

ANDY SODE ANKER



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



andy@chem.ku.dk



+45 21 30 68 67



andysanker.github.io

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 how experimental scattering- and spectroscopy data can be analysed with machine learning. This has led to 16 publications, several awards and grants, international collaborations, co-supervision of 6 students and the installation of 2 software packages at beamline DanMAX, MAX IV. I am now interested to pursue an academic career in the interface of machine learning and materials chemistry.

CURRENT POSITION

2018 – present

Department of Chemistry, University of Copenhagen, Denmark

PhD Student, supervisor: Associate Professor Kirsten Marie Ørnsbjerg Jensen

EDUCATION

University of Copenhagen (UCPH), Denmark, supervision: Kirsten M. Ø. Jensen

Integrated 3+5 MSc & PhD

2018 – Aug. 2023

Dissertation: *"Using machine learning to analyse experimental scattering data in materials chemistry"*

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"*

SCHOLARLY FIRST-AUTHOR PUBLICATIONS

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

ClusterFinder: A fast tool to find cluster structures from pair distribution function data, A. S. Anker, et al., to be submitted 2023

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



github.com/AndySAnker



andysanker.github.io



bit.ly/AndyGoogleScholar

OTHER RELEVANT POSITIONS

Sept. 2021 – Mar. 2022

Scientific Machine Learning Group, Rutherford Appleton Laboratory, England

Visiting PhD Student, Supervisor: Sr. Lecturer Keith T. Butler

AWARDS AND HONORS

Best Talk, PhD Seminar, Department of Chemistry, University of Copenhagen	2022
Winning Team in the Danish Fungi Challenge – ML Hackathon	2022
Travel Research Grant, Danish Data Science Academy (15 000 DKK)	2022
Poster Prize, ISIS Student Meeting, Harwell, England	2021
Travel Research Grant, Augustinus Foundation (22 500 DKK)	2021
Travel Research Grant, Manufacturer Vilhelm Pedersen and wife Foundation (9000 DKK)	2021
Travel Research Grant, Haynmann Foundation (15 000 DKK)	2021
Travel Research Grant, Henry and Mary Skovs Foundation (6000 DKK)	2021
Travel Research Grant, Thomas B. Thriges Foundation (25 000 DKK)	2021
Travel Research Grant, Viet Jacobsen Foundation (9000 DKK)	2021
Travel Research Grant, Knud Højgaard Foundation (16 000 DKK)	2021
Poster Prize, Analysis of Diffraction Data, Grenoble, France	2019
Poster Prize, Inorganic Student Seminar, Odense, Denmark	2019
Siemens Foundation Research Grant, (20 000 DKK)	2018
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

"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 20 contributed summer schools(1), national-(9) 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)

Twitter takeover (@RealSci_Nano) and outreach video (https://youtu.be/PywCje9_YF4) 2022



TEACHING EXPERIENCE

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

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 3 Chemistry courses at 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

- Organizing 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 “Introduction to the Mathematics for the Chemical Sciences” 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) 12 (4)

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

Number of preprints (first-author) 2 (0)

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

Number of citations 41

REVIEW

ACS Reviewer Lab Course 2022

Reviewed 4 papers for the AI4PS workshop at NeurIPS 2022

SOFTWARE SKILLS

Co-responsible for an AI workstation, High Performance Computing, GPU-accelerated Computing, Multiprocessing, Cloud Computing, Version Control, Job Scheduler (Slurm), Python, Numpy, Pandas, Scikit-learn, SQL, Machine Learning, PyTorch, PyTorch Lightning, PyTorch Geometric, Generative Modelling, XGBoost, SHAP, autoML, visualization tools (Matplotlib, Seaborn, Bokeh, Plotly), Linux, MacOS, Windows, app development, frequent user of AI image and text generation.

REFERENCES

Keith T. Butler, Ph.D.

Senior Lecturer

School of Engineering and

Materials Science

Queen Mary University of London

k.butler@qmul.ac.uk

Raghavendra Selvan, Ph.D.

Assistent Professor

Department of Computer Science

Department of Neuroscience

University of Copenhagen

raghav@di.ku.dk

Kirsten M. Ø. Jensen, Ph.D.

Associate Professor

Department of Chemistry

Nano-Science Center

University of Copenhagen

kirsten@chem.ku.dk



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