ANDY SODE ANKER

Postdoc, Department of Chemistry, University of Copenhagen

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I have recently been awarded a 4 000 000 DKK (~ £460 000) postdoctoral grant to pursue an academic career in the interface of materials chemistry, machine learning and robotics. Here, I will build a self-driving laboratory for controlled synthesis of inorganic nanomaterials starting from 1st December 2023.

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

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 13(4) journal-, 3(3) ML-venue-, and 5(3) preprint publications (submitted) where the paranthesis indicate (co)first authorships. 2 papers are as corresponding author. I am cited 93 times in total.

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

POMFinder: Identifying polyoxometalate cluster structures from pair distribution function data using explainable machine learning, **A. S. Anker**, et al., (Submitted IUCrJ) 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 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

Characterising the Atomic Structure of Mono-Metallic Nanoparticles from X-Ray Scattering Data Using Conditional Generative Models, **A. S. Anker** & E. T. S. Kjær, et al., SIGKDD, 16th International Workshop on Mining and Learning with Graphs 2020

FUNDING

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)
2 invited talks:

"*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 | General and Inorganic Chemistry | 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 9 papers: (AI4PS workshop at NeurIPS: 4 (2022) & 3 (2023), *npj* Computational Materials: 2)


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