NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE | Graduate College

Joint Projects

NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE | Graduate College

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

Date Posted	01 July 2024	
Home University	Nanyang Technological University	
Partner University	Technical University of Denmark	
Supervisors	**Home**	**Partner**
Name	Asst. Prof. Tej S. Choksi	Prof. Thomas Bilgaard
School	School of Chemistry, Chemical Engineering and Biotechnology	Department of Energy Conversion and Storage
Email	tej.choksi@ntu.edu.sg	tbli@dtu.dk
Website	https://www.ntu.edu.sg/research/faculty-directory/detail/rp00567	https://orbit.dtu.dk/en/persons/thomas-bligaard
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

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

Date Posted	1 July 2024	
Home University	Nanyang Technological university	
Partner University	Technical University of Denmark	
Supervisors	**Home**	**Partner**
Name	SHI Chao	DONG Yuepeng
School	School of Civil and Environmental Engineering	Department of Environmental and Resource Engineering
Email	Chao.shi@ntu.edu.sg	yuedo@dtu.dk
Website	https://dr.ntu.edu.sg/cris/rp/rp02150	https://orbit.dtu.dk/en/persons/yuepeng-dong
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	