# ANDY SODE ANKER, PhD


Postdoc, Principal Investigator

Department of Energy, Technical University of Denmark

Department of Chemistry, University of Oxford

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I have recently been awarded a 4 000 000 DKK (~ £500 000) grant to pursue an academic career in the interface of materials chemistry, machine learning and robotics. I will as principal investigator build a self-driving laboratory for controlled synthesis of inorganic nanomaterials.

## POSITIONS

Visiting Postdoctoral Fellow, Department of Chemistry, University of Oxford, England 2024 –

Postdoc, Department of Energy, Danish Technical University, Denmark 2023 –

Postdoc, Department of Chemistry, University of Copenhagen, Denmark 2023

PhD, Department of Chemistry, University of Copenhagen, Denmark 2018 – 2023
Supervisor: Associate Professor Kirsten Marie Ørnsbjerg Jensen
Dissertation: "Towards Automated Structure Analysis of Nanoparticles"

Visiting Researcher, Rutherford Appleton Laboratory, England 2021 – 2022
Mentor: Sr. Lecturer Keith T. Butler

## EDUCATION

**University of Copenhagen, Denmark, supervision: Kirsten M. Ø. Jensen**

PhD in Chemistry 2018 – 2023
Dissertation: *"Towards automated structure analysis of nanoparticles"*

MSc in Nanoscience, (4.0 / 4.0 GPA) 2018 – 2021
Dissertation: *"Pushing the boundaries of nanocluster modelling from PDF and SAXS Analysis"*

BSc in Nanoscience, (4.0 / 4.0 GPA) 2015 – 2018
Dissertation: *"The formation of {$Bi_{38}O_{45}$} clusters from crystalline [$Bi_6O_8$] suspended in DMSO characterised with PDF and SAXS"*

## SELECTED PUBLICATIONS (ORCID: 0000-0002-7403-6642) (Google Scholar: bit.ly/AndyGoogleScholar)

I have published 18(6) journal-, 3(3) ML-venue-, and 3(1) preprint publications (submitted) where the paranthesis indicate (co)first authorships. 2 papers are as corresponding author. My work is cited 123 times in total.

*Machine learning for analysis of experimental spectroscopy and scattering data in materials chemistry*, **A. S. Anker**, et al., Chemical Science 2023

*Using generative adversarial networks to match experimental and simulated inelastic neutron scattering data*, **A. S. Anker**, et al., Digital Discovery **(Front cover)** 2023

*DeepStruc: Towards structure solution from pair distribution function data using deep generative models*, **A. S. Anker** & E. T. S. Kjær, et al., Digital Discovery **(Front cover)**+AI4MAT NeurIPS 2022

*Extracting Structural Motifs from Pair Distribution Function Data of Nanostructures using Explainable Machine Learning*, **A. S. Anker**, et al., npj Computational Materials + AI4MAT NeurIPS **(MAX IV annual report highlight)** 2022

*Structural Changes during the Growth of Atomically Precise Metal Oxido Nanoclusters from Combined Pair Distribution Function and Small-Angle X-ray Scattering Analysis*, **A. S. Anker**, et al., Angewandte Chemie **(Back cover)** 2021

## FUNDING

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|---|---|---|---|
| 2023 – Today | Research Grant | Postdoctoral Fellowship from Novo Nordisk Foundation | 4 000 000 DKK |
| | | Granted ten other grants of total | ~143 000 DKK |

## AWARDS AND HONORS

AI-Generated Art Challenge: Nordic Landscapes – Nordic AI 2023 2023

Best Talk, PhD Seminar, Department of Chemistry, University of Copenhagen 2022

Winning Team in the Danish Fungi Challenge – ML Hackathon 2022

Poster Prize, ISIS Student Meeting, Harwell, England 2021

Poster Prize, Analysis of Diffraction Data, Grenoble, France 2019

Poster Prize, Inorganic Student Seminar, Odense, Denmark 2019

Best Bachelor Thesis, Department of Chemistry, University of Copenhagen 2018

## PRESENTATIONS

9 contributed talks to summer schools(1), seminars (2), national-(3) and international conferences(1)
22 contributed posters summer schools(1), national-(10) and international conferences (10)
3 invited talks:

*"AI in Science: Transforming Communication, Data Analysis, and Laboratory Practices", DTU NanoLab, Copenhagen, Denmark* *2024*

"*Towards Automated Structure Analysis of Nanoparticles*", Materials Innovation Factory, Liverpool, England 2023

"Using Generative Adversarial Networks to match experimental and simulated inelastic neutron scattering data", European Spallation Source Data Management and Software Centre, Copenhagen, Denmark 2022

**BEAMTIMES** ~20 scattering and spectroscopy experiments at international radiation facilities

## TEACHING AND OUTREACH

Paper in the danish popular science journal - Aktuel Naturvidenskab

Twitter takeover (@RealSci_Nano) and outreach video (https://youtu.be/PywCje9_YF4)

Co-supervised 6 students, Department of Chemistry, University of Copenhagen
- 2 MSc students in machine learning for structure solution from pair distribution function data
- 3 BSc students using machine learning to analyse scattering data
- 1 BSc student using scattering to understand the formation process of nanomaterials

Teaching assistant for chemistry courses, 740 hrs., Department of Chemistry, University of Copenhagen
- Applied Spectroscopy I General and Inorganic Chemistry I General Chemistry for Life Sciences

Student assistant at Nano-Science Center & Skoletjenesten, University of Copenhagen 2016 – 2018
- Organising and teaching 1–5 days teaching events for primary and high school students
- Teaching nanoscience, chemistry and physics for primary school students

Teaching qualification course, Department of Science Education, University of Copenhagen, 3ECTS

Guest lecture "Applied Mathematics for Chemists" 2023

## REVIEW EXPERIENCE

ACS Reviewer Lab Course 2022

Reviewed 16 papers: (AI4PS workshop at NeurIPS: 4 (2022) & 3 (2023), AI4Mat workshop at NeurIPS: 2 (2023), *npj* Computational Materials: 7)

github.com/AndySAnker
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