

Mie Andersen

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www.phys.au.dk/forskning/forskningsomraader/catalytic-structure-activity-relationships-with-machine-learning

Education and career:

- 2021 – : AIAS Fellow and Associate Professor, Aarhus University, Denmark.
- 2022 – 2023: Maternity leave (18.6.2022–13.3.2023). One working day per week.
- 2021: Habilitation, September 8th 2021, TU Munich, Germany.
Mentor: Prof. Karsten Reuter.
Thesis: *Adsorption enthalpies for catalysis modeling through machine-learned descriptors*
- 2017 – 2021: Group leader and Habilitandin, TU Munich, Germany.
Part of EU-funded *LMCat* project coordinated by Prof. Irene Groot (U Leiden, NL).
- 2019 – 2020: Maternity leave (12.6.2019–17.5.2020). Worked half time 18.11.2019–17.5.2020.
- 2014 – 2017: Alexander von Humboldt Fellow / postdoc, TU Munich, Germany.
Host: Prof. Karsten Reuter.
Project: *Scaling-relation-based kinetic Monte Carlo modelling of higher alcohol synthesis.*
- 2014: PhD degree in nanoscience, November 12th 2014, Aarhus University, Denmark.
Supervisor: Prof. Bjørk Hammer.
Thesis: *Graphene and polycyclic aromatic hydrocarbons modeled with density functional theory.*
- 2013: Research stay (6 months), CEMES-CNRS, Toulouse, France.
Host: Dr. Xavier Bouju.
Project: *Simulation of STM images using the ESQC code.*
- 2012: Master's degree in nanoscience, June 1st 2012, Aarhus University, Denmark.
Specialization in physics and materials science.
- 2009: Study and research stay (4 months), University of Wisconsin-Madison, USA.
- 2009: Bachelor's degree in nanoscience, August 30th 2009, Aarhus University, Denmark.

Fellowships, grants and awards:

- 2023 – 2025: Marie Skłodowska-Curie Global Fellowship for Raffaele Cheula (project coordinator and supervisor for return phase).
- 2023 – 2026: Project grant from the Novo Nordisk Foundation. Volume: DKK 2.6 million.
Host: Department of Physics and Astronomy, Aarhus University.
- 2021 – 2026: VILLUM Young Investigator grant. Volume: DKK 8 million.
Host: Department of Physics and Astronomy, Aarhus University.
- 2021 – 2024: AIAS-COFUND fellowship at Aarhus Institute of Advanced Studies.
- 2019 and 2020: Computing grants on Jülich's JUWELS with Prof. Karsten Reuter.
Total volume: 19 million core hours.
- 2018: Gerhard Ertl Young Investigator Award for excellence of research in surface science.
- 2017 – 2019: MPG fellowship for distinguished visiting scientists.

Host: Prof. Matthias Scheffler.

Research visits to the Theory Department of the Fritz Haber Institute, Berlin, Germany.

2016: Computing grant on Jülich's JURECA with Prof. Karsten Reuter.
Volume: 4 million core hours.

2015 – 2017: Alexander von Humboldt postdoctoral fellowship.

Scientific publications:

44 articles published in international peer-reviewed journals (11 first authorships and 16 corresponding authorships).

Total number of citations (Google Scholar): 4043

H-index (Google Scholar): 26

Selected invited talks and seminars (from a total of 36):

2023: *Modeling and Design of Single-Atom Alloy Catalysts for CO₂ hydrogenation reactions.*
AIChE Annual Meeting, Orlando, FL, USA.

2023: *Modeling and design of single-atom alloy catalysts using graph-based machine learning.*
Surface Science Discussions 2023 (virtual seminar).

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).

2022: *Machine learning in surface science and catalysis.*
Plenary talk at Physics Days, Aalto University, Finland (virtual).

2021: *Active site representation in computational catalyst screening.*
Invited speaker and panelist for session on "Data-driven Catalyst Discovery", SUNCAT Center for Interface Science and Catalysis, Stanford University, USA (virtual).

2021: *Active sites in solid and liquid surface catalysis.*
14th European Conference on Surface Crystallography and Dynamics (virtual).

2019: *Scaling relations and beyond for kinetic Monte Carlo models in heterogeneous catalysis.*
DPG Spring Meeting, Regensburg, Germany.

2019: *Liquid metal catalysis: role of liquid copper in high-quality graphene synthesis.*
Open Science Seminar, Aarhus University, Denmark.

2018: *Scaling-relation-based kinetic Monte Carlo modelling of syngas reactions on stepped metals.*
ECOSS34, Aarhus, Denmark.

2018: *Multi-scale simulation methods.*
Hands-On DFT and Beyond Workshop, Peking University, Beijing, China

Teaching experience:

2023: Tutoring: "Quantum Mechanics" (Bachelor level), Aarhus University, Denmark.

2021, 2023: Perspective lecture in course "Mechanics and Thermodynamics" (Bachelor level), Aarhus University, Denmark.

2018: Design and teaching of new course: "Advanced Laboratory Methods: Physical Chemistry" (Bachelor level), TU Munich, Germany.

- 2017-2018: Hands-on sessions in “*European Summer School on Multiscale Modelling in Chemical Reaction Engineering*”, Porto Carras, Halkidiki, Greece.
- 2017: Lectures and hands-on sessions in “*Topical Summer School on Theoretical and Computation Chemistry: Kinetic Monte Carlo Modelling*”, Academia Sinica, National Taiwan University of Science and Technology, Taipei, Taiwan.
- 2017 – 2021: Lectures: “*Advanced electronic structure*” (Master level), TU Munich, Germany.
- 2016: Hands-on sessions in “*College on Multiscale Computational Modeling of Materials for Energy Applications*”, ICTP, Trieste, Italy.
- 2015 – 2020: Lectures: “*Molecular catalysis and kinetics*” (Master level), TU Munich, Germany.
- 2014 – 2015: Tutoring: “*Quantum Chemistry: Electronic structure*”, “*Measurement, analysis & simulation*” (Master level), TU Munich, Germany.
- 2010 – 2014: Tutoring: Undergraduate courses in physics, Aarhus University, Denmark.

Supervision of students and postdocs:

Currently: 2 postdocs, 4 PhD students, 1 Master's students, 2 Bachelor's students.

Previously: 3 PhD students, 1 visiting PhD student, 5 Master's students, 3 visiting Master's students, 5 Bachelor's students, 4 project (*Forschungspraktikum*) students.

Other professional activities:

- Reviewer for Nature, Nature Catalysis, Nature Computational Science, Nature Communications, Angewandte Chemie, ACS Catalysis, ACS Omega, JACS, Chemical Science, Journal of Chemical Physics.
- Member of “Institutforum” at the Department of Physics and Astronomy, Aarhus University (advisory body for the head of the department).
- Co-organizer of the international workshop “Astrochemistry meets Surface Science: Theoretical Frontiers” held April 5-8 2022 at Aarhus Institute of Advanced Studies, Aarhus University, Denmark.

Languages:

Danish: Mother tongue

English: Fluent

French: High level

German: Advanced (CEFR level B2 certificate from Goethe Institute, 2015)