Computational Heterogeneous Catalysis Engineering for on-line optimization of Catalytic Reforming Processes

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The Integrated Carbon Capture and Conversion (ICCC) is a promising catalytic process to produce syngas from CO_2 and CH_4 via a combined separation and reactor unit. Besides, its performance can fluctuate from the inconsistent feed ratio resulting from the flue gas unit. Herein, the Ratings concept workflow based on density functional theory (DFT) is applied to overcome these problems in a two-step protocol: (i) catalyst identification designating the catalyst characteristics and predicts performance and (ii) catalyst optimization determining new operating condition setpoint accounted for its deactivation over time.

Dr. Supareak is the Director of the Center of Excellence on Catalysis and Catalytic Reaction Engineering (CECC), Chulalongkorn University, Thailand. His work on computational heterogeneous catalysis engineering employs density functional theory, microkinetic modeling, and machine learning to design the catalyst screening workflow in gas-phase and liquid-phase reactions. The workflow called the Ratings Concept was developed by the group in 2017 and can be used to screen for dry reforming catalysts at high accuracy validated by experiments. Recently, the group proposed a screening workflow for high-entropy alloys (HEA) as three-way catalysts, where the HEA catalysts database was published by the group at http://www.hcu.cecc.eng.chula.ac.th/hea-database/

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Research field:

- Computational Heterogeneous Catalysis Engineering
- Catalyst Deactivation