

Data science for catalyst discovery and process intensification

Dion G. Vlachos

Department of Chemical and Biomolecular Engineering, Catalysis Center for Energy Innovation (CCEI), RAPID Manufacturing Institute, Delaware Energy Institute (DEI),
University of Delaware

vlachos@udel.edu

Abstract

Over the past two decades, multiscale modeling has advanced tremendously. Yet, our ability to apply first principles modeling to process design and catalyst development is seriously limited due to multiple challenges. At the same, energy transformations due to the introduction of shale gas, cheaper wind and solar-based electricity, feedstock diversification, and sustainability require new materials, reactors, and processes. In this talk, we will outline these challenges and discuss computational and experimental methods to overcome of them. We will place emphasis on data science methods for improving catalysts and for design of novel reactors.