

ANDY SODE ANKER



Integrated 3+5 MSc & PhD, Department of Chemistry, University of Copenhagen



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Through my Master's and doctoral degree, I have established an international research profile within applied data science for materials chemistry. I am specifically interested in experimental scattering- and spectroscopy data analysis using machine learning. This has led to 17 publications, several awards and grants, international collaborations, co-supervision of six students and the installation of two software packages at the MAX IV synchrotron in Sweden. I have recently been awarded a 4 000 000 DKK (~ £500 000) postdoctoral grant to pursue an academic career in the interface of materials chemistry, machine learning and automation. 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 Supervisor: Associate Professor Kirsten Marie Ørnsbjerg Jensen Dissertation: "Towards Automated Structure Analysis of Nanoparticles"	2018 – 2023
Visiting Researcher, Rutherford Appleton Laboratory, England Mentor: Sr. Lecturer Keith T. Butler	2021 – 2022

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

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

Using generative adversarial networks to match experimental and simulated inelastic neutron scattering data, A. S. Anker, et al., RSC 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., RSC 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 Oxide 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



github.com/AndySAnker



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bit.ly/AndyGoogleScholar

FUNDING

2023	Travel Grant	AI in Chemistry 2023 Bursary	700 £
2023	Research Grant	Postdoctoral Fellowship from Novo Nordisk Foundation	4 000 000 DKK
2022	Travel Grant	Danish Data Science Academy	15 000 DKK
2021	Travel Grant	Augustinus Foundation	22 500 DKK
2021	Travel Grant	Manufacturer Vilhelm Pedersen and wife Foundation	9000 DKK
2021	Travel Grant	Haynmann Foundation	15 000 DKK
2021	Travel Grant	Henry and Mary Skovs Foundation	6000 DKK
2021	Travel Grant	Thomas B. Thriges Foundation	25 000 DKK
2021	Travel Grant	Viet Jacobsen Foundation	9000 DKK
2021	Travel Grant	Knud Højgaard Foundation	16 000 DKK
2018	Research Grant	Siemens Foundation	20 000 DKK

AWARDS AND HONORS

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

TALKS

Using generative adversarial networks to match experimental and simulated INS data:

- UK Neutron & Muon Science and User Meeting (NMSUM), Warwick, England 2022

Machine helping the chemist - towards automated modelling of pair distribution function Data:

- SMART Meeting, Copenhagen, Denmark 2022
- **Best talk award** to PhD Seminar, Department of Chemistry, University of Copenhagen 2022
- SMART Student Meeting, Århus, Denmark 2022
- SMART Lighthouse PhD Summer School , Sønderborg, Denmark 2021

Formation mechanism of metal oxido clusters: A complex modelling study using PDF and SAXS:

- Danscatt Annual Meeting, Århus, Denmark 2019
- Nanoscience Symposium, Copenhagen, Denmark 2018

INVITED TALKS

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

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

POSTERS 21 contributed summer schools(1), national-(10) and international conferences (10)

BEAMTIMES ~20 scattering and spectroscopy experiments (PDF, SAXS, XRD and INS) at international radiation facilities (MAX IV, DESY, ESRF, Soleil, ILL, APS)



TEACHING EXPERIENCE

Paper in the danish popular science journal - Aktuel Naturvidenskab – “Med et atomart blik på verden: MATERIALEUDVIKLING PÅ NANOSKALA”

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 “Introduction to University Pedagogy”, Department of Science Education, University of Copenhagen, 3ECTS

Guest lecture “Applied Mathematics for Chemists” 2023

PUBLICATIONS (ORCID: [0000-0002-7403-6642](https://orcid.org/0000-0002-7403-6642)) (Google Scholar: bit.ly/AndyGoogleScholar)

Number of peer-reviewed journal publications (first-author) 14 (4)

Number of peer-reviewed ML-venues publications (first-author) 3 (3)

Number of preprints (first-author) 1 (0)

Number of corresponding-author publications (preprints) 1 (0)

Number of citations 70

REVIEW EXPERIENCE

ACS Reviewer Lab Course 2022

Reviewed 5 papers: (AI4PS workshop at NeurIPS: 4, npj Computational Materials: 1)

SOFTWARE SKILLS

Co-responsible for an AI workstation, High Performance Computing, GPU-accelerated Computing, Cloud Computing, Version Control, Job Scheduler, Python, Machine Learning, App development, frequent user of AI image and text generation.

REFERENCES

Keith T. Butler, Ph.D.

Senior Lecturer

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Materials Science

Queen Mary University of London

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Volker Deringer, Ph.D.

Associate Professor

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Kirsten M. Ø. Jensen, Ph.D.

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