ANDY SODE ANKER, PhD

Principal Investigator, Postdoctoral Fellow

Department of Energy, Technical University of Denmark

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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.

CURRENT POSITIONS

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

Postdoctoral Fellow, Department of Energy, Danish Technical University, Denmark — Dec 2023 –

PREVIOUS POSITIONS

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 20(8) journal-, 3(3) ML-venue-, and 3(0) preprint publications (submitted) where the parentheses indicate (co)first authorships. 2 papers are as a corresponding author. My work is cited 134 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

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

3 Poster Prizes, (England 2019, France 2019, Denmark 2021)

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)
5 invited talks:

"TBA", Chemical Compound Space Conference, *Heidelberg, Germany* *2024*

"TBA", Conference: Machine Learning Modalities for Materials Science, *Ljubljana, Slovenia* *2024*

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

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

"Using Generative Adversarial Networks to match experimental and simulated inelastic neutron scattering data", Seminar: ESS Data Management and Software Centre, Copenhagen, Denmark 2022

1 invited keynote talk:

"Generative machine learning for scattering and spectroscopy data analysis", Machine Learning Conference for X-Ray and Neutron-Based Experiments, *Garching, Germany* *2024*

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

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


github.com/AndySAnker


bit.ly/AndyGoogleScholar


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andysanker.github.io