NaWuReT
Early Career Reaction Engineers, Germany

ProcessNet
EINE INITIATIVE VON DECHEMA UND VDI-GVC

NaWuReT online Colloquium

Being an early career reaction engineering scientist does not only impose scientific challenges. The career path towards a professorship is full of challenges and obstacles that are not well known. NaWuReT is inviting the chemical reaction engineering community to a virtual colloquium in the fall of 2021 entitled

„From PhD student to assistant professor – Early career chemical engineers in academia“

The colloquium will be held on every Monday from September 27th to October 25th. In this series of lectures, we will discuss the career path of five distinguished, international early career researchers who successfully became an assistant professor. Each of them will provide insights into their current research topics, which cover a wide range of multiscale modeling: from the computational investigation of the catalyst surface to the modeling and design of reactors. The colloquium is directed to everyone who is curious about possible career pathways in science and to those interested in our speaker's research.

Speaker of NaWuReT:

Prof. Dr.-Ing. Gregor D. Wehinger
Institute for Chemical and Electrochemical Process Engineering
Clausthal University of Technology
Email: wehinger@icvt.tu-clausthal.de

Program 2021

Monday, September 27th (time zone: CEST)
5 – 6 pm *„Pushing the limits of large datasets and machine learning in computational catalysis“*

Zachary Ulissi, Carnegie Mellon University, USA

Monday, October 4th
3 – 4 pm "Hierarchical multiscale modelling in heterogeneous catalysis: the quest for computational holism."

Ivo Filot, TU Eindhoven, Netherlands

Monday, October 11th
5 – 6 pm *"Tuning catalyst activity, selectivity, and stability through fundamental understanding"*

Charlotte Vogt, Technion, Israel

Monday, October 18th
5 – 6 pm *„Hierarchical multi-scale modelling of high temperature solid oxide cell stacks“*

Aayan Banerjee, University of Twente, Netherlands

Monday, October 25th
5 – 6 pm *„Hierarchical analysis and advanced design of catalytic structures for process intensification via Computational Fluid Dynamics reactive simulations“*

Mauro Bracconi, Politecnico di Milano, Italy

Registration

Participation is free of charge. The talks will be held via Zoom and the link will be provided after registration. We kindly ask for registration via email to *wehinger@icvt.tu-clausthal.de*

Zachary Ulissi is assistant professor at the Carnegie Mellon University in the College of Engineering in Pittsburgh, USA. Machine learning models are increasingly popular in chemistry, but many challenges remain for day-to-day use in complex areas like catalysis. He'll discuss his path towards working in this area, current excitement about large datasets and models for catalysis (and the Open Catalyst Project), and some of the outstanding issues that he hopes other young researchers will help address.

Aayan Banerjee is assistant professor in computational chemical engineering at the University of Twente in the Catalytic Process and Materials group. His research centers on the development of high-fidelity multiscale models to predict the performance and lifetime of novel reaction systems. The models help actualize his research aims of efficiently scaling up and reducing the time-to-market of next generation chemical and electrochemical technologies.

Ivo Filot is an assistant professor in computational and theoretical catalysis at Eindhoven University of Technology. His research focuses on the development of novel computational methods in multiscale modeling of heterogeneous catalysis utilizing modern computational strategies. An important focal point in this research endeavor is the elucidation of kinetic mechanisms at the nanoscale utilizing advanced microkinetic models. For the description of reaction kinetics in larger scale CFD and reactor models, the kinetic responses of nanoscale models are encapsulated in simplified descriptor based functionals using machine learning approaches.

Mauro Bracconi is an assistant professor at the Laboratory of Catalysis and Catalytic Processes of Politecnico di Milano. His research interest is in the context of process intensification with a focus on innovative reactor configuration through CFD and multiscale modeling. He is also interested in the coupling of Machine Learning and AI with Chemical Reaction Engineering to facilitate the coupling of first-principles based kinetic models into CFD and to build computationally efficient surrogate models of chemical reactors.

Charlotte Vogt is an assistant professor at the Technion in Israel. The aim of her work is to develop special (micro)spectroscopic methodologies to study details of catalytic reactions at work that we couldn't study before. By studying fundamental phenomena of non-model catalysts under realistic process conditions, she then use that understanding to come up with novel concepts to manipulate these reactions for higher efficiency, selectivity, and/or other desired properties necessary to bridge the energy, climate, and materials crises that our global society are facing.

Interested in becoming a member of the NaWuReT ?

NaWuReT is always looking for new members who want to engage with the early career reaction engineering community. Whether you are PhD student, postdoc, assistant professor, or an early career reaction engineer in the industry - you are welcome to join. If you are interested, reach out to Gregor Wehinger for further information.

NaWuReT is now on Linkedin. Be sure to connect with us to stay up-to-date with our latest activities.

Click here!