

### Invited talks (total 36):

- Nov 2023: *Modeling and Design of Single-Atom Alloy Catalysts for CO<sub>2</sub> hydrogenation reactions.* AIChE Annual Meeting, Orlando, FL, USA.
- Oct 2023: *Machine learning and atomistic modelling for CO<sub>2</sub> hydrogenation catalysis.* Colloquium on computational catalysis, Chalmers University, Sweden / virtual.
- Sep 2023: *Effektiv omdannelse af CO<sub>2</sub> ved hjælp af kunstig intelligens.* Popular talk at high school (Aarhus Tech) for the Festival of Natural Science.
- May 2023: *Accelerated kinetic Monte Carlo simulations with lateral interactions applied to higher oxygenate synthesis over Rh-based catalysts.* Workshop: KMC as a Tool for Understanding Catalytic Function, Berlin, Germany / virtual.
- Mar 2023: *Modeling and design of single-atom alloy catalysts.* DPG Spring Meeting, Dresden, Germany.
- Feb 2023: *Machine learning methods for heterogeneous catalysis.* Lennard-Jones Centre Discussion Group, University of Cambridge, UK / virtual.
- Jan 2023: *Modeling and design of single-atom alloy catalysts using graph-based machine learning.* Surface Science Discussions 2023, virtual seminar.
- May 2022: *Machine learning for catalysis modelling.* Seminar, Hannu Häkkinen Group, University of Jyväskylä, Finland / virtual.
- Apr 2022: *Data-efficient and physics-inspired machine-learning models to treat complex catalyst materials and reaction networks.* TACO Colloquium, Technical University of Vienna, Austria.
- Apr 2022: *Machine learning for catalysis modelling.* Distinguished iNANO lecture, interdisciplinary Nanoscience Center, Aarhus University, Denmark.
- Mar 2022: *Combining machine learning and microkinetic modelling to treat complex reactions in surface catalysis.* Spring Meeting of the American Chemical Society, San Diego, USA / virtual.
- Mar 2022: *Machine learning in surface science and catalysis.* Plenary talk at Physics Days, Aalto University, Finland / virtual.
- Mar 2022: *Catalysis and CO<sub>2</sub>.* Popular science talk in Science Slam at the Planetarium, Copenhagen, Denmark.
- Nov 2021: *Adsorption.* CatLab lecture series on heterogeneous catalysis. CatLab, IRIS Adlershof, Berlin, Germany.
- Aug 2021: *Adsorption energies for catalysis modeling through machine-learned descriptors.* Center for High Entropy Alloy Catalysis, Technical University of Denmark. Retreat at Sonnerupgård Gods, Hvalsø, Denmark.
- June 2021: *Structure-activity relationships of catalytic materials with machine learning.* Annual meeting of the Danish Physical Society, Brogaarden Konferencenter, Middelfart, Denmark.
- June 2021: *Active site representation in computational catalyst screening.* Invited speaker and panelist for the online June SUNCAT session on "Data-driven Catalyst Discovery", SUNCAT Center for Interface Science and Catalysis, Stanford University, USA.
- May 2021: *Active sites in solid and liquid surface catalysis.* 14th European Conference on Surface Crystallography and Dynamics (ECSCD-14), virtual conference.

- Mar 2021: *Machine-learned adsorption energies for catalysis modeling.*  
Virtual seminar, Department of Energy Conversion and Storage: Atomic Scale Materials Modelling, Technical University of Denmark.
- Mar 2021: *Microkinetic and thermodynamic modeling in heterogeneous catalysis with machine learning input.*  
Virtual seminar, Center for Interstellar Catalysis, Aarhus University, Denmark.
- Apr 2019: *Scaling relations and beyond for kinetic Monte Carlo models in heterogeneous catalysis.*  
DPG Spring Meeting, Regensburg, Germany.
- Mar 2019: *Liquid metal catalysis: role of liquid copper in high-quality graphene synthesis.*  
Open Science Seminar, Aarhus University, Denmark.
- Jan 2019: *2D material growth on liquid metals: role of liquid copper in high-quality graphene synthesis.*  
6th Munich 2D Materials Meeting, Ludwig-Maximilians-Universität, München, Germany.
- Aug 2018: *Scaling-relation-based kinetic Monte Carlo modelling of syngas reactions on stepped metals.*  
ECOSS34, Aarhus, Denmark.
- Aug 2018: *Kinetic Monte Carlo.*  
Tutorial Seminar on Theoretical Methods in Surface Science, ECOSS34, Aarhus, Denmark.
- Aug 2018: *Multi-scale simulation methods.*  
Hands-On DFT and Beyond Workshop, Peking University, Beijing, China
- Jun 2018: *Scaling-relation-based kinetic Monte Carlo modelling of syngas reactions on stepped metals.*  
Japan-German Joint Symposium on Advanced Catalysis Material and Characterization, Catalysis Research Center, TU Munich, Germany.
- Mar 2018: *Syngas reactions on metal surfaces studied using scaling-relation-based kinetic Monte Carlo.*  
DPG Spring Meeting, Berlin, Germany.
- Aug 2017: *Applications and current frontiers of kinetic Monte Carlo simulations.*  
"Topical Summer School on Theoretical and Computation Chemistry: Kinetic Monte Carlo Modelling", Academia Sinica, National Taiwan University of Science and Technology, Taipei, Taiwan.
- Jan 2017: *Scaling-relation based analysis of bifunctional catalysis.*  
Institute of theoretical chemistry, Ulm University, Ulm, Germany.
- Oct 2016: *First-principles microkinetic modeling of bifunctional catalysts.*  
Inorganic Chemistry Department, Fritz Haber Institute, Berlin, Germany.
- Sep 2016: *First-principles microkinetic modeling of bifunctional catalysts.*  
European Physical Society: Condensed Matter Division, Groningen, The Netherlands.
- Mar 2016: *Analyzing the case for bifunctional catalysis.*  
School of Chemical & Biomolecular Engineering, Georgia Tech, Atlanta, USA.
- Mar 2016: *Analyzing the case for bifunctional catalysis.*  
American Chemical Society National Meeting, San Diego, USA.

- Jan 2015: *Graphene on metal surfaces and its efficiency as a coating material.*  
BASF, Ludwigshafen, Germany.
- Mar 2014: *Graphene on metal surfaces and its efficiency as a coating material.*  
Haldor Topsøe, Kgs. Lyngby, Denmark.
- Apr 2013: *Superhydrogenated coronene.*  
Workshop: "*Exploring mechanisms for H<sub>2</sub> formation on very small carbonaceous grains and PAHs of astrophysical interest*", Toulouse, France.