim to identify factors that optimize reaction conditions and improve the overall efficiency of gypsum reduction. This research continues our ongoing work in both commercial and fundamental projects focused on reducing hazardous industrial wastes. To the best of our knowledge, no previous studies have comprehensively investigated the molecular mechanisms behind the interaction of molten salts with solid reagents during the thermal reduction of phosphogypsum. The findings will contribute to advancing molten salt science and provide a foundation for developing more sustainable, cost-effective approaches to environmental remediation and waste treatment in industrial settings. The supervisory team, led by Dr. Yong SUN (kinetic modeling, reaction engineering characterization, and molten salt synthesis, molecular simulation), supported by Dr. Kow Kien Woh (solid waste and reaction engineering) and Prof. Jonathan D. Hirst (theoretical modeling), combines both hands-on and theoretical expertise, ensuring a well-rounded approach to the project's success, which is also pivtal to smooth running of this PhD project.
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Supervisory Team	Prof. Bencan Tang (UNNC) Prof. Jonathan D. Hirst (UNNC) Dr Kam Loon Fow (UNNC)
Short introduction & description of research project	**Project Title:** **Development of Automated Flow Chemistry Reaction Platform for the Production of 1,3-Propanediol** Developing new reaction technology to realize challenging chemical reactions as such with automatic reaction control would increase the production efficiency of many important chemicals and is to be embraced by chemical industry. This research aims to establish a fully automated intelligent flow chemistry reaction platform for the optimization of reaction conditions and pilot production of important chemicals. The intelligent flow chemistry reaction platform will be based on flow chemistry and Bayesian optimization theory. It will enable the injection of raw materials via an HPLC pump, with parameters such as substrate type, concentration, solvent, and catalyst being controlled. By integrating Bayesian

	optimization algorithms, the platform will optimize the reaction conditions, leading to the identification of the optimal production conditions. This method will significantly reduce human, material, and time resources during the optimization process. Moreover, when scaling up to production, the flow chemistry equipment can be easily adapted for increased scale and capacity, while minimizing potential hazards and waste in the production process. The ideal candidate would be students with bachelor's and master's degrees from Chemistry and Chemical Engineering. The candidate should have strong interests in flow chemistry, programing and coding, and should have good problem-solving skills, including technical and theorical problems. We only encourage hardworking and ambitious students to apply for this position.
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Supervisory Team	Bo Li (UNNC) Kow Kien Woh (UNNC) Sreeram, Anand (UNNC)
Short introduction & description of research project	**Engineered controlled low-strength materials using multiple solid waste-derived binders and excavated soil: mechanical performances and stabilisation mechanisms** Controlled Low-Strength Material (CLSM) is a flowable, low-strength construction material commonly used for backfilling. The properties of most existing CLSM depend on carbon-intensive cement. Furthermore, its high-water content results in slow setting times and limited early strength, which negatively impacts construction efficiency. Therefore, developing a novel type of binder that is more environmentally friendly, cost-effective, and capable of providing higher early strength for CLSM is crucial for enhancing its overall performance and eco-friendliness. Novel low-carbon cementitious materials can be prepared using industrial residues. Therefore, the proposed project aims to develop an innovative CLSM using multiple solid wastes as binders and excavated waste soil as the aggregate. The specific objectives include: 1) to develop a novel low-carbon binder with both high early strength and improved durability based on a deep understanding of cementitious mechanisms within a multi-solid waste system; 2) to investigate the impact of chemical addition on accelerating the reaction process of waste-based cementitious materials; 3) to develop a CLSM with comprehensive performance improvements across all stages by analysing the time-dependent microstructural evolution of the binder-water-soil triphasic system; and 4) to assess the environmental benefits of CLSM through a Life Cycle Assessment, considering its green composition, low-effort construction methods, and shortened construction cycles. Overall, developing eco-friendly binders from industrial by-products presents significant potential for producing low-carbon CLSM with superior engineering performance.
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Supervisory Team	Prof. Cheng Heng Pang (UNNC)
Short introduction & description of research project	AI-Assisted Green Conversion of Biomass towards Energy Security and Carbon Neutrality This PhD project is focused on simultaneously deriving clean energy and developing advanced functional materials from renewable materials, including biomass and solid wastes, via AI-assisted green chemistry and clean processing. A combined experimental and computational studies will be used to ensure conversion efficiency, selectivity and sustainability. The ability to transform waste materials into value-added end-products is pivotal in the collective efforts towards carbon-neutrality.
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