UNIVERSITY OF DELAWARE
DELAWARE ENERGY INSTITUTE

DEI WEBINAR

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HTTPS://UDEL.ZOOM.US/J/95422002732

ALEXANDER MITSOS

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Alexander Mitsos is a Full Professor (W3) in RWTH Aachen University, and the Director of the Laboratory for Process Systems Engineering (AVT.SVT), comprising 40 research and administrative staff. He also has a joint appointment at Forschungszentrum Juelich where he is a Director of ICE-1 Energy Systems Engineering. Mitsos received his Dipl-Ing from University of Karlsruhe in 1999 and his Ph.D. from MIT in 2006, both in Chemical Engineering. Prior appointments include military service, free-lance engineering, involvement in a start-up company, a junior research group leader position in the Aachen Institute of Computational Engineering Science and the Rockwell International Assistant Professorship at MIT. Mitsos' research focuses on optimization of energy and chemical systems and development of enabling numerical algorithms. He is (associate) editor in multiple journals including AAAS Science Advances, Computers & Chemical Engineering, Journal of Global Optimization and Journal of Optimization Theory & Applications.

MACHINE-LEARNED PHYSICAL PROPERTIES FOR MOLECULAR DESIGN

This talk gives an overview of our work on the predictions of physical properties and the use of these predictions for molecular design. We have been employing Graph Neural Networks and Generative Machine Learning. The calculation, estimation and prediction of physical properties is crucial for the design of chemical products and processes. As such chemical engineering has devoted substantial effort over decades, spanning experimental work, macroscopic semi-empirical thermodynamic models to a-priori predictive models. In the last years many research groups have employed modern techniques from machine learning. A particular challenge is the relatively small number of data. We present an overview of our employed and developed methods, the various physical properties predicted, and the effect of physics-informed machine learning. We also demonstrate how the predictions can be used for molecular design, with a focus on fuel synthesis from biomass and hydrogen.

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