

# Data-Driven Material and Process Design for Sustainable Energy and Environment



Date: 15 April 2021 (Thursday)

Time: 10am - 11am

Seminar link: <https://cityu.zoom.us/j/92645472480>

## ABSTRACT

In order to successfully transfer the traditional fossil fuels into renewable energies, the optimal design of functional molecules or materials that are used in the energy storage, utilization, and emission reduction processes is significant. Due to the large diversity of material structure, it is necessary to develop theoretical methods to help identify promising candidates for experimental investigation. Unfortunately, the complex relationship between material structure and its property makes it challenging for theoretical material design. In this talk, the significance of machine learning for molecular or material property prediction is first highlighted. A generic framework for machine learning-based functional materials design is then proposed. Several successful applications are introduced, including solvent design for CO<sub>2</sub> capture, extractant design for gasoline desulfurization, phase-change material design for solar thermal storage, and nanoporous material design for industrial gas separations. In the second part of the talk, the speaker will introduce a data-driven modeling approach for the analysis and optimization of complex energy conversion systems. He will also point out how artificial intelligence can help develop high-value and sustainable chemical products.



## Dr Teng ZHOU GUEST SPEAKER'S PROFILE

Dr Teng Zhou is currently a Junior Professor (Assistant Professor) at the Max Planck Institute (MPI) for Dynamics of Complex Technical Systems, Germany and the Otto-von-Guericke University (OvGU) of Magdeburg, Germany. He received his doctoral degree with the highest distinction in Process Systems Engineering in 2016 from OvGU. Afterwards, he worked as a postdoctoral scientist at the MPI and TU Denmark before he got appointed as an assistant professor in 2019.

Dr Zhou's research lies at the intersection of chemical and energy engineering, systems engineering, material science, and data science. He is currently interested in the development of artificial intelligence and machine learning tools for sustainable chemical product design and energy & environment-related functional materials design. Besides, he is also interested in the analysis and optimization of complex chemical production and energy conversion systems using the data-driven modeling approach. Dr. Zhou has already published 38 articles in top-ranked journals and his works have received more than 1000 citations. He has earned many prestigious honors and awards including the AIChE CAST Directors Award and CGCA Young Researchers Award. He is a founding Associate Editor of two international journals and an Editorial Board Member for several SCI-indexed journals.

**Enquiries: [hkids@cityu.edu.hk](mailto:hkids@cityu.edu.hk)**

**All are welcome**