NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE | Graduate College

Joint Projects

NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE | Graduate College

1. Sustainable cascade conversion of carbohydrates to nitrogen heterocycles

Date Posted	5 July 2024	
Home University	Nanyang Technological University	
Partner University	Technical University of Denmark	
Supervisors	**Home**	**Partner**
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Project Description (200-300 words)	The project will develop one-pot, three-component cascade reaction to obtain nitrogen heterocycles sustainably by reacting native carbohydrates, active methylene compounds and primary amines in a selective fashion. The reaction will be developed under benign conditions of water and room temperature using common cheap catalysts such as mineral acids and inorganic bases. The developed process will be beneficial for the pharmaceutical industry to develop drug intermediates that can be converted to final drugs in a sustainable fashion. The innovation in this project relies on introducing nitrogen from an external source (e.g. ammonium acetate) and keeping the atom economy of the reaction high. Precedents of such reactions in the literature is scares due to the difficulty in using native carbohydrates for such reactions without protection /deprotection methodologies.	
Program/Center Website(s)		
Additional Information (e.g., files with project details)	https://pubs.acs.org/doi/abs/10.1021/acs.joc.2c01270 https://aces.onlinelibrary.wiley.com/doi/abs/10.1002/ajoc.202200367 https://www.mdpi.com/1420-3049/28/3/1265	

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2. Registration of Safety-Related Behavior of Cyclists Using Privacy Preserving Computer Vision and Federated Learning

Date Posted	5 July 2024	
Home University	Nanyang Technological University	
Partner University	Technical University of Denmark	
Supervisors	**Home**	**Partner**
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Project Description (200-300 words)	In Singapore and Denmark, the rise in urban cycling has intensified during the COVID-19 pandemic, leading to improved cycling infrastructure. However, cyclists' behavior, particularly mobile phone use while riding, poses significant safety risks. This behavior is a key performance indicator for road safety globally, yet there is no broad method to monitor it. Computer vision, though proposed for detecting road users' safety-related behavior, has not been applied to cyclists and faces challenges in different environments. Additionally, collecting such data raises privacy concerns. Researchers from DTU and NTU aim to address these issues by investigating privacy-preserving detection of cyclists' safety-related behavior using computer vision and federated learning. They will collect a diverse video dataset of cyclists in Copenhagen and Singapore to develop an automated detection approach. This project will generate accurate and comprehensive data on cyclists' safety behavior in Denmark and Singapore. A DTU-based PhD will analyze factors affecting the behavior and ensure the algorithm's robustness in different environments. An NTU-based PhD will focus on maintaining detection accuracy under privacy regulations and improving the algorithm using federated learning. The project will enhance road safety in Denmark and Singapore by providing data on mobile phone use and other safety behaviors (e.g., helmet and bicycle light use). This data will inform public debates and support evidence-based decisions on rule enforcement and education. Collaborative activities and research stays between DTU and NTU will expand the researchers' perspectives on computer vision in transport safety.	
Program/Center Website(s)	-	
Additional Information (e.g., files with project details)	-	

3. Designing Catalysts for Dehydrogenating Liquid Organic Hydrogen Carriers using First Principles Methods and Machine Learning

Date Posted	1 July 2024	
Home University	Nanyang Technological University	
Partner University	Technical University of Denmark	
Supervisors	**Home**	**Partner**
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Project Description (200-300 words)	Hydrogen will be an important energy vector that will drive Singapore's decarbonisation strategy to achieve net zero CO_2 emissions by 2050. The trans-oceanic shipment of low-carbon hydrogen into Singapore will be enabled through hydrogen carriers. The hydrogen carriers are those molecules that can be reversibly hydrogenated and dehydrogenated, and store more than 5.5 wt.% of hydrogen. Ammonia, methyl cyclohexane, formic acid, methanol etc. are examples of such hydrogen carriers. In fact, Singapore recently set up its first proof of concept hydrogen ecosystem using methyl cyclohexane as an example. The critical step in this technology is dehydrogenating the hydrogen carrier to extract the hydrogen. A catalyst is required to accelerate the rate of the dehydrogenation reactions. There are stringent criteria for the long-term stability of the catalyst and in terms of the selectivity of dehydrogenation reactions such that the hydrogen carrier can be recycled. Catalysts for dehydrogenating hydrogen carriers are designed using trial-and-error experiments. Most often, these catalysts include precious metals like Pt. It is vital to accelerate the pace of catalyst discovery, and generate a library of cost-effective, stable, and selective catalysts for dehydrogenating hydrogen carriers. Moreover, each hydrogen carrier has different C-H, O-H, and N-H bond strengths, requiring tailored catalysts for each type of hydrogen carrier. Experimental methods alone cannot be used to discover these tailored catalysts because trial-and-error methods are limited by time and resource requirements. First principles calculations together with machine learning can be used to guide the design of catalysts that are tailored for each type of hydrogen carrier. These methods need to overcome	

	challenges associated with describing the reactivity of large molecules on low-symmetry active sites. In this project, we will develop such advanced machine learning models that identify optimal catalysts for several classes of hydrogen carriers. These models will rapidly predict the reactivity, selectivity, and stability of candidate catalysts for dehydrogenation. The machine learning models will also be used to build detailed reaction networks for dehydrogenation that are difficult to establish using experiments alone. Insights from the reaction networks will be used to identify and mitigate unselective steps of the dehydrogenation process, and prevent deactivation through coke formation.
Program/Center Website(s)	N.A.
Additional Information (e.g., files with project details)	Please see additional-information.docx for details for preliminary results that support the hypotheses governing the project. Additional-information Tej Salil Choksi.pdf

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4. Risk-informed Digital Twin of Energy Geostructures for Resilient Urban Communities

Date Posted	1 July 2024	
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Partner University	Technical University of Denmark	
Supervisors	**Home**	**Partner**
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Project Description (200-300 words)	Space heating and cooling dominate the overall thermal demand. There is a pressing need to decarbonize the energy sector to achieve carbon neutrality by 2050. Energy geostructures (e.g., energy piles and diaphragm walls) have proven to be viable solutions for exploiting shallow geothermal energy and reducing reliance on fossil fuels, thereby significantly cutting greenhouse gas emissions. However, there are several critical technical issues need to be addressed in the application of energy geostructures: (a) the understanding of thermo-hydro-mechanical behavior of soil-structure interaction under long-term cyclic thermal loadings is still limited, posing significant uncertainties to the serviceability and safety of geostructures; (b) there is a lack of a unified framework for life-cycle analyses of energy geostructures, taking into account uncertainties from design, construction, and operation stages. To address these challenges, this project aims to develop a risk-informed digital twin of geostructures for resilient urban communities. Advanced soil constitutive models will be developed and implemented in commercial software for long-term thermo-mechanical analysis of soil-structure interaction. Moreover, multi-fidelity physics-informed machine learning models will be developed to predict the long-term resilience of geostructures in real time. The success of this project will offer a sustainable urban solution that can expedite the pace of developing livable, sustainable, and resilient urban communities.	
Program/Center Website(s)	NA	
Additional Information (e.g., files with project details)	NA	