

Validation of the Reliability of Photocatalysis Machine Learning Model based on the Understanding from Experiments

School:

Chemical Engineering

Supervisory Team:

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Research Area:

Renewable Energy – Photocatalysis

Description of field of research:

Photoreforming is a process that utilizes solar energy to activate photocatalysts (i.e. TiO₂) for the reduction of H⁺ into H₂ gas and at the same time oxidation of harmful organic substrates.^[1-2] Despite its applicability to various organic waste products, the overall efficiency of photoreforming reaction is still relatively low. Implementation of machine learning framework to discovery efficient photocatalyst for photoreforming reaction has recently attracted significant attention. With the aid of artificial intelligent, photocatalyst design and screening can be accelerated.^[3] To ensure the reliability of machine learning model, this project aims to validate the predicted outcomes from the machine via experimental approaches.

Research Environment

The student will have the opportunity to work in Particles and Catalysis Research Group (PartCat) under the guidance of Prof. Rose Amal, Dr. Cui Ying Toe and Dr. Hassan Masood. The student will have the access to well-equipped laboratories with experimental facilities and computational tools for photocatalysis research. The student will work in a multidisciplinary research environment and learn various functional skills to facilitate future career in academic or industry.

Expected Outcomes

The student is expected to gain experience in catalyst synthesis, characterizations and photocatalytic activity measurement techniques. The project will also allow the student to work with other research students to gain valuable interdisciplinary experience. Continuing of the research as an 4th year honour thesis project is possible.

Reference Material/Links

^[1] Navarro, R. M., Sanchez-Sanchez, M. C., Alvarez-Galvan, M. C., Del Valle, F., & Fierro, J. L. G. (2009). Hydrogen production from renewable sources: biomass and photocatalytic opportunities. *Energy & Environmental Science*, 2(1), 35-54.

^[2] Shimura, K., & Yoshida, H. (2011). Heterogeneous photocatalytic hydrogen production from water and biomass derivatives. *Energy & Environmental Science*, 4(7), 2467-2481.

^[3] Masood, H., Toe, C. Y., Teoh, W. Y., Sethu, V., & Amal, R. (2019). Machine Learning for Accelerated Discovery of Solar Photocatalysts. *ACS Catalysis*, 9(12), 11774-11787.