

Rapportskema - forskningsinfrastruktur

Styrelsen for Forskning og Innovation

Bredgade 40

1260 København K



Uddannelses- og
Forskningsministeriet

Styrelsen for Forskning og Innovation

Dato

Bevilling og bevillingshaver

Bevillingens akronym og titel

Sagsnr. (f.eks. 5072-01234B)

Bevillingshavers navn, stilling,
arbejdsplads, adresse, telefonnr.
og e-mail

Bevillingens hjemmeside

Bevilling

Egen
finansiering

Anden
finansiering

Bevilling i alt

Oprindelig projektperiode (dd-mm-åååå)

Fra

Til

Senest godkendte
projektperiode (dd-mm-åååå)

Fra

Til

Årsagerne til eventuelle
ændringer i bevillingsperioden

Ledelse og konsortium

Faglig leders navn, stilling,
arbejdsplads, adresse, telefonnr.
og e-mailadresse

Konsortium-deltagere, f.eks.
universiteter, virksomheder og
offentlige institutioner (nævnes
på institutionsniveau)

Øvrige parter

Status og resultater for projektet

Der redegøres for status og resultater for projektets fremdrift i henhold til det senest godkendte projektforslag, -budget og –periode, herunder redegøres for eventuelle afvigelser fra disse. Redegørelsen skal i videst muligt omfang beskrive nedenstående punkter hvad angår henholdsvis forskningsinfrastrukturen, det videnskabelige udbytte og værdiskabelsen for samfund, innovation og erhverv.

Forskningsinfrastrukturen

Konstruktion, etablering og indkøb (f.eks. apparatur og software)

Projekt- og tidsplan

Adgangspolitik (alle nationale forskningsinfrastrukturer skal have en klart defineret adgangspolitik for akademiske og industrielle brugere)

Data management og tilgængelighed

Brugerstøtte (for akademiske og industrielle brugere)

Kompetenceopbygning (f.eks. kurser, informations- og undervisnings-materiale)

Opsøgende aktiviteter (f.eks. informations- og opstartsmøder, nyhedsbreve, mv.)

Planer for driften efter
bevillingsperiodens udløb (kun
ved slutrapport)

Det forventes, at de involverede
forskningsinstitutioner påtager
sig ansvar for den videre drift af
forskningsinfrastrukturen efter
dens etablering

Videnskabeligt udbytte

Antal brugere
(forskningsformål), herunder
om muligt institutionel
fordeling af brugere samt evt.
internationale brugere

Publikationer (som eksplicit er
baseret på brug af/data fra
forskningsinfrastrukturen)

Internationalt samarbejde
(herunder f.eks. samarbejder
med ESFRI-projekter)

Mobilitet, uddannelse og
tiltrækning (f.eks. ph.d. og
postdocs)

Værdiskabelse for samfund og erhverv

Samarbejder med andre uden
for forskningsinstitutioner,
f.eks. virksomheder, GTS-
institutter, innovationsnetværk

Brugere uden for
forskningsinstitutioner, f.eks.
fra virksomheder, GTS-
institutter, innovationsnetværk,
m.fl.

Nye teknologier, metoder,
processer, mv. baseret på
resultater fra
forskningsinfrastrukturen

Nye produkter baseret på
resultater fra
forskningsinfrastrukturen

Nye virksomheder baseret på
resultater fra
forskningsinfrastrukturen

Samfundsmæssig værdi (f.eks.
samarbejder med andre
myndigheder, organisationer,
m.fl.)

Andet

Nye ansøgninger til
forskningsinfrastruktur eller
forskningsprojekter, der er
direkte afledt af bevillingens
resultater (f.eks. til EU-midler,
private fonde, osv.)

Ny finansiering til
forskningsinfrastruktur eller
forskningsprojekter, der er
direkte afledt af bevillingens
resultater (f.eks. fra EU-midler,
private fonde, osv.)

Anmodninger om faglige ændringer i bevillingsgrundlag som kræver FI's godkendelse (kun ved årsrapporter)

Jf. Vilkår for bevillinger anses ændring af administrator, bevillingshaver, forskergruppe og aktivitetens ledelse altid for større ændringer og kræver forhåndsgodkendelse. Det samme gælder ændringer af faglig karakter. Anmodninger om faglige ændringer i bevillingsgrundlag skal her begrundes. Anmodning om ændring af projektperiode skal ske via separat skema. Se desuden Vilkår for bevillinger.

Er der tidligere anmodet om og
godkendt faglige ændringer?

Ændringer i
forskningsinfrastrukturen

Ændringer af faglig kontakt

Ændringer af konsortium

Andre ændringer

Formidlingseget sammenfatning egnet til offentliggørelse på www.fi.dk (udfyldes kun, når skemaet bruges til faglig slutrapportering)

Beskriv på en enkel og forståelig måde forskningsinfrastrukturen på maksimum 1.000 anslag på dansk og 1.000 anslag på engelsk. Beskrivelsen vil blive offentliggjort uredigeret på Styrelsen for Forskning og Innovations hjemmeside www.fi.dk. Beskrivelsen bør tage udgangspunkt i følgende spørgsmål:

- Hvad er forskningsinfrastrukturens formål, forventede videnskabelige udbytte og værdiskabelse for samfund, innovation og erhverv?
- Hvad har forskningsinfrastrukturen ind til videre opnået i relation til ovenstående?

Formidlingseget præsentation
på dansk

Formidlingseget præsentation
på engelsk

Bilag 1: DANSCATT personoversigt 2017

I nedenstående tabeller er oplistet de personer, der har haft DANSCATT-relaterede aktiviteter i 2017. I alt drejer det sig om

102 VIP's (professors, senior scientists etc.)

102 Postdocs, assistant professors etc.

146 PhD studerende

81 studerende

31 TAP'ere (technicians, administrative staff) and scientific assistants

Department of Chemistry, Aarhus University

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIP's (professors, senior scientists etc.) 7 personer	Bo Brummerstedt Iversen (gruppeleder)	VIP, Beamtime	
	Henrik Birkedal	VIP, Beamtime	
	Martin Bremholm	VIP, Beamtime	
	Mogens Christensen	VIP, Beamtime	
	Hidetaka Kasai	VIP, Beamtime	
	Nina Lock	VIP, Beamtime	
	Mads Ry Vogel Jørgensen	VIP, Beamtime	
Postdocs, assistant professors etc. 9 personer	Yigang Yan	Beamtime	Hydrides for batteries
	Samera Siddiqui	Beamtime	Structure of Bio-inspired Inorganic Materials
	Chen Gao	Beamtime	Single molecule magnets
	Kasper Andersen Borup	Beamtime	Thin film synthesis
	Matilde Saura-Muzquiz	Beamtime	Magnetic Materials
	Cecilia Granados-Miralles	Beamtime	Magnetic Materials
	Lars Haahr Jepsen	Beamtime	Hydrogen Storage Materials
	Morten Bormann Nielsen	Beamtime	Structure of Bio-inspired Inorganic Materials
	Lennard Krause	Beamtime	Single molecule magnets
TAPs (technicians, administrative staff) and scientific assistants 5 personer	Jacob Becker	Beamtime, Admin	Vacuum diffractometer (AVID)
	Hazel Reardon	Beamtime, Admin	Thermoelectric Materials
	Bo Richter	Sample Preparation, Admin	
	Aref Mamakhel	Sample Preparation	
	Marianne Sommer	Admin	
PhD Students 25 personer	Hao Tang	Beamtime	Magnetic materials
	Mathias Salomon Hvid	Beamtime	Functional Nanoparticles
	Steffen R. H. Jensen	Beamtime	Hydrogen storage materials

Bilag 1: DANSCATT personoversigt 2017

	Jakob B. Grinderslev	Beamtime	Hydrogen storage materials
	Mattia Sist	Beamtime	Semiconductors
	Elisabeth Grube	Beamtime	Hydrogen storage materials
	Mathias Jørgensen	Beamtime	Magnetic materials
	Sanna Sommer	Beamtime	Functional nanoparticles
	Simone Kevy	Beamtime	Topological insulators
	Camilla Kronbo	Beamtime	Topological insulators
	Jakob Voldum Ahlburg	Beamtime	Magnetic Materials
	Martin Roelsgaard	Beamtime	In situ synthesis and X-ray analysis of thin films
	Kasper T. Møller	Beamtime	Hydrogen storage materials
	Pelle Gorm Garbus	Beamtime	Magnetic Materials
	Nina Kølln Wittig	Beamtime	Structure of Bio-inspired Inorganic Materials
	Frederik Munkeholm Søndergaard-Pedersen	Beamtime	In situ studies on the synthesis and morphology control of nano-oxides for catalysis
	Jinlong Yu	Beamtime	Tailored design and synthesis of nano-oxide catalysts
	Nils Laue Nyborg Broge	Beamtime	In situ studies on the synthesis and morphology control of nano metallic alloys for catalysis
	Emil Andreasen Klahn	Beamtime	Single molecule magnets
	Kasper Tolborg	Beamtime	Charge density studies
	Nikolaj Roth	Beamtime	3D Pair Distribution Function (PDF) analysis
	Bjarke Svane Boysen	Beamtime	Vacuum diffractometer (AVID)
	Christian Bonar Zeuthen	Beamtime	Synthesis of chalcogenides for thermoelectrics
	Lasse Rabøl Jørgensen	Beamtime	Combined PXRD and PDF analysis of thermoelectrics at high temperature
Students 21 personer	Jakob Mikkelsen	Beamtime	Piezoelectric Materials
	Mathias Mørch	Beamtime	Magnetic Materials
	Jonas Beyer	Beamtime	Hydrothermal synthesis of functional nano-oxides
	Jacob G. Andreasen	Beamtime	Hydrogen storage materials
	Steffan Schmidt	Beamtime	Topological insulators
	Ahmad Rinno	Beamtime	Topological insulators
	Ida Gjerlevsen Nielsen	Beamtime	Nanoparticles
	Frederik Gjørup	Beamtime	Magnetic Materials
	Anette Gert Kielland	Beamtime	Charge Density
	Thomas Bjørn Grønbech	Beamtime	Charge Density
	Mads Folkjær	Beamtime	Topological Insulators
	Xenia Hansen	Beamtime	In situ studies on the synthesis and morphology control of nano metallics for catalysis
	Kristoffer Holm	Beamtime	Charge Density
	Jonas Sandemann	Beamtime	Synthesis and structure of exotic Tye-1

Bilag 1: DANSCATT personoversigt 2017

			clathrates
	Maja Østergaard	Beamtime	Structure of Bio-inspired Inorganic Materials
	Henrik Jeppesen	Beamtime	Functional Nanomaterials
	Alexander Bernthz Jensen	Beamtime	Structure of Bio-inspired Inorganic Materials
	Jonas Palle	Beamtime	Structure of Bio-inspired Inorganic Materials
	Laiyang Li	Beamtime	Hydrogen storage materials
	Yigang Yi	Beamtime	Hydrogen storage materials
	Shaiq Ghorwal	Beamtime	Hydrogen storage materials
External persons present at beamtime:			
Assistant Professor (Bordeaux Université)	Gilles Phillipot (GCAM)	Beamtime	
PhD students	Aimery Auxmery	Beamtime	In situ hydrothermal synthesis of nanoparticle
	Ola Grøndal	Beamtime	In situ hydrothermal synthesis of nanoparticle
	Isaiah Chua	Beamtime	In situ hydrothermal synthesis of nanoparticle
	Petr Pridhochenko	Beamtime	In situ hydrothermal synthesis of nanoparticle

Department of Molecular Biology, Aarhus University

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 8 personer	P. Nissen	Vejleder, tolkning	
	G.R.Andersen	Vejleder, tolkning, x-experiment	
	T.Boesen	Vejleder, tolkning, x-experiment	
	D.E.Brodersen	Vejleder, tolkning, x-eksperiment	
	R.Hartmann	Vejleder, tolkning, x-eksperiment	
	L.B. Jenner	Vejleder, tolkning, x-eksperiment	
	S.S.Thirup (gruppeleder)	Vejleder, tolkning, x-eksperiment	
	C. B. F. Andersen	Vejleder, tolkning, x-eksperiment	
Postdocs, assistant professors etc. 3 personer	B.P.Pedersen	Vejleder, tolkning, x-eksperiment	
	N.S.Laursen	Sample prep, x-eksperiment, tolkning	
	K.R.Andersen	Vejleder, tolkning, x-eksperiment	

Bilag 1: DANSCATT personoversigt 2017

TAPs (technicians, administrative staff etc) 9 personer	J.L.Karlsen	Computing infrastructure	
	L.B.Van	Sample prep.	
	L. T. Pedersen	Sample prep.	
	A.M. Nielsen	Sample prep.	
	T. Klymchuk	Sample prep.	
	D. Strandbygård	Sample prep.	
	K.M. Nielsen	Sample prep	
	S. Vends	Sample prep	
	G. Ratz	Sample prep.	
Postdocs 18 personer	J. L. Andersen	sample prep., x-eksperiment, tolkning	Structural studies of drug/biotek targets, industry collaborations
	A.Bøggild	sample prep., x-eksperiment, tolkning	LINX researcher, Ca ²⁺ -ATPase crystallization in lipid nanodiscs
	C. E. Olesen	sample prep., x-eksperiment, tolkning	Structural studies of Ca ²⁺ -ATPase from heart muscle
	H.H. Gad	sample prep. x-eksperiment, tolkning	cytokines
	R. Kidmose	sample prep., x-eksperiment, tolkning	Sugar transporters
	Kristian Stødkilde Jørgensen	sample prep. x-eksperiment	Structural studies of Isg75
	Azadeh Shasavar	sample prep. x-eksperiment, tolkning	Human neurotransmitter transporters
	Joseph Lyons	sample prep. x-eksperiment, tolkning	Lipid flippases and P5-ATPases
	Meriem Senissar	sample prep. x-eksperiment, tolkning	Structure of archaeal persistence factors
	J.L. Gregersen	Sample prep, x-eksperiment, tolkning	Ribosomes
	Kira Gysel	sample prep. x-eksperiment, tolkning	Structural studies of LysM receptors.
	P.A. Paulsen	sample prep. x-eksperiment, tolkning	Sugar transport
	Prasad Kasaragod	sample prep. x-eksperiment, tolkning	Ca ²⁺ -ATPase:peptide complexes
	Dennis V Pedersen	sample prep. x-eksperiment, tolkning	Complement antibody-complexes
	J.M. Wong	Sample prep, x-eksperiment, tolkning	Structural studies of LysM receptor like kinases
	Casper Larsen	sample prep. x-eksperiment	Sugar transporters
	Jakob Mikkelsen	sample prep. x-eksperiment	Structural studies of Isg75
	Antoni Kowalski	sample prep. x-eksperiment	Plasma-membrane Ca ²⁺ -ATPase

Bilag 1: DANSCATT personoversigt 2017

PhD students 27 personer	Ewa Anna Terczynska-Dyla	Sample prep	Structure and function of Interferon receptors
	J. A. Schatz-Jakobsen	sample prep. x-eksperiment, tolkning	Complement and danger sensing receptors
	Mateusz Dyla	sample prep. x-eksperiment, tolkning	Listeria Ca ²⁺ -ATPase
	Morten Torvund-Jensen	sample prep. x-eksperiment	Structural studies of the hemoglobin scavenging receptor CD163
	Sigrid T. Larsen	sample prep. x-eksperiment, tolkning	Calmodulin activated Ca ²⁺ -ATPases
	Jeryl Cheng	sample prep. x-eksperiment, tolkning	Structural studies of plant Lysm receptor like kinases
	Rasmus K Jensen	sample prep. x-eksperiment, tolkning	Complement receptors
	Alessandra Zarantonello	sample prep. x-eksperiment, tolkning	Complement receptors
	Trine AF Gadeberg	sample prep. x-eksperiment, tolkning	Complement proteases
	Caroline Neumann	sample prep. x-eksperiment	Neurotransmitter transporters, chloride transporters
	Jacob Ulstrup	sample prep. x-eksperiment	Lipid flippases
	Marlene Sørensen	sample prep. x-eksperiment	Na ⁺ ,K ⁺ -ATPase, RSK/MSK kinases, neutron crystallography
	Melek Cemre Manav	sample prep. x-eksperiment, tolkning	Structural studies of the bacterial stringent response
	Rasmus K Flygaard	sample prep. x-eksperiment	Ribosomes
	Joachim Vilstrup	sample prep. x-eksperiment	PCSK9, Vps10p and CLC-CLF
	Aljona Kotsubei	sample prep. x-eksperiment,	Ca ²⁺ -ATPase from heart muscle
	Jeppe A. Nielsen	sample prep. x-eksperiment	Structure of the Vps10p domain
	Tania Custodio	sample prep. x-eksperiment	Sugar transport
	Mikael Winkler	sample prep. x-eksperiment	Sterol transport
	Andreas Holleufer	sample prep. x-eksperiment, tolkning	Antiviral proteins
	Hao Zhou	sample prep	Antiviral proteins
	Sara Basse	sample prep. x-eksperiment	Listeria Ca ²⁺ -ATPase
	Milena Laban	sample prep. x-eksperiment	Lipid flippases
	Josephine Nissen	sample prep. x-eksperiment	Plasma-membrane Ca ²⁺ -ATPase
	Sofia Trampari	Sample prep. X-eksperiment	Krystallisation af Membranproteiner
	Samuel Hjort-Jensen	Sample prep. X-ray og Neutron diffraktion	Sarco/endoplasmic reticulum Ca ²⁺ -ATPase
	Henrik Pedersen	sample prep. X-	Complement-nanobody complexes

Bilag 1: DANSCATT personoversigt 2017

		eksperiment	
Students 3 personer	Thea G. Birkefeldt	sample prep. x-eksperiment	Nanobodies and LysM receptors
	Simon B Hansen	sample prep. x-eksperiment	Nanobodies and LysM receptors
	René Bærentsen	sample prep. x-eksperiment	Bacterial stringent response

DTU Cen

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 1 person	Christian Damsgaard	Combination of x-ray and electron microscopy	

DTU Chemistry

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 6 personer	René Wugt Larsen	Beam-time at SOLEIL	"Exploring the Potential Energy Landscapes of Weakly Bound Molecular Dimers: High-Resolution Synchrotron Terahertz Spectroscopy"
	Klaus B. Møller	Teori for og computersimulering af strukturel dynamik studeret med XFELs	
	Kenny Stahl (gruppeleder)	PXRD, XAS	
	Hans Mølager Christensen	Synkrotronstudier, PX	
	Pernille Harris	MX, SAXS, XAS	
	Günther Peters	SAXS	
Postdocs, assistant professors etc. 5 personer	Peter Westergaard Jakobsen	Beam-time at SOLEIL	"Exploring the Potential Energy Landscapes of Weakly Bound Molecular Dimers: High-Resolution Synchrotron Terahertz Spectroscopy"
	Mátyás Imre Pápai	Computersimuleringer af strukturel dynamik studeret med XFELs	Kortlægning af photoinduceret strukturel dynamik i overgangsmetal komplekser.
	Christian Engelbrekt	Synkrotronstudier, pulverdiffraktion, EXAFS	EXAFS og pulverdiffraktion på Cu-nano-systemer
	Pernille Sønderby	SAXS	Protein-protein interactions

Bilag 1: DANSCATT personoversigt 2017

	Sanaullah Kahn	SAXS	Protein-oligosaccharide interactions
PhD students	Dmytro Mihrin	Beam-time at SOLEIL	"Exploring the Potential Energy Landscapes of Weakly Bound Molecular Dimers: High-Resolution Synchrotron Terahertz Spectroscopy"
12 personer	Alexandre Paolo Voute	Beam-time at SOLEIL	"Exploring the Potential Energy Landscapes of Weakly Bound Molecular Dimers: High-Resolution Synchrotron Terahertz Spectroscopy"
	Gianluca Levi	XFEL-eksperimenter: Dataanalyse og computersimuleringer	Kortlægning af photoinduceret strukturel dynamik i overgangsmetal komplekser.
	Mats Simmermacher	Teori for kemisk dynamik studeret med XFELs	Udarbejdelse af teori for signaturer af elektroners dynamik i XFEL eksperimenter
	Mostafa Abedi	Computersimuleringer strukturel dynamik studeret med XFELs	Kortlægning af photoinduceret strukturel dynamik i overgangsmetal komplekser.
	Ulf Molich	XAS	Radiation damage, metalloproteins
	Alina Kulakova	SAXS	PIPPI
	Sujata Mahapatra	SAXS	PIPPI
	Christin Pohl	SAXS	PIPPI
	Sowmya Indrakumar	Teoretiske simuleringer af SAXS	PIPPI
	Natalia Skawinska	SAXS	Tryptophan hydroxylase
	Line Ryberg	SAXS	Protein-protein interactions
Chemist	Maria Blanner	Sample preparation	
1 person			

DTU Energy

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.)	Jacob R. Bowen	Beamtime participant	
10 personer	Peter Stanley Jørgensen	Beamtime participant	
	Karin V. Hansen	Planning experiment for beamtime	
	Jens W. Andreassen (gruppeleder)	Beamtime participant	
	Nini Pryds	Beamtime participant	
	Yunzhong Chen	Beamtime participant	
	Didier Blanchard	Beamtime participant	
	Luise Theil Kuhn	Beamtime participant	

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Postdocs, assistant professors etc. 5 personer	Poul Norby	Beamtime participant	
	Torben Jacobsen	Planning experiment for beamtime	
	Salvatore De Angelis	Beamtime participant	<i>In situ</i> 3D solid oxide cell electrode microstructure evolution
	Rune E. Johnsen	Travel activities in connection to experiments at large facilities (X-ray and neutron)	<i>In operando</i> studies of the structure and microstructure of Li-rich FCC electrode materials for battery applications
	Christian Rein	Beamtime participant	Time-resolved X-ray absorption spectroscopy of kesterite nanoparticles
PhD students 11 personer	Dennis Christensen	Beamtime participant	Investigating the band inversion in g-Al ₂ O ₃ /STO and its relation to content of oxygen vacancies using Angle-Resolved Photoelectron Emission (ARPES) and Resonant Inelastic X-ray Scattering (RIXS) experiments to directly measure the resulting electronic structure. Understanding that can help understanding the origin of the mobility in this sample.
	Roberto Scipioni	Beamtime participant	<i>In situ</i> synchrotron studies of lithium ion batteries.
	José Xavier Sierra Trujillo	Beamtime participant	<i>In situ</i> dark field X-ray microscopy of solid oxide cell electrolyte degradation
	Martina Trini	Beamtime participant	Helping other project
	Giovanni Fevola	Beamtime participant	MAX IV Expert Commissioning scanning fluorescence and ptychography
	Tiago Ramos	Beamtime participant	MAX IV Expert Commissioning scanning fluorescence and ptychography
	Khadijeh Khalili	Planning experiment for beamtime	Time-resolved X-ray scattering and spectroscopy of polymer heterojunctions
	Mariana M. Lucas	Planning experiment for beamtime	3D X-ray diffraction of kesterite solar cell absorber layers
	Anders S. Gertsen	Planning experiment for beamtime	X-ray scattering of polymer heterojunctions
	Lea H. Rossander	Planning experiment for beamtime	X-ray scattering of polymer heterojunctions
	Jessica Lefevr	Beamtime participant	Development and characterization of emerging battery electrodes and electrolytes
	Monica-Elisabeta Lacatusu	Beamtime participant	Phase distribution visualisation in solid oxide cells by monochromatic Bragg edge tomography
	Simone Santucci	Beamtime participant	Study Giant Electrostriction effect in Gd-doped Ceria thin film, for electromechanical application. Giant-E has been discovered only recently, and it

Bilag 1: DANSCATT personoversigt 2017

			can have a high impact in different field application, like actuators and transducers. The project ongoing is aimed to explain the main mechanism behind giant electrostriction, and find the best condition to enhance this effect. To do this experiments in a synchrotron are needed to analyze x-ray absorption in CGO samples.
Students 1 person	Jette Katja Mathiesen	Beamtime participant	<i>In situ</i> synchrotron studies of lithium-ion and sodium ion batteries using diffraction and scattering (pdf analysis)
TAPs (technicians, administrative staff etc.)	Ebtisam Abdellahi	Sample preparation for beamtime	
	Pernille H. Nielsen	Sample preparation for beamtime	
	Lene Knudsen	Sample preparation for beamtime	
	Karen Brodersen	Sample preparation for beamtime	
	John Johnson	Preparing setup for sample preparation	
	Søren Koch,	Preparing sample environments for <i>in situ</i> measurements	
	Jens V. T. Høgh	Preparation of in-operando setup	

DTU Mechanical Engineering

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 10 personer	Wolfgang Pantleon (gruppeleder)	Synkrotroneksperimenter	
	Seunghwan Lee	Neutroneksperimenter	
	Karen Pantleon	Synkrotroneksperimenter	
	Marcel Somers	Synkrotroneksperimenter	
	Grethe Winther	Synkrotroneksperimenter	
	Thomas Christiansen	Synkrotroneksperimenter	
	Matteo Villa	Synkrotroneksperimenter	
	Jesper Hattel	Synkrotroneksperimenter	

Bilag 1: DANSCATT personoversigt 2017

	Dorte Juul Jensen	Synkrotroneksperiment	*
	Yubin Zhang	Synkrotroneksperiment	*
Postdocs, assistant professors etc.	Tianbo Yu	Synkrotroneksperiment	*
5 personer	Tito Andriollo	Synkrotroneksperiment	<i>Modelling the effects of process induced defects on subsequent mechanical behaviour of cast components</i>
	Chitta Ranjan Das	Synkrotroneksperiment	<i>Creep resistant steels and welds for ultra super critical power plants</i>
	Nikolai Ytterdal Juul	Synkrotroneksperiment	<i>Characterisation and modelling of crystallographic orientation changes at the grain scale during plastic deformation</i>
	Troels Røn	Neutroneksperiment	<i>Spontaneously Segregated Polymer Brush Structure</i>
PhD students	Jacob Obitsø Nielsen	Synkrotroneksperiment	<i>Surface engineering of Fe-C coatings</i>
3 personer	Frank Nissen	Synkrotroneksperiment	<i>Supermartensitic Stainless Steels for oil and gas applications</i>
	Annika Martina Diederichs	Synkrotroneksperiment	<i>Structural reorganization during cyclic deformation</i>
TAPs (technicians, administrative staff etc.) and scientific assistants	Fleming Bjerg Grumsen	Synkrotroneksperiment	
2 personer	Yichen Meng	Synkrotroneksperiment	
Students	Chloe Devos	Synkrotroneksperiment	<i>Cryotreatment of tool steels</i>
1 person			

* from DTU Vind, joined DTU MEK 01.10.2017

DTU Physics

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.)	Anders Dahl (DTU Compute)	Synkrotron	
9 personer	Cathrine Frandsen	Neutron	
	Henning Friis Poulsen (Gruppeleder)	Synkrotron, direktør for DANSCATT	
	Kristoffer Haldrup	XFEL	
	Martin Meedom Nielsen	XFEL, bestyrelsesmedlem	
	Matti Knaapila	Neutron, synkrotron	
	Niels Bech Christensen	Neutron, bestyrelsesmedlem	
	Søren Schmidt	Synkrotron, neutron	
	Innokenty Kantor	Synkrotron	
Postdocs, assistant professors etc.	Alberto Cereser	Synkrotron	
13 personer	Anders Clemen Jakobsen	Synkrotron	
	Anders Filsøe Pedersen	Synkrotron	
	Elisa Biasin	XFEL	
	Hanna Leemreize	Synkrotron	
	Hugh Simons	Synkrotron	
	Kasper Skov Kjær	XFEL	
	Morten Sales	Synkrotron, neutron	
	Mika Torkkeli	Neutron, synkrotron	
	Nanna Wahlberg	Synkrotron	
	Rasmus Toft-Petersen	Neutron	
	Tobias Harlang	XFEL	
	Yi Zheng	Synkrotron	
PhD students	Diana Zederkof	XFEL	
7 personer	Ellen Fogh	Neutron	
	Jeppe Ormstrup	Synkrotron	
	Jin Zhang	Synkrotron	
	Mads Laursen	XFEL	
	Peter Vester	XFEL	
	Sonja Rosenlund Ahl	Synkrotron	
TAPs (technicians, administrative staff etc.) and scientific assistants	Carsten Gundlach	Outreach	
5 personer	Erik B Knudsen	McStas, McXtrace	
	Finn Saxild	Instrumentering	
	Marianne Sundby	DANSCATT sekretær	
	Peter Kjær Willendrup	McStas, McXtrace	
Students	Asbjørn Moltke	XFEL	

Bilag 1: DANSCATT personoversigt 2017

9 personer	Andreas Lauritzen	Neutron, synkrotron	
	Frederik W Isaksen	Neutron	
	Marie Hansteen	Neutron, synkrotron	
	Mathias Huss-Hansen	Neutron, synkrotron	
	Michael Korning Sørensen	Synkrotron	
	Rasmus Eilkær Hansen	Neutron	
	Steffen Sloth	Neutron	
	Wenjie Wan	Neutron	

DTU Space

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 1 person	Finn Christensen (gruppeleder)	Udvikling af røntgenoptik til rumforskning	Udvikling af røntgenreflekterende spejle til røntgen teleskoper
Postdocs, assistant professors etc. 2 personer	Desiree Ferreira	Samme	Samme
	Atefeh Jafari	Samme	Samme
PhD students 2 personer	Sonny Masahi	Samme	Samme
	Sara Svendsen	Samme	Samme

DTU Wind Energy

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 2 personer	Dorte Juul Jensen (gruppeleder)	Synkrotroneksperimenter	
	Yubin Zhang	Attending beam time At ESRF and APS	1)3D characterization of Goss-grained Fe-3%Si sample 2)Fitting materials parameters by comparing 3D movies and 3D simulations of growing grains 3)Strain gradient measurements near interfaces in laminated Ti-Al composites 4)The influence of local residual stresses on recrystallization of deformed iron

Bilag 1: DANSCATT personoversigt 2017

Postdocs, assistant professors etc.	Tianbo Yu	Attending beam time At ESRF and APS	1) Strain gradient measurements near interfaces in laminated Ti-Al composites 2) The influence of local residual stresses on recrystallization of deformed iron
1 person			

Niels Bohr Institute, Copenhagen University

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 8 personer	Kell Mortensen (gruppeleder)	SAXS, SANS	Soft matter sciences, biophysics
	Lise Arleth	SAXS, SANS	Soft matter sciences, biophysics
	Heloisa N. Bordallo	Inelastic Neutron Scattering	Materials Dynamics, Instrumentation
	Kim Lefmann	Inelastic neutron scattering	Magnetism, superconductivity, Instrumentation
	Brian Møller Andersen,	Theory, Neutron data	Magnetism, superconductivity
	Jacob Kirkensgaard	SAXS, SANS	Soft matter sciences, biophysics
	Linda Udby	Neutron Education, Neutron scattering	Magnetism, superconductivity, instrumentation
	Robert Feidenhans'l	X-ray scattering, X-ray imaging	Food sciences, materials science. Instrumentation.
Postdocs, assistant professors etc. 11 personer	Aghiad Ghazal	SAXS	In situ SAXS / microfluids
	Erik Brok	SAXS / SANS	Soft matter materials, biophysics
	Gregory Smith	SAXS / SANS	Soft matter materials, biophysics
	Jonas Okkels Birk	Inelastic neutron scattering	Instrument design
	Mads Bertelsen	Inelastic neutron scattering	Instrument design
	Martin Nors Pedersen	SAXS, SANS	Biophysics
	Martin Schmiele	SAXS / SANS	Soft matter materials, biophysics
	Raul Secchi	SAXS / SANS	Soft matter materials, biophysics
	Sergey Kapishnikov	X-ray Imaging	Bio-systems
	Søren Roi Midtgaard	SAXS / SANS	Soft matter materials, biophysics
	Nicholas Skar-Gislinge	SAXS / SANS	Soft matter materials, biophysics
PhD students 19 personer	Ana-Elena Tutueanu,	Neutron Scattering, TAS	Superconductivity, Magnetism
	Andreas Larsen	SAXS / SANS	Biophysics
	Anine L Borger	SAXS / SANS	Polymer physics
	Anton Kovyakh	X-ray/Neutron diffraction	Green chemistry
	Dainius Jakubauskas	SAXS / SANS	Biophysics
	Éverton C. Dos Santos	Quasielastic Neutron scattering	Water/Liquid Dynamics in solid materials
	Frederik G Tidemand	SAXS / SANS	Biophysics
	Jakob Lass	Neutron Scattering, TAS	Superconductivity, Magnetism

Bilag 1: DANSCATT personoversigt 2017

	Jose E.M. Pereira	Quasielastic Neutron scattering	Water/Liquid Dynamics in solid materials
	Kristian Rix	X-ray Imaging	Materials Sciences
	Lasse Sander Dreyer	SAXS, SANS	Biophysics
	Lise Sandberg	Neutron Scattering, TAS	Superconductivity, Magnetism
	Marcella C Berg	Quasielastic Neutron scattering	Water/Liquid Dynamics in solid materials
	Nicolai Johansen	SAXS, SANS	Biophysics
	Pia Jensen Ray	Neutron Scattering, TAS	Superconductivity, Magnetism
	Sofie Janas	Neutron Scattering, TAS	Superconductivity, Magnetism
	Tim Tejsner	Neutron Scattering, TAS	Superconductivity, Quantum Chemistry
	Torsten Lauritsen	X-ray imaging	Biomaterials, materials sciences
	Ursula B. Hansen	Neutron Scattering, TAS	Superconductivity, Magnetism
Students	Anders Komar Ravn	Neutron Scattering, TAS	Superconductivity, Magnetism
3 personer	Simon R. Larsen,	Quasielastic Neutron scattering	Water/Liquid Dynamics in solid materials
	Helle Leerberg	Neutron Scattering, TAS	Superconductivity, Magnetism
Emeritus prof.	Jens Als Nielsen	X-ray imaging, X-ray scattering	Biosystems etc
	Poul Erik Lindelof	X-ray spectroscopy	Archeology
2 personer			

Department of Chemistry, University of Copenhagen

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 13 personer	Sine Larsen	Crystallography, SAXS	
	Leila Lo Leggio (gruppeleder)	Macromolecular crystallography, SAXS(SANS)	
	Anders Kadziola	Crystallography	
	Jesper Bendix	Mest XMCD, EXAFS, INS, PND, MuSR	
	Stergios Piligkos	XMCD, INS	
	Høgni Weihe	XMCD, INS	
	Henning Osholm Sørensen	Advisor, synchrotron X-ray radiation techniques (tomography, PXRD, 3DXRD, CTR, reflectometry)	
	Susan Stipp	Advisor	

Bilag 1: DANSCATT personoversigt 2017

	Nicolas Bovet	Advisor, synchrotron X-ray radiation techniques (STXM, reflectometry)	
	Kim N. Dalby	Synchrotron IR and tomography	
	Knud Dideriksen	Pair-distribution function analysis and PXRD	
	Martin Andersson	Synchrotron IR and Raman	
	Tue Hassenkam	X-ray tomography	
Postdocs, assistant professors etc.	Heidi A. Ernst	Macromolecular crystallography	Laccases
14 personer	Kim K. Rasmussen	Macromolecular crystallography and SAXS	Genetic switch of TP901-1
	Folmer Fredslund	Macromolecular crystallography	Industrial enzymes
	Morten Ejby (Guest from DTU)	Crystallization and macromolecular crystallography	Carbohydrate esterases and soluble binding proteins
	Kristian Frandsen	Macromolecular crystallography and SAXS	Lytic polysaccharide monooxygenases
	Janina Sprenger	Macromolecular crystallography	Method development
	Scott Mazurkewich (guest from Chalmers)	Crystallization and macromolecular crystallography	Glucuronoyl esterases
	Dmitri Mitcov	XMCD, XAS	
	Mauro Perfetti	INS, XMCD	
	Yi Yang	In situ X-ray microtomography	In situ 3D imaging of the evolution of the microstructure of chalk caused by flow of CO ₂ in pore network
	Dominique Tobler	Pair-distribution function analysis, PXRD and X-ray tomography	Studies of the formation of amorphous CaCO ₃ nanoparticles and the transformation to the crystalline phases, vaterite and calcite and the influence of organic compounds on this process. Bacteria transport properties in natural porous materials.
	Kirsten Marie Ørnsbjerg Jensen	Synkrotronmålinger	
	Dirk Mütter	X-ray tomography and SAXS	
	Case van Genuchten	EXAFS, PXRD and PDF analysis	
PhD students	Monika Kovacic	Inelastic X-ray and	Jumping crystals

Bilag 1: DANSCATT personoversigt 2017

12 personer		neutron scattering	
	Mads Østergaard (Chemical Biology section)	Crystallization and macromolecular crystallography	Modified insulin
	Daniel Krska (guest from Chalmers)	Crystallization, SAXS, macromolecular crystallography	Glucuronoyl esterases
	Mikkel Agerbæk Sørensen	INS, MuSR, XMCD	Single molecule magnets based on lanthanides and actinides
	Anders Reinholdt	XAS, EXAFS	Metal Carbide Chemistry
	Morten G. Vinum	INS, XMCD	Molecular magnetism and magnetism of condensed phases
	Emil Hansen	INS	Lanthanide-based molecular magnetism
	Troels Lindahl Christiansen	Synkrotronmålinger	Structure and formation of nanoscale molybdenum oxides
	Mikkel Juelsholt	Synkrotronmålinger	Material synthesis studies - from clusters to nanoparticles
	Sepide Hakim	Reflectometry, surface diffraction, tomography and PXRD	Interaction between organic compounds and the surfaces of calcite and quartz
	Marco Mangayayam	PXRD and PDF analysis	Development and investigation of layered double hydroxides.
	Arash Moaddel	X-ray tomography	Determination of pore and fracture networks in chalk.
Students 14 personer	Tobias Tandrup	Crystallization and macromolecular crystallography	Lytic polysaccharide monooxygenases
	Anders Varming	Crystallization and macromolecular crystallography	Genetic switch of TP901-1
	Rasmus Meland Knudsen	Crystallization and macromolecular crystallography	Glucuronoyl esterases
	Yusuf Ahmad Theibich	Sample preparation and crystallization	Lytic polysaccharide monooxygenases
	Sebastian Muderspach	Crystallization and macromolecular crystallography	Lytic polysaccharide monooxygenases
	Emil Elholm	Synkrotronmålinger	Formation of NiO nanoparticles in organic solvents
	Elly Kim Bathke	Synkrotronmålinger	X-ray total scattering studies of the formation of CuO nanoparticles
	Triana Wulandari	Synkrotronmålinger	PDF studies of nanoscale structures in molybdenum oxide catalysts
	Joanna Symonowicz	Synkrotronmålinger	Synthesis and structure of CZTS nanoparticles for solar cells
	Mathias Helmsøe-Zinck	Synkrotronmålinger	Synthesis of disordered MoO ₂ materials
	Emil Skaaning Kjær	Synkrotronmålinger	Synthesis and structure of delafossite

Bilag 1: DANSCATT personoversigt 2017

			nanoparticles
	Andy Sode Anker	Synkrotronmålinger	PDF studies of Bi oxido clusters in solution
	Jake Thomas Cook	X-ray tomography	Investigation of the mechanical properties of sea urchins using X-ray imaging.
	Marie Bjerrum	X-ray tomography	Studies of microstructure developments in DeNOx selective reduction catalysts during use.
TAPs (technicians, administrative staff etc.) and scientific assistants	Jens-Christian N. Poulsen	Macromolecular crystallization and crystallography	
2 personer	Melania Rogowska	X-ray tomography, PXRD	In situ 3D imaging of the evolution of the microstructure of chalk caused by flow of CO ₂ in pore network.

Department of Drug Design and Pharmacology, University of Copenhagen

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.)	Michael Gajhede (gruppeleder)	Kromatin modificerende enzymer	
6 personer	Jette Sandholm Kastrup	Ionotrope glutamat receptorer	
	Karla Frydenvang	Ionotrope glutamat receptorer Cytochrome P450 enzymes	
	Bente Vestergaard	Amyloid Fibrillation	
	Annette Langkilde	Amyloid Fibrillation and neutron krystallografi	
	Osman Mirza	Cytochrome P450 enzymes	
Postdocs, assistant professors etc.	Saara Laulumaa	Ionotrope glutamat receptorer	NMX on iGluR LBD
7 personer	Thor Seneca Thorsen	Ionotrope glutamat receptorer	X-ray crystal diffraction studies, SANS on full-length and LBDs of iGluRs
	Jerzy Dorosz	Ionotrope glutamat receptorer	X-ray crystal diffraction studies, SANS on full-length and LBDs of iGluRs
	Carlotta Marasini	Amyloid Fibrillation	Influence of crowding agents, chemical probes or solvent conditions on amyloid fibrillation. Fibril surface layer.
	Saskia Bucciarelli	Amyloid Fibrillation	Amyloid interaction with lipid membranes
	Folmer Fredslund	Amyloid Fibrillation	Fiber diffraction

Bilag 1: DANSCATT personoversigt 2017

	Dilip Narayanan	Keap1 structure	Fragment based drug discovery
PhD students	Anja Probst Larsen	Ionotrope glutamat receptorer	X-ray crystal diffraction studies on LBDs of iGluRs
8 personer	Stine Møllerud	Ionotrope glutamat receptorer	X-ray crystal diffraction studies on LBDs of iGluRs
	Sarah E. Jones	Kromatin modificerende enzymer	X-ray crystal diffraction studies on chromatin modifying enzymes
	Thomas Skamris Pedersen	Amyloid Fibrillation	Advanced probes on amyloid fibrils
	Nils Skovgaard	Amyloid Fibrillation	Fibril surfaces produced with microfluidics
	Ersoy Cholak	Amyloid Fibrillation	Amyloid interaction with lipid membranes
	Kirstine Bendtsen	Amyloid Fibrillation	LAG3 interactions with synuclein fibrils
	Line K. Skaaning	Amyloid Fibrillation	Amyloid strain formation
Students	Mathias Poulsen	Ionotrope glutamat receptorer	X-ray crystal diffraction studies on LBDs of iGluRs
11 personer	Aura Leahu	Ionotrope glutamat receptorer	X-ray crystal diffraction studies on LBDs of iGluRs
	Sebastian Winther	Ionotrope glutamat receptorer	X-ray crystal diffraction studies on LBDs of iGluRs
	Arpan Sharma	Cytochrome P450 enzymes	X-ray crystal diffraction studies
	Liv Damgaard	Amyloid Fibrillation	Amyloid interaction with lipid membranes
	Daniel Rønnow Schacht	Cytochrome P450 enzymes	Expression and purification of protein
	Adriana Lauroba	Cytochrome P450 enzymes	Expression and purification of protein
	Kristoffer Brasen	Kromatin modificerende enzymer	Expression and purification of protein
	Ina Dai	Ionotrope glutamat receptorer	X-ray crystal diffraction studies on LBDs of iGluRs
	Lise Nielsen	Ionotrope glutamat receptorer	X-ray crystal diffraction studies on LBDs of iGluRs
	Rikke Lousen	Kromatin modificerende enzymer	Expression and purification of protein

The Novo Nordisk Foundation Center for Protein Research, University of Copenhagen

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.)	Pablo Mesa	Synchrotron/data collection SLS (2 trips)	CCT project
	Stefano Stella	16-02-2017 SLS swiss synchrotron	Determination of various Crystall Structures
3 personer			

Bilag 1: DANSCATT personoversigt 2017

		01-04-2017 SLS swiss synchrotron 28-06-2017 MAXIV Swedish synchrotron 02-12-2017 SLS swiss synchrotron 14-12-2017 MAXIV Swedish synchrotron	
	Guillermo Montoya (gruppelider)	Synchrotron/data collection	
Postdocs, assistant professors etc. 1 person	Nicholas Sofos	Synchrotron/data collection PSI/SLS (1 trip), MaxIV (2 trips)	Structural determination of a nuclease complex involved in CRISPR-Cas biology.
PhD students 1 person	Danyang Wang	Synchrotron/data collection SLS (4 trips)	CCT project
Students 1 person	Claudia Weidling	Trip to Synchrotron MaxIV	Structural characterization of CRISPR proteins
TAPs (technicians, administrative staff etc.) and scientific assistants 1 person	Kamila Kamuda	SLS	CCT project

Department of Biomedical Sciences, University of Copenhagen

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 1 person	Pontus Gourdon (gruppelider)	Gruppelider	
Postdocs, assistant professors etc. 3 personer	Md Tamim Al-Jubair	Synchrotron trip to collect protein crystals diffraction data.	Crystallization and structure determination of the PIB-4 ATPases
	Annette Duelli	No synchrotron trips in 2017	
	Kamil Gotfryd	No synchrotron trips in 2017	
PhD students 6 personer	Qiaoxia Hu	Synchrotron trip to collect protein crystals diffraction data.	Crystallization and structure determination of the PIB-4 ATPases
	Elena Longhin	Synchrotron trip to collect protein crystals diffraction data.	Crystallization and structure determination of PIB-2 ATPases and related targets.

Bilag 1: DANSCATT personoversigt 2017

	Julie Winkel Missel	Synchrotron trip to collect protein crystals diffraction data.	Crystallization and structure determination of the human Aquaporins using X-ray and neutron scattering.
	Liying Zhang	Synchrotron trip to collect protein crystals diffraction data	Crystallization and structure determination of a light gated channel-----Channelrhodopsin2
	Eva Ramos Becares	No synchrotron trip in 2017	
	Christina Grønberg	Synchrotron trips to collect data on protein crystals	Crystallization and structure determination of the P _{1B-4} -ATPases, a group of proteins involved in the homeostasis of heavy metals.
TAPs (technicians, administrative staff etc.) and scientific assistants 1 person	Nancy Mutsaers	No synchrotron trip in 2017	

Department of Pharmacy, University of Copenhagen

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 5 personer	Anan Yaghmur (gruppeleder)	Nanostructural characterization of drug nanocarriers by synchrotron SAXS	
	Martin Malmsten	Neutron scattering of biological and soft matter interfaces	
	Kathryn Browning	Neutron scattering of biological and soft matter interfaces	
	Vito Fodera	Biophysical studies including X-ray scattering on amyloid-like aggregation	
	Anders Østergaard Madsen	X-ray and neutron inelastic and diffuse scattering studies of drug crystals	
PhD students 3 personer	Gizem Bor	Cubosomes and Hexosomes as Drug Nanocarriers for Brain Cancer Therapy	Formulation and characterization of cubosomes and hexosomes loaded with anticancer drugs for brain cancer treatment. The project will focus on the combination of the structural characterization with relevant in vitro and in vivo evaluations.

Bilag 1: DANSCATT personoversigt 2017

	Shen Yu Helvig	NANO-engineered LYMPHotropic Cubosomes and Hexosomes	Formation of multifunctional lymphotropic cubosomes and hexosomes. The project focuses on precision surface nano-engineering for efficient targeting of designated lymph node elements.
	Mark Gontsarik	Tailoring Antimicrobial Peptides for Bacteria Membrane Destruction	Formation and characterization of soft lipidic nanocarriers loaded with antimicrobial peptide (A joint PhD project with Dr. Stefan Salentinig from EMPA (St. Gallen, Switzerland))
Students 9 personer	Sabah Al-Hosayni	Structural characterization of nano-self-assemblies based on novel omega-3 monoglycerides	Formation and characterization of bulk and dispersed phases of three new omega-3 monoglycerides
	Xianrong Shao	Structural characterization of nano-self-assemblies based on novel omega-3 monoglycerides	Formation and characterization of bulk and dispersed phases of three new omega-3 monoglycerides
	Hasan Akram	Characterization of Isosomes loaded with thymoquinone	Formation and characterization of non-lamellar liquid crystalline nanocarriers loaded with the natural anticancer drug thymoquinone
	Umar Asghar	Characterization of Isosomes loaded with thymoquinone	Formation and characterization of non-lamellar liquid crystalline nanocarriers loaded with the natural anticancer drug thymoquinone
	Ghulam Sadat	Characterization of nanoparticles based on binary egg yolk phospholipid (EPC)/citrem mixtures	EPC/citrem Nanocarriers for delivery of anticancer drugs
	Rama Prajapati	Effect of temperature on the structure of binary soybean phospholipid (SPC)/citrem mixtures	SPC/citrem nanocarriers for intra-articular administration
	Boi Vi Tran	Characterization of nanocarriers loaded with thymoquinone	Formation and characterization of non-lamellar liquid crystalline nanocarriers loaded with the natural anticancer drug thymoquinone
	Wael Al-Hallaq	Characterization of curcumin nanocarriers	Formation and characterization of non-lamellar liquid crystalline nanocarriers loaded with the natural anticancer drug curcumin
	Firas Alturk	Characterization of curcumin nanocarriers	Formation and characterization of non-lamellar liquid crystalline nanocarriers loaded with the natural anticancer drug curcumin

Department of Science and Environment, Roskilde University

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 4 personer	Dorthe Posselt (gruppeleder)	Nanoscale structure and dynamics, soft materials science, GISAXS, SAXS, SANS, inelastic neutron scattering	
	Kristine Niss	Viscous liquid dynamics, crystallization, inelastic neutron scattering, and neutron diffraction	
	Håvard Jenssen	Antimicrobial peptides seen by X-ray and Neutron scattering	
	Kornelius Zeth	Protein crystallography	
Postdocs, assistant professors etc. 1 person	Alejandro Sanz	Viscous liquid dynamics, crystallization, inelastic neutron scattering, and neutron diffraction	Development of a high-pressure device for simultaneous dielectric and neutron spectroscopy measurements
PhD students 4 personer	Henriette Wase Hansen	Viscous liquid dynamics, crystallization, inelastic neutron scattering, and neutron diffraction	Testing the isomorph theory for liquids by combined neutron and dielectric high pressure measurements.
	Mikkel Hartmann Jensen	Viscous liquid dynamics, crystallization, inelastic neutron scattering, and neutron diffraction	Studying dynamics and structure in liquids with combined dielectric and neutron spectroscopy.
	Sina Ariaee	Nanoscale structure and dynamics, soft materials science, GISAXS, SAXS, SANS, inelastic neutron scattering	filmSTAR - Characterization and modelling of star block co-polymer thin-film materials and their restructuring behaviour by time-resolved GISAXS
	Abdullah Lone	Antimicrobial peptides seen by X-ray and Neutron scattering	Antimicrobial peptides seen by X-ray and Neutron scattering
TAPs (technicians, administrative staff etc.) and scientific assistants 6 personer	Bo Jakobsen	Sample environment development for Neutron and X-ray scattering.	
	Ib Høst Pedersen	Sample environment development for Neutron and X-ray scattering.	
	Preben Olsen	Sample environment development for Neutron and X-ray scattering.	
	Torben Steen Rasmussen	Sample environment development for Neutron and X-ray scattering.	
	Ebbe Hyldahl	Sample environment	

Bilag 1: DANSCATT personoversigt 2017

		development for Neutron and X-ray scattering.	
	Marianne Lauridsen	Sample preparation	

Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
VIPs (professors, senior scientists etc.) 5 personer	Ulla Gro Nielsen	APS, Chicago – PDF+XRD	
	Sven Taugaard	Beamtime	HAXPEEM of deeply buried interfaces in novel TaAl alloys for gating of AlGaN high-electron mobility transistors
	Dorthe B. Ravnsbæk (gruppeleder)		Operando diffraction studies of electrode materials for rechargeable batteries
	Beate Klösgen	project: experiments, supervision of projects, data analysis; assistance for DANSCATT meeting 2017	
	Jakob Kjelstrup-Hansen	Sample preparation, GIXRD measurements at ESRF	
Postdocs, assistant professors etc. 4 personer	Luciana Tavares	Sample preparation	
	Daniel R. Sørensen	Beamtime at ESRF and Petra	Operando diffraction studies of electrode materials for rechargeable batteries
	Jeanette Hvam	Beamtime at Petra	Operando diffraction studies of electrode materials for rechargeable batteries
	Priscilla Huen	Beamtime at Petra	Operando diffraction studies of electrode materials for rechargeable batteries
PhD students 6 personer	Laura Lundehøj	APS, Chicago - PDF+XRD	In situ studies LDHs
	Nicholai Daugaard Jensen	ANKA, Karlsruhe - EXAFS	Synthesis and characterization of ZnAl ₄ -LDH
	Chen Shen	experiments, data analysis, participation in DANSCATT meeting	molecular switches in lipid layers: - GISAXS on lateral structure of lipid monolayers - reflectometry on lipid monolayers - structure of lipid bilayers - dynamics in lipid bilayers
	Charlotte Zborowski	Beamtime	HAXPEEM of deeply buried interfaces in novel TaAl alloys for gating of AlGaN high-electron mobility transistors
	Christian Henriksen	Beamtime at ESRF and Petra	Operando diffraction studies of electrode materials for rechargeable batteries
	Christian K. Christiansen	Beamtime at ESRF and Petra	Operando diffraction studies of electrode materials for rechargeable batteries
Students	Jes Linnet	Sample preparation,	Organic photodiodes and

Bilag 1: DANSCATT personoversigt 2017

8 personer		GIXRD measurements at ESRF	phototransistors
	Jeppe Udegaard Jørgensen	data analysis	molecular switches in lipid layers: X-ray reflectometry on lipid monolayers
	Jens Kristian Greve Schmidt	data analysis	molecular switches in lipid layers: neutron reflectometry on lipid monolayers
	Henrik Siboni	"observing" student during experiments	polyelectrolyte layers
	Christian L. Jakobsen	Beamtime at Petra	Operando diffraction studies of electrode materials for rechargeable batteries
	Jonas H. Kristensen	Beamtime at Petra	Operando diffraction studies of electrode materials for rechargeable batteries
	Anders K. Clausen	Beamtime at Petra	Operando diffraction studies of electrode materials for rechargeable batteries
	Martin A. Karlsen	Beamtime at ESRF	Operando diffraction studies of electrode materials for rechargeable batteries

Haldor Topsoe A/S

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
Senior Principal Scientist	Lars Lundegaard (gruppeleder)	To synchrotron ture til ESRF	Methanol to hydrocarbon conversion, in collaboration with Oslo university.
Principal Scientist	Christoffer Tyrsted	Organisering af EXAFS beamtid udført ved ANKA.	
Research Specialist	Robin Christensen		

Xnovo

Stilling	Navn	DANSCATT-relateret aktivitet	Generel beskrivelse af projekt (for studenter + post docs)
CEO	Erik Lauridsen	Commercial synchrotron beamtime	

Bilag 2: Liste over peer-reviewed artikler 2017

Department of Chemistry, Aarhus University

Zhao, Kunpeng; Blichfeld, Anders Bank; Chen, Hongyi; Song, Qingfeng; Zhang, Tiansong; Zhu, Chenxi; Ren, Dudi; Hanus, Riley; Qiu, Pengfei; Iversen, Bo B.; Xu, Fangfang; Snyder, G. Jeffrey; Shi, Xun; Chen, Lidong. (2017) Enhanced Thermoelectric Performance through Tuning Bonding Energy in $\text{Cu}_2\text{Se}_{1-x}\text{S}_x$ Liquid-like Materials. *Chemistry of Materials* 29(15), p. 6367-6377.

Zhao, Kunpeng; Blichfeld, Anders Bank; Eikeland, Espen; Qiu, Pengfei; Ren, Dudi; Iversen, Bo Brummerstedt; Shi, Xun; Chen, Lidong. Extremely low thermal conductivity and high thermoelectric performance in liquid-like $\text{Cu}_2\text{Se}_{1-x}\text{S}_x$ polymorphic materials. (2017) *Journal of Materials Chemistry A* 5(34), 18148-18156.

Zhao, Kunpeng; Zhu, Chenxi; Qiu, Pengfei; Blichfeld, Anders B.; Eikeland, Espen; Ren, Dudi; Iversen, Bo B.; Xu, Fangfang; Shi, Xun; Chen, Lidong. (2017) High thermoelectric performance and low thermal conductivity in $\text{Cu}_2-\gamma\text{S}_{1/3}\text{Se}_{1/3}\text{Te}_{1/3}$ liquid-like materials with nanoscale mosaic structures. *Nano Energy* 42, 43-50.

Zhao, Kunpeng; Qiu, Pengfei; Song, Qingfeng; Blichfeld, Anders Bank; Eikeland, Espen Zink; Ren, Dudi; Ge, Binghui; Iversen, Bo Brummerstedt; Shi, Xun; Chen, Lidong. (2017) Ultrahigh thermoelectric performance in $\text{Cu}_2-\gamma\text{Se}_{0.5}\text{S}_{0.5}$ liquid-like materials. *Materials Today Physics* 1, 14-23.

Zhang, Jiawei; Song, Lirong; Pedersen, Steffen Hindborg; Yin, Hao; Hung, Le Thanh; Iversen, Bo Brummerstedt. (2017) Discovery of high-performance low-cost n-type Mg_3Sb_2 -based thermoelectric materials with multi-valley conduction bands. *Nature Communications*, 8, 13901.

Zhang, Jiawei; Song, Lirong; Mamakhel, Mohammad Aref Hasen; Jørgensen, Mads Ry Vogel; Iversen, Bo Brummerstedt. (2017) High-Performance Low-Cost n-Type Se-Doped Mg_3Sb_2 -Based Zintl Compounds for Thermoelectric Application. *Chemistry of Materials* 29(12), 5371-5383.

Voisin, T.; Erriguible, A.; Philippot, G.; Ballenghien, D.; Mateos, D.; Cansell, F.; Iversen, B. B.; Aymonier, C. Investigation of the precipitation of Na_2SO_4 in supercritical water. *Chemical Engineering Science* 174, 268-276.

Tolborg, Kasper; Jørgensen, Mads R.V.; Christensen, Sebastian; Kasai, Hidetaka; Becker, Jacob; Walter, Peter; Dippel, Ann Christin; Als-Nielsen, Jens; Iversen, Bo B. (2017) Accurate charge densities from powder X-ray diffraction - a new version of the Aarhus vacuum imaging-plate diffractometer. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials* 73(4), 521-530.

Tamtogl, Anton; Kraus, Patrick; Avidor, Nadav; Bremholm, Martin; Hedegaard, Ellen M. J.; Iversen, Bo B.; Bianchi, Marco; Hofmann, Philip; Ellis, John; Allison, William; Benedek, Giorgio; Ernst, Wolfgang E. (2017) Electron-phonon coupling and surface Debye temperature of $\text{Bi}_2\text{Te}_3(111)$ from helium atom scattering. *Physical Review B* 95(19), 195401.

Song, Lirong; Zhang, Jiawei; Iversen, Bo Brummerstedt. (2017) Simultaneous improvement of power factor and thermal conductivity via Ag doping in p-type Mg_3Sb_2 thermoelectric materials. *Journal of Materials Chemistry A* 5(10), 4932-4939.

Sommer, Sanna; Bøjesen, Espen Drath; Blichfeld, Anders Bank; Iversen, Bo Brummerstedt. (2017) Tailoring band gap and thermal diffusivity of nanostructured phase-pure ZnAl_2O_4 by direct spark plasma sintering synthesis. *Journal of Solid State Chemistry* 256, 45-52.

Skjaervo, Susanne Linn; Sommer, Sanna; Norby, Peter; Bojesen, Espen Drath; Grande, Tor; Iversen, Bo B.; Einarsrud, Mari-Ann. (2017) Formation mechanism and growth of MnNbO_3 , $\text{M}=\text{K}$, Na by insitu X-ray diffraction. *American Ceramic Society. Journal* 100(9), 3835-3842.

Sist, Mattia; Gatti, Carlo; Nørby, Peter; Cenedese, Simone; Kasai, Hidetaka; Kato, Kenichi; Iversen, Bo Brummerstedt. (2017) High-Temperature Crystal Structure and Chemical Bonding in Thermoelectric Germanium Selenide (GeSe). *Chemistry: A European Journal* 23(28), 6888-6895.

Sist, Mattia; Fischer, Karl Frederik Færch; Kasai, Hidetaka; Iversen, Bo Brummerstedt. Low-Temperature Anharmonicity in Cesium Chloride (CsCl). (2017) *Angewandte Chemie (International Edition)* 56(13), 3625-3629.

Saha, Dipankar; Bojesen, Espen D.; Mamakhel, Mohammad Aref Hasen; Bremholm, Martin; Iversen, Bo B. (2017) In Situ PDF Study of the Nucleation and Growth of Intermetallic PtPb Nanocrystals. *ChemNanoMat* 3(7), 472-478.

Reardon, Hazel; Blichfeld, Anders B.; Kasai, Hidetaka; Yin, Hao; Bojesen, Espen Drath; Iversen, Bo B. (2017) Revealing the slow decomposition kinetics of type-I clathrate $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30}$. *Physical Chemistry Chemical Physics* 19(24), 15734-15744.

Mirhosseini, Mojtaba; Rezaei, Alireza; Blichfeld, Anders B.; Iversen, Bo B.; Rosendahl, Lasse A. (2017) Experimental Investigation of Zinc Antimonide Thin Film Thermoelectric Element over Wide Range of Operating Conditions. *Physica Status Solidi (A) Applications and Materials Science* 214(11), 1-7.

Mi, Jian Li; Ying, Ping Jun; Sist, Mattia; Reardon, Hazel; Zhang, Peng; Zhu, Tie Jun; Zhao, Xin Bing; Iversen, Bo Brummerstedt. (2017) Elaborating the Crystal Structures of MgAgSb Thermoelectric Compound: Polymorphs and Atomic Disorders. *Chemistry of Materials* 29(15), 6378-6388.

Mi, Jian Li; Nørby, Peter; Bremholm, Martin; Iversen, Bo B. (2017) Insight into Nucleation and Growth of $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_3$ ($x = 0-2$) Nanoplatelets in Hydrothermal Synthesis. *Chemistry of Materials* 29(12), 5070-5079.

Manna, S; Kamalpure, A; Cornils, L; Hänke, T; Hedegaard, E M J; Bremholm, M; Iversen, B B; Hofmann, Philip; Wiebe, J; Wiesendanger, R. (2017) Interfacial superconductivity in a bi-collinear antiferromagnetically ordered FeTe monolayer on a topological insulator. *Nature Communications* 8(14074), 1-8.

Kasai, Hidetaka; Song, Lirong; Andersen, Henrik Lyder; Yin, Hao; Iversen, Bo Brummerstedt. (2017) Multi-temperature structure of thermoelectric Mg₂Si and Mg₂Sn. *Acta Cryst. B* 73, 1158-1163.

Jørgensen, Mads Ry Vogel; Piccoli, Paula M B; Hathwar, Venkatesha R.; Wang, Xiaoping; Hoffmann, Christina M.; Yakovenko, Andrey A.; Halder, Gregory J.; Schlueter, John A.; Iversen, Bo B.; Schultz, Arthur J. (2017) Neutron and X-ray investigations of the Jahn-Teller switch in partially deuterated ammonium copper Tutton salt, (NH₄)₂[Cu(H₂O)₆](SO₄)₂. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials* 73(1), 87-93.

Jiang, Binbin; Qiu, Pengfei; Eikeland, Espen Zink; Chen, Hongyi; Song, Qingfeng; Ren, Dudi; Zhang, Tiansong; Yang, Jiong; Iversen, Bo Brummerstedt; Shi, Xun; Chen, Lidong. (2017) Cu₈GeSe₆-based thermoelectric materials with an argyrodite structure. *Journal of Materials Chemistry C* 5(4), 943-952.

Jensen, Mads Mørk; Madsen, René Bjerregaard; Becker, Jacob; Iversen, Bo Brummerstedt; Glasius, Marianne. (2017) Products of hydrothermal treatment of lignin and the importance of ortho-directed repolymerization reactions. *Journal of Analytical and Applied Pyrolysis* 126, 371-379.

Hänke, Torben; Singh, Udai Raj; Cornils, Lasse; Manna, Sujit; Kamlapure, Anand; Bremholm, Martin; Hedegaard, Ellen Marie Jensen; Iversen, Bo Brummerstedt; Hofmann, Philip; Hu, Jin; Mao, Zhiqiang; Wiebe, Jens; Wiesendanger, Roland. (2017) Reorientation of the diagonal double-stripe spin structure at Fe_{1+y}Te bulk and thin-film surfaces. *Nature Communications* 8(13939), 1-8.

Hung, Le Thanh; Ngo, Duc The; Han, Li; Iversen, Bo Brummerstedt; Yin, Hao; Pryds, Nini; Van Nong, Ngo. (2017) In Operando Study of High-Performance Thermoelectric Materials for Power Generation : A Case Study of β -Zn₄Sb₃. *Advanced Engineering Materials* 3(10), 1700223.

Hathwar, Venkatesha Rama; Stingaciu, Marian; Richter, Bo; Overgaard, Jacob; Iversen, Bo B. (2017) Variable-temperature structural studies on valence tautomerism in cobalt bis(dioxolene) molecular complexes. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials* 73(2), 304-312.

Eikeland, Espen Zink; Blichfeld, Anders Bank; Borup, Kasper; Zhao, Kunpeng; Overgaard, Jacob; Shi, Xun; Chen, Lidong; Iversen, Bo Brummerstedt. (2017) Crystal structure across the β to α phase transition in thermoelectric Cu_{2-x}Se. *IUCrJ* 4, 476-485.

Eikeland, Espen Zink; Thomsen, Maja; Overgaard, Jacob; Spackman, Mark A.; Iversen, Bo Brummerstedt. (2017) Intermolecular Interaction Energies in Hydroquinone Clathrates at High Pressure. *Crystal Growth & Design* 17(7), 3834-3846.

Datzer, Christian; Zumbielte, Anna; Braun, Juergen; Foerster, Tobias; Schmidt, Anke B.; Mi, Jianli; Iversen, Bo Brummerstedt; Hofmann, Philip; Minar, Jan; Ebert, Hubert; Krueger, Peter; Rohlfing, Michael; Donath, Markus. (2017) Unraveling the spin structure of unoccupied states in Bi₂Se₃. *Physical Review B* 95(11), 115401.

Bondesgaard, Martin; Mamakhel, Mohammad Aref Hasen; Becker, Jacob; Kasai, Hidetaka; Philippot, Gilles; Bremholm, Martin; Iversen, Bo B. (2017) Supercritical Flow Synthesis of Pt₁-xRu Nanoparticles : Comparative Phase Diagram Study of Nanostructure versus Bulk. *Chemistry of Materials* 29(7), 3265-3273.

Birgisson, Steinar; Shen, Yanbin; Iversen, Bo B. (2017) In operando observation of sodium ion diffusion in a layered sodium transition metal oxide cathode material, P2 Na_xCo_{0.7}Mn_{0.3}O₂. *Chemical Communications* 53(6), 1160-1163.

Andersen, Casper Welzel; Borfecchia, Elisa; Bremholm, Martin; Jørgensen, Mads Ry Vogel; Vennestrøm, Peter Nicolai Ravnborg; Lamberti, Carlo; Lundegaard, Lars Fahl; Iversen, Bo Brummerstedt. (2017) Redox-Driven Migration of Copper Ions in the Cu-CHA Zeolite as Shown by the In Situ PXRD/XANES Technique. *Angewandte Chemie (International Edition)*, 56(35), 10367-10372.

Andersen, Henrik Lyder; Zhang, Jiawei; Yin, Hao; Iversen, Bo B. (2017) Structural stability and thermoelectric properties of cation- and anion-doped Mg₂Si_{0.4}Sn_{0.6}. *Inorganic Chemistry Frontiers* 4(3), 456-467.

Andersen, Amanda; Krogsgaard, Marie; Birkedal, Henrik. (2017) Mussel-Inspired Self-Healing Double-Cross-Linked Hydrogels by Controlled Combination of Metal Coordination and Covalent Cross-Linking. *Biomacromolecules*, DOI:10.1021/acs.biomac.7b01249.

Azevedo, Sara; Costa, Ana M. S.; Andersen, Amanda; Choi, Insung S.; Birkedal, Henrik; Mono, Joao F. (2017) Bioinspired Ultratough Hydrogel with Fast Recovery, Self-Healing, Injectability and Cytocompatibility. *Advanced Materials* 29(28), 1700759.

Frølich, Simon; Weaver, James C.; Dean, Mason N.; Birkedal, Henrik. (2017) Uncovering Nature's Design Strategies through Parametric Modeling, Multi-Material 3D Printing, and Mechanical Testing. *Advanced Engineering Materials*, 19(6), 201600848.

Schlafer, Sebastian; Ibsen, Casper Jon Steenberg; Birkedal, Henrik; Nyvad, Bente. (2017) Calcium-Phosphate-Osteopontin Particles Reduce Biofilm Formation and pH Drops in in situ-Grown Dental Biofilms. *Caries Research* 51, 26-33.

Birkedal, Henrik. (2017) Cation- π Interactions : Mimicking mussel mechanics. *Nature Chemistry* 9(5), 408-409.

Birkbak, Mie; Nielsen, Ida; Frølich, Simon; Stock, Stuart R.; Kenesei, Peter; Almer, Jonathan D.; Birkedal, Henrik. (2017) Concurrent determination of nanocrystal shape and amorphous phases in complex materials by diffraction scattering computed tomography. *Journal of Applied Crystallography* 50(1), 192-197.

Bilag 2: Liste over peer-reviewed artikler 2017

Flinker, Mathias ; Yin, Hongfei; Juhl, Rene W. ; Eikeland, Espen Zink; Overgaard, Jacob; Nielsen, Dennis Ulsøe; Skrydstrup, Troels. (2017) Efficient Water Reduction with sp³-sp³ Diboron(4) Compounds: Application to Hydrogenations, H-D Exchange Reactions and Carbonyl Reductions. *Angewandte Chemie (International Edition)*, 56(50), 15910-15915.

Enevoldsen, Martin V.; Overgaard, Jacob; Pedersen, Maja Staffeldt; Lindhardt, Anders Thyboe. (2017) Organocatalyzed Decarboxylative Trichloromethylation of Morita-Baylis-Hillman Adducts in Batch and Continuous Flow. *Chemistry: A European Journal* 24(5), 1204-1208.

Meninno, Sara; Zullo, Luca; Overgaard, Jacob; Lattanzi, Alessandra. (2017) Tunable Cinchona-Based Thioureas-Catalysed Asymmetric Epoxidation to Synthetically Important Glycidic Ester Derivatives. *Advanced Synthesis & Catalysis* 359(6), 913-918.

Meninno, Sara; Overgaard, Jacob; Lattanzi, Alessandra. (2017) Amine Thiourea Catalysed Double Michael Reaction : An Approach for the Asymmetric Synthesis of Spiro[pyrazolone-4,3'-tetrahydrothiophenes]. *Synthesis* 49(7), 1509-1518.

Meninno, Sara; Roselli, Angelo; Capobianco, Amedeo; Overgaard, Jacob; Lattanzi, Alessandra. (2017) Diastereodivergent and Enantioselective Access to Spiroepoxides via Organocatalytic Epoxidation of Unsaturated Pyrazolones. *Organic Letters* 19(19), 5030-5033.

Andersen, Thomas; Kramer, Søren; Overgaard, Jacob; Skrydstrup, Troels. (2017) Evidence for Single-Electron Pathways in the Reaction between Palladium(II) Dialkyl Complexes and Alkyl Bromides under Thermal and Photoinduced Conditions. *Organometallics* 36(11), 2058-2066.

Nielsen, Morten B.; Ceresoli, Davide; Jørgensen, Jens Erik; Prescher, Clemens; Prakapenka, Vitali B.; Bremholm, Martin. (2017) Experimental evidence for pressure-induced first order transition in cerium nitride from B1 to B10 structure type. *Journal of Applied Physics* 121(2), 1-9.

Stingaciu, Marian; Andersen, Henrik Lyder; Granados-Miralles, Cecilia; Mamakhel, Mohammad Aref Hasen; Christensen, Mogens. (2017) Magnetism in CoFe₂O₄ nanoparticles produced at sub- and near-supercritical conditions of water. *CrystEngComm* 19(28), 3986-3996.

Eikeland, Anna Zink; Stingaciu, Marian; Granados-Miralles, Cecilia; Saura-Múzquiz, Matilde; Andersen, Henrik Lyder; Christensen, Mogens. (2017) Enhancement of magnetic properties by spark plasma sintering of hydrothermally synthesised SrFe₁₂O₁₉. *CrystEngComm* 19(10), 1400-1407.

Stefanescu, I.; Christensen, Mogens; Fenske, J.; Hall-Wilton, R.; Henry, P. F.; Kirstein, O.; Mueller, M.; Nowak, G.; Pooley, D.; Raspino, D.; Rhodes, N.; Saroun, J.; Schefer, J.; Schooneveld, E.; Sykora, J.; Schweika, W. (2017) Neutron detectors for the ESS diffractometers. *Journal of Instrumentation* 12, 2017.

Hvid, Mathias Salomon; Lamagni, Paolo; Lock, Nina. (2017) Light absorption engineering of a hybrid (Sn₃S₇₂)-(n) based semiconductor - from violet to red light absorption. *Scientific Reports* 7, 45822.

Bilag 2: Liste over peer-reviewed artikler 2017

Møller, Kasper T.; Sheppard, Drew; Ravensbaek, Dorte B.; Buckley, Craig E.; Akiba, Etsuo; Li, Hai-Wen; Jensen, Torben R. (2017) Complex Metal Hydrides for Hydrogen, Thermal and Electrochemical Energy Storage. *Energies* 10(10), 1645.

Møller, Kasper T.; Jørgensen, Mathias; Fogh, Alexander S.; Jensen, Torben R. (2017) Perovskite alkali metal samarium borohydrides : crystal structures and thermal decomposition. *Dalton Transactions (Print Edition)* 46, 11905-11912.

Hansen, Bjarne R. S.; Tumanov, Nikolay A.; Santoru, Antonio; Pistidda, Claudio; Bednarcik, Jozef; Klassen, Thomas; Dornheim, Martin; Filinchuk, Yaroslav; Jensen, Torben R. (2017) Synthesis, structures and thermal decomposition of ammine $MxB_{12}H_{12}$ complexes ($M = Li, Na, Ca$). *Dalton Transactions (Print Edition)* 46(24), 7770-7781.

Wolczyk, Anna; Paik, Biswajit; Sato, Toyoto; Nervi, Carlo; Brighi, Matteo; GharibDoust, SeyedHosein Payandeh; Chierotti, Michele; Matsuo, Motoaki; Li, Guanqiao; Gobetto, Roberto; Jensen, Torben R.; Cerny, Radovan; Orimo, Shin ichi; Baricco, Marcello. (2017) $Li-5(BH_4)(3)NH$: Lithium-Rich Mixed Anion Complex Hydride. *Journal of Physical Chemistry Part C: Nanomaterials, Interfaces and Hard Matter* 121(21), 11069-11075.

Møller, Kasper Trans; Grinderslev, Jakob; Jensen, Torben René. (2017) A $NaAlH_4$ - $Ca(BH_4)_2$ composite system for hydrogen storage. *Journal of Alloys and Compounds* 720, 497-501.

Hansen, Bjarne R. S.; Paskevicius, Mark; Jørgensen, Mathias; Jensen, Torben R. (2017) Halogenated Sodium-closo-Dodecaboranes as Solid-State Ion Conductors. *Chemistry of Materials* 29(8), 3423-3430.

Plerdsranoy, Prapatsorn; Javadian, Payam; Jensen, Nicolai Dagaard; Nielsen, Ulla Gro; Jensen, Torben René; Utke, Rapee. Compaction of $LiBH_4$ - $LiAlH_4$ nanoconfined in activated carbon nanofibers : Dehydrogenation kinetics, reversibility, and mechanical stability during cycling. *International Journal of Hydrogen Energy* 42(2), 1036–1047.

Heere, Michael; GharibDoust, Seyed Hosein Payandeh; Sørby, Magnus H.; Frommen, Christoph; Jensen, Torben R.; Hauback, Bjørn C. (2017) In situ investigations of bimetallic potassium erbium borohydride. *International Journal of Hydrogen Energy* 42(35), 22468-22474.

Richter, Bo; Ravensbaek, Dorte B.; Sharma, Manish; Spyratou, Alexandra; Hagemann, Hans; Jensen, Torben R. (2017) Fluoride substitution in $LiBH_4$; destabilization and decomposition. *Physical Chemistry Chemical Physics* 19(44), 30157-30165.

Møller, Kasper Trans; Jensen, Torben René; Akiba, Etsuo; Li, Hai-wen. (2017) Hydrogen - A sustainable energy carrier. *Progress in Natural Science: Materials International* 27(1), 34-40.

Heere, Michael ; Payandeh GharibDoust, SeyedHosein; Brighi, Matteo; Frommen, Christoph; Sørby, Magnus H.; Cerný, Radovan; Jensen, Torben René; Hauback, Bjørn C. (2017) Hydrogen Sorption in Erbium Borohydride Composite Mixtures with $LiBH_4$ and/or LiH . *Inorganics* 5(2), 31.

Bilag 2: Liste over peer-reviewed artikler 2017

Paskevicius, Mark; Jepsen, Lars Haahr; Schouwink, Pascal; Černý, Radovan; Ravnsbæk, Dorthe B.; Filinchuk, Yaroslav; Dornheim, Martin; Besenbacher, Flemming; Jensen, Torben René. (2017) Metal borohydrides and derivatives - synthesis, structure and properties. *Chemical Society Reviews* 46(5), 1565-1634.

Paskevicius, Mark; Hansen, Bjarne R. S.; Jorgensen, Mathias; Richter, Bo; Jensen, Torben R. (2017) Multifunctionality of silver closo-boranes. *Nature Communications* 8, 15136.

Huen, Priscilla; Peru, Filippo ; Charalambopoulou, Georgia; Steriotis, Theodore; Jensen, Torben René; Ravnsbæk, Dorthe Bomholdt. (2017) Nanoconfined NaAlH₄ Conversion Electrodes for Li Batteries. *ACS Omega* 2(5), 1956-1967.

Dematteis, Erika M.; Pinatel, Eugenio R.; Corno, Marta; Jensen, Torben R.; Baricco, Marcello. (2017) Phase diagrams of the LiBH₄-NaBH₄-KBH₄ system. *Physical Chemistry Chemical Physics* 19(36), 25071-25079.

Javadian-Deylami, Seyd Payam; Payandeh GharibDoust, SeyedHosein; Li, Hai-Wen; Sheppard, Drew A.; Buckley, Craig E.; Jensen, Torben René. (2017) Reversibility of LiBH₄ Facilitated by the LiBH₄-Ca(BH₄)₂ Eutectic. *Journal of Physical Chemistry C* 121(34), 18439-18449.

Payandeh GharibDoust, SeyedHosein; Ravnsbæk, Dorthe B.; Černý, Radovan; Jensen, Torben R. (2017) Synthesis, structure and properties of bimetallic sodium rare-earth (RE) borohydrides, NaRE(BH₄)₄, RE = Ce, Pr, Er or Gd. *Dalton Transactions (Print Edition)* 46(39), 13421-13431.

Jorgensen, Jens Erik; Filinchuk, Yaroslav; Dmitriev, Vladimir. (2017) Tilting of semi-rigid GaF₆ octahedra in GaF₃ at high pressures. *Powder Diffraction* 32(S1), S69-S73.

Nielsen, Morten B.; Ceresoli, Davide; Jørgensen, Jens Erik; Prescher, Clemens; Prakapenka, Vitali B.; Bremholm, Martin. (2017) Experimental evidence for pressure-induced first order transition in cerium nitride from B1 to B10 structure type. *Journal of Applied Physics* 121(2), 025903, 1-9.

Department of Molecular Biology, Aarhus University

Janulien D, Andersen JL, Nielsen JA, Quistgaard EM, Hansen M, Strandbygaard D, Moeller A, Petersen CM, Madsen P, Thirup SS. (2017) Acidic Environment Induces Dimerization and Ligand Binding Site Collapse in the Vps10p Domain of Sortilin. *Structure* 25, 1809-1819.

Andersen JL, Lindberg S, Langgård M, Maltas PJ, Rønn LCB, Bundgaard C, Strandbygaard D, Thirup S, Watson SP. (2017) The identification of novel acid isostere based inhibitors of the VPS10P family sorting receptor Sortilin. *Bioorg Med Chem Lett.* 27, 2629-2633.

Senissar, M., Manav, M. C., Brodersen, D. E. (2017) Structural conservation of the PIN domain active site across all domains of life, *Protein Sci* 26(8), 1474-1492.

Bendtsen, K. L., Xu, K., Luckmann, M., Winther, K. S., Shah, S. A., Pedersen, C. N. S., and Brodersen, D. E. (2017) Toxin inhibition in *C. crescentus* VapBC1 is mediated by a flexible pseudo-palindromic protein motif and modulated by DNA binding, *Nucleic Acids Res* 45(5), 2875-2886.

Hansen SB, Laursen NS, Andersen GR, Andersen KR*. Introducing site-specific cysteines into nanobodies for mercury labeling allow de novo phasing of their crystal structures. *Acta Crystallogr D Struct Biol.* 2017 Oct 1;73(Pt 10):804-813.

Bozsoki Z, Cheng J, Feng F, Gysel K, Vinther M, Andersen KR, Oldroyd G, Blaise M, Radutoiu S, Stougaard J. Receptor-mediated chitin perception in legume roots is functionally separable from Nod factor perception. *PNAS.* 2017 Sep 5. pii: 201706795. doi: 10.1073/pnas.1706795114. PMID: 28874587.

Andersen KR#*. Insights into Rad3 kinase recruitment from the crystal structure of the DNA damage checkpoint protein Rad26. *J Biol Chem.* 2017 Mar 17.

Gustafsen, C., Olsen, D., Vilstrup, J., Lund, S., Reinhardt, A., Wellner, N., Larsen, T., Andersen, C. B. F., Weyer, K., Li, J., Seeberger, P. H., Thirup, S., Madsen, P. and Glerup, S. (2017) Heparan sulfate proteoglycans present PCSK9 to the LDL receptor, *Nature communications* 8, 503

Mortensen SA, Sander B, Jensen RK, Pedersen JS, Golas MM, Jensenius JC, Hansen AG, Thiel S, Andersen GR. Structure and activation of C1, the complex initiating the classical pathway of the complement cascade. *Proc Natl Acad Sci U S A.* 2017 Jan 31;114(5):986-991.

Pedersen DV, Roumenina L, Jensen RK, Gadeberg TA, Marinozzi C, Picard C, Rybkine T, Thiel S, Sørensen UB, Stover C, Fremeaux-Bacchi V, Andersen GR. Functional and structural insight into properdin control of complement alternative pathway amplification. *EMBO J.* 2017 Apr 13;36(8):1084-1099.

He Y, Staley JP, Andersen GR, Nielsen KH. Structure of the DEAH/RHA ATPase Prp43p bound to RNA implicates a pair of hairpins and motif Va in translocation along RNA. *RNA.* 2017 Jul;23(7):1110-1124.

Mortensen SA, Sander B, Jensen RK, Pedersen JS, Golas M, Jensenius JC, Hansen AG, Thiel S, Andersen GR. Reply to Arlaud et al.: Structure of the C1 complex and the unbound C1r(2)s(2) tetramer. *Proc Natl Acad Sci U S A.* 2017 Jul 18;114(29):E5768-E5770

Jabs F, Plum M, Laursen NS, Jensen RK, Mølgaard B, Miehe M, Mandolesi M, Rauber MM, Pfützner W, Jakob T, Möbs C, Andersen GR, Spillner E. Trapping IgE in a closed conformation by mimicking CD23 binding prevents and disrupts FcεRI interaction. *Nat Commun.* 2018 Jan 2;9(1):7.

Midtgaard S, Darwish T, Pedersen M, Huda P, Larsen A, Jensen G, Kynde S, Skar-Gislinge N, Nielsen A, Olesen C, Blaise M, Venskutonyte R, Krintel C, Møller J, Frielinghaus H, Gilbert E, Martel A, Kastrup J, Jensen PE, Nissen P, Arleth L (2017). Invisible detergents for structure determination of membrane proteins by small-angle neutron scattering. *FEBS J* [in press] doi: 10.1111/febs.14345. **Sampublicering med anden Danscatt-gruppe.**

Dyla M, Terry DS, Kjaergaard M, Sørensen TLM, Andersen JL, Andersen JP, Knudsen CR, Altman RA, Nissen P*, Blanchard SB* (2017). Dynamics of P-type ATPase transport cycle revealed by single-molecule FRET. *Nature* 551, 346-351 doi:10.1038/nature24296.

Sehgal P, Szalai P, Olesen C, Praetorius HA, Nissen P, Christensen SB, Engedal N, Møller JV (2017). Inhibition of the sarco/endoplasmic reticulum (ER) Ca²⁺-ATPase by thapsigargin analogs induces cell death via ER Ca²⁺ depletion and the unfolded protein response. *J Biol Chem* 292, 19656-19673 doi: 10.1074/jbc.M117.796920

Skjørringe T, Amstrup Pedersen P, Salling Thorborg S, Nissen P, Gourdon P, Birk Møller L (2017). Characterization of ATP7A missense mutants suggests a correlation between intracellular trafficking and severity of Menkes disease. *Sci Rep* 7, 757. doi: 10.1038/s41598-017-00618-6.

Focht D, Croll T, Pedersen BP, Nissen P (2017). Improved model of proton pump crystal structure obtained by interactive molecular dynamics flexible fitting expands the mechanistic model for proton translocation in P-type ATPases. *Front Mol Biosci* 8, 202. doi: 10.3389/fphys.2017.00202

Azouaoui H, Montigny C, Dieudonné T, Champeil P, Jacquot A, Vázquez-Ibar JL, Le Maréchal P, Ulstrup J, Ash MR, Lyons JA, Nissen P, Lenoir G (2017). A High and Phosphatidylinositol-4-phosphate (PI4P)-dependent ATPase Activity for the Drs2p/Cdc50p Flippase after Removal of its N- and C-terminal Extensions. *J Biol Chem* 292, 7954-7970, doi: 10.1074/jbc.M116.751487

Stolzenberg S, Li Z, Quick M, Malinauskaite L, Nissen P, Weinstein H, Javitch JA, Shi L (2017). The Role of TM5 in Na² Release and the Conformational Transition of Neurotransmitter:Sodium Symporters toward the Inward-Open State. *J Biol Chem* 292, 7372-7384. doi: 10.1074/jbc.M116.757153

Lyons JA, Bøggild A, Nissen P, Frauenfeld J (2017). Saposin-Lipoprotein Scaffolds for Structure Determination of Membrane Transporters. *Methods Enzymol* 594, 85-99. doi: 10.1016/bs.mie.2017.06.035.

DTU Cen

Reinhardt, J., Hoppe, R., Hofmann, G., Damsgaard, C. D., Patommel, J., Baumbach, C., Baier, S., Rochet, A., Grunwaldt, J. D., Falkenberg, G. & Schroer, C. G. Beamstop-based low-background ptychography to image weakly scattering objects. *Ultramicroscopy* 173, 52–57 (2017).

Baier, S., Damsgaard, C. D., Klumpp, M., Reinhardt, J., Sheppard, T., Balogh, Z., Kasama, T., Benzi, F., Wagner, J. B., Schwieger, W., Schroer, C. G. & Grunwaldt, J.-D. Stability of a Bifunctional Cu-Based Core@Zeolite Shell Catalyst for Dimethyl Ether Synthesis under Redox Conditions Studied by Environmental Transmission Electron Microscopy and in Situ X-Ray Ptychography. *Microsc. Microanal.* 23, (2017).

DTU Chemistry

Y. Jiao, B.W. Adams, A.O. Dohn, K.B. Møller, H. Jónsson, C. Rose-Petruck (2017) Ultrafast X-ray absorption study of longitudinal-transverse phonon coupling in electrolyte aqueous solution, *Physical Chemistry Chemical Physics* 19, 27266-27274.

B. K. Brink, K. Ståhl, T.L. Christiansen and M.A.J. Somers (2017). The ternary Fe-C-N system: Homogeneous distribution of nitrogen and carbon. *JALCOM*. 690, 431-437.

B. K. Brink, K. Ståhl, T. L. Christiansen, C. Frandsen, M. F. Hansen, P. Beran and M.A.J. Somers (2017). Effect of carbon on interstitial ordering and magnetic properties of ϵ -Fe₂(N,C)_{1-z}. *JALCOM* 694, 282-291.

Q. Yu, A.S. Ahmad, K. Ståhl, X.D. Wang, Y. Su, K. Glazyrin, H. P. Liermann, H. Franz, Q.P. Cao, D.X. Zhang and J.Z. Jiang (2017) . Pressure-induced structural change in liquid GaIn eutectic alloy. *Scientific Reports* 7, 1139.

DTU Energy

Makowska, M. G., Kuhn, L., Theil, Frandsen, H. L., Lauridsen, E. M., De Angelis, S., Cleemann, L. N., Morgano, M., Trtik, P., Strobl, M. (2017) Coupling between creep and redox behavior in nickel - yttria stabilized zirconia observed in-situ by monochromatic neutron imaging, *Journal of Power Sources* 340, 167-175. **Collaboration with other DANSCATT institution.**

Makowska, M. G., Strobl, M., Kardjilov, N., Frandsen, H. L., Manke, I., Morgano, M., Lacatusu, M.-E., De Angelis, S., Lauridsen, E. M., Kuhn, L. Theil (2017) Investigating phase behavior and structural changes in NiO/Ni-YSZ composite with monochromatic in-situ 2D and static 3D neutron imaging, *Physica B: Condensed Matter* (in press, available online). **Collaboration with other DANSCATT institution.**

Cunha Ramos, T. J., Jørgensen, J. S., & Andreasen, J. W. (2017). Automated angular and translational tomographic alignment and application to phase-contrast imaging. *Journal of the Optical Society of America A*, 34(10), 1830-1843. DOI: 10.1364/JOSAA.34.001830.

De Angelis, S., Jørgensen, P.S., Esposito, V., Tsai, E.H.R., Holler, M., Kreka, K., Abdellahi, E., Bowen, J.R. (2017) Ex-situ tracking solid oxide cell electrode microstructural evolution in a redox cycle by high resolution ptychographic nanotomography. *Journal of Power Sources* 360, 520–527.

Rossander, L. H., Dam, H. F., Carlé, J. E., Helgesen, M., Rajkovic, I., Corazza, M., Krebs, F. C. & Andreasen, J. W. (2017) In-line, roll-to-roll morphology analysis of organic solar cell active layers *Energy & Environmental Science*, 11, 2411-2419. DOI: 10.1039/C7EE01900A.

DTU Mechanical Engineering

Das, C. R., and Hald, J. (2017) Microstructural evolution in advanced 12Cr steels during creep, 14th International Conference on Creep and Fracture of Engineering Materials and Structures, Creep 2017, Saint Petersburg, Russia, 19-21 June 2017, 138.

Diederichs, A. M., Thiel, F., Fischer, T., Lienert, U., and Pantleon, W. (2017), Monitoring microstructural evolution in-situ during cyclic deformation by high resolution reciprocal space mapping, Journal of Physics: Conference Series, 843, 012031:1-9.

Diederichs, A. M., Thiel, F., Lienert, U., and Pantleon, W. (2017), In-situ investigations of structural changes during cyclic loading by high resolution reciprocal space mapping. Procedia Structural Integrity, 7, 268-274.

Niessen, F., Grumsen, F.B., Hald, J., and Somers, M.A.J. (2017), Formation and stabilization of reversed austenite in supermartensitic stainless steel, Proc. 24th IFHTSE Congr. 2017, 138–145.

Niessen, F., Villa, M., Apel, D., Keßler, O., Reich, M., Hald, J. and Somers, M.A.J. (2017), In situ techniques for the investigation of the kinetics of austenitization of supermartensitic stainless steel, Mater. Sci. Forum., 879, 1381–1386.

Niessen, F., Villa, M., Hald, J. and Somers, M.A.J. (2017), Kinetics analysis of two-stage austenitization in supermartensitic stainless steel, Materials & Design, 116, 8–15.

Lienert, U., Gábor; R., Tamas, U., Wejdemann, C., and Pantleon, W. (2017) High-Resolution Single-Grain Diffraction of Polycrystalline Materials, Synchrotron Radiation News, 30, 35-40.

Okoro, S.C., Nießen, F., Villa, M., Apel, D., Montgomery, M., Jappe Frandsen, F., Pantleon, K. (2017) Complementary Methods for the Characterization of Corrosion Products on a Plant-Exposed Superheater Tube, Metallography, Microstructure, and Analysis, 6, 22-35.

Villa, M., Niessen, F. and Somers, M.A.J. (2017), In Situ Investigation of the Evolution of Lattice Strain and Stresses in Austenite and Martensite During Quenching and Tempering of Steel, Metallurgical and Materials Transactions A, 49, 1–13.

DTU Physics

A low-spin Fe(III) complex with 100-ps ligand-to-metal charge transfer photoluminescence. / Chabera, Pavel; Liu, Yizhu; Prakash, Om; Thyraug, Erling; El Nahhas, Amal; Honarfar, Alireza; Essen, Sofia; Fredin, Lisa A.; Harlang, Tobias C. B.; Kjær, Kasper Skov; Handrup, Karsten; Ericson, Fredric; Tatsuno, Hideyuki; Morgan, Kelsey; Schnadt, Joachim; Haggstrom, Lennart; Ericsson, Tore; Sobkowiak, Adam; Lidin, Sven; Huang, Ping; Styring, Stenbjorn; Uhlig, Jens; Bendix, Jesper; Lomoth, Reiner; Sundstrom, Villy; Persson, Petter; Warnmark, Kenneth. In: Nature, Vol. 543, No. 7647, 2017.

Coherent structural trapping through wave packet dispersion during photoinduced spin state switching. / Lemke, Henrik T.; Kjær, Kasper Skov; Hartsock, Robert; Brandt van Driel, Tim; Chollet, Matthieu; Glowia, James M.; Song, Sanghoon; Zhu, Diling; Pace, Elisabetta; Matar, Samir F.; Nielsen, Martin Meedom; Benfatto, Maurizio; Gaffney, Kelly J.; Collet, Eric; Cammarata, Marco. In: Nature Communications, Vol. 8, 15342, 2017.

Damped spin excitations in a doped cuprate superconductor with orbital hybridization. / Ivashko, O.; Shaik, N. E.; Lu, X.; Fatuzzo, C. G.; Dantz, M.; Freeman, P.G.; McNally, D. E.; Destraz, D.; Christensen, Niels Bech; Kurosawa, T.; Momono, N.; Oda, M.; Matt, C. E.; Monney, C.; Rønnow, H. M.; Schmitt, T.; Chang, J. In: Physical Review B, Vol. 95, No. 21, 214508, 2017.

Determining material parameters using phase-field simulations and experiments. / Zhang, Jin; Poulsen, Stefan O.; Gibbs, John W.; Voorhees, Peter W.; Poulsen, Henning Friis. In: Acta Materialia, Vol. 129, 2017, p. 229-238.

FELIX: an algorithm for indexing multiple crystallites in X-ray free-electron laser snapshot diffraction images. / Beyerlein, Kenneth R.; White, Thomas A.; Yefanov, Oleksandr; Gati, Cornelius; Kazantsev, Ivan G.; Gade-Nielsen, Nicolai Fog; Larsen, Peter Mahler; Chapman, Henry N.; Schmidt, Søren. In: Journal of Applied Crystallography, Vol. 50, No. 4, 2017, p. 1075-1083.

Field-induced reentrant magnetoelectric phase in LiNiPO₄. / Toft-Petersen, Rasmus; Fogh, Ellen; Kihara, Takumi; Jensen, Jens; Fritsch, Katharina; Lee, Jooseop; Granroth, Garrett E.; Stone, Matthew B.; Vaknin, David; Nojiri, Hiroyuki; Christensen, Niels Bech. In: Physical Review B, Vol. 95, No. 6, 064421, 2017.

From concept to in vivo testing: Microcontainers for oral drug delivery. / Mazzoni, Chiara; Tentor, Fabio; Andersen, Sophie Strindberg; Nielsen, Line Hagner; Keller, Stephan Sylvest; Alstrøm, Tommy Sonne; Gundlach, Carsten; Müllertz, Anette; Marizza, Paolo; Boisen, Anja. In: Journal of Controlled Release, Vol. 268, 2017, p. 343-351.

Improved orientation sampling for indexing diffraction patterns of polycrystalline materials. / Larsen, Peter Mahler; Schmidt, Søren. In: Journal of Applied Crystallography, Vol. 50, No. 6, 2017.

Induced Mesocrystal-Formation, Hydrothermal Growth and Magnetic Properties of α -Fe₂O₃ Nanoparticles in Salt-Rich Aqueous Solutions. / Brok, Erik; Larsen, Jacob; Varón, Miriam; Hansen, Thomas W.; Frandsen, Cathrine. In: Crystals, Vol. 7, No. 8, 2017, p. 248.

In-Situ X-ray Tomography Study of Cement Exposed to CO₂ Saturated Brine. / Chavez Panduro, E. A.; Torsæter, M.; Gawel, K.; Bjørge, R.; Gibaud, A.; Yang, Yan; Bruns, S.; Zheng, Yi; Sørensen, H. O.; Breiby, D. W. In: Environmental Science and Technology, Vol. 51, No. 16, 2017, p. 9344-9351. (with KU Chem)

Ligand manipulation of charge transfer excited state relaxation and spin crossover in [Fe(2,2'-bipyridine)₂(CN)₂]. / Kjær, Kasper Skov; Zhang, Wenkai; Alonso-Mori, Roberto; Bergmann, Uwe; Chollet, Matthieu; Hadt, Ryan G.; Hartsock, Robert W.; Harlang, Tobias C. B.; Kroll, Thomas; Kubiček, Katharina; Lemke, Henrik T.; Liang, Huiyang W.; Liu, Yizhu; Nielsen, Martin Meedom; Robinson, Joseph S.; Solomon, Edward I.; Sokaras, Dimosthenis; van Driel, Tim B.; Weng, Tsu-Chien; Zhu, Diling; Persson, Petter; Wärnmark, Kenneth; Sundström, Villy; Gaffney, Kelly J. In: Structural Dynamics, Vol. 4, No. 4, 044030, 2017.

Magnetic order, hysteresis, and phase coexistence in magnetoelectric LiCoPO₄. / Fogh, Ellen; Toft-Petersen, Rasmus; Ressouche, Eric; Niedermayer, Christof; Holm, Sonja Lindahl; Bartkowiak, Maciej; Prokhnenko, Oleksandr; Sloth, Steffen; Isaksen, Frederik Werner; Vaknin, David; Christensen, Niels Bech. In: Physical Review B, Vol. 96, No. 10, 104420, 2017.

Manipulating charge transfer excited state relaxation and spin crossover in iron coordination complexes with ligand substitution. / Zhang, Wenkai; Kjær, Kasper Skov; Alonso-Mori, Roberto; Bergmann, Uwe; Chollet, Matthieu; Fredin, Lisa A.; Hadt, Ryan G.; Hartsock, Robert W.; Harlang, Tobias; Kroll, Thomas; Kubiček, Katharina; Lemke, Henrik T.; Liang, Huiyang W.; Liu, Yizhu; Nielsen, Martin Meedom; Persson, Petter; Robinson, Joseph S.; Solomon, Edward I.; Sun, Zheng; Sokaras, Dimosthenis; Brandt van Driel, Tim; Weng, Tsu Chien; Zhu, Diling; Wärnmark, Kenneth; Sundström, Villy; Gaffney, Kelly J. In: Chemical Science, Vol. 8, No. 1, 2017, p. 515-523.

Measured resolved shear stresses and Bishop-Hill stress states in individual grains of austenitic stainless steel. / Juul, Nicolai Ytterdal; Oddershede, Jette; Beaudoin, Armand ; Chatterjee, Kamalika ; K.A. Koker, Margaret; Dale, Darren; Shade, Paul; Winther, Grethe. In: Acta Materialia, Vol. 141, 2017, p. 388-404. (with DTU MEK)

Methodology for in situ synchrotron X-ray studies in the laser-heated diamond anvil cell. / Mezouar, M.; Giampaoli, R.; Garbarino, G.; Kantor, I.; Dewaele, A.; Weck, G.; Boccato, S.; Svitlyk, V.; Rosa, A. D.; Torchio, R.; Mathon, O.; Hignette, O.; Bauchau, S. In: High Pressure Research, Vol. 37, No. 2, 03.04.2017, p. 170-180.

Monte Carlo Particle Lists: MCPL. / Kittelmann, Thomas ; Klinkby, Esben Bryndt; Bergbäck Knudsen, Erik; Willendrup, Peter Kjær; Cai, Xiao Xiao; Kanaki, Kalliopi . In: Computer Physics Communications, Vol. 218, 2017, p. 17-42. (with DTU NUTECH)

MultiFLEXX - The new multi-analyzer at the cold triple-axis spectrometer FLEXX. / Groitl, Felix; Toft-Petersen, Rasmus; Quintero-Castro, Diana Lucia; Meng, Siqin; Lu, Zhilun; Huesges, Zita; Le, Manh Duc; Alimov, Svyatoslav; Wilpert, Thomas; Kiefer, Klaus; Gerischer, Sebastian; Bertin, Alexandre; Habicht, Klaus. In: Scientific Reports, Vol. 7, No. 1, 13637, 2017.

Bilag 2: Liste over peer-reviewed artikler 2017

Off-axis spin orientation in goethite nanoparticles. / Brok, Erik; Lefmann, Kim; Nilsen, Gøran Jan; Kure, Mathias; Frandsen, Cathrine. In: Physical Review B, Vol. 96, No. 10, 104426, 2017. (with Niels Bohr Institute)

On the elusive crystal structure of expanded austenite. / Brink, Bastian; Ståhl, Kenny; Christiansen, Thomas Lundin; Oddershede, Jette; Winther, Grethe; Somers, Marcel A. J. (with DTU MEK and DTU CHEM). In: Scripta Materialia, Vol. 131, 2017, p. 59-62. Publication: Research - peer-review › Journal article – Annual report year: 2017

Operando XAS Study of the Surface Oxidation State on a Monolayer IrO_x on RuO_x and Ru Oxide Based Nanoparticles for Oxygen Evolution in Acidic Media. / Pedersen, Anders Filsøe; Escibano, Maria Escudero; Sebok, Bela; Bodin, Anders; Paoli, Elisa Antares; Frydendal, Rasmus; Friebe, Daniel; Stephens, Ifan; Rossmesl, Jan; Chorkendorff, Ib; Nilsson, Anders. In: Journal of Physical Chemistry Part B: Condensed Matter, Materials, Surfaces, Interfaces & Biophysical, 2017.

Powder embossing method for selective loading of polymeric microcontainers with drug formulation. / Abid, Zarmeena; Gundlach, Carsten; Durucan, Onur; von Halling Laier, Christoffer; Nielsen, Line Hagner; Boisen, Anja; Keller, Stephan Sylvest. In: Microelectronic Engineering, Vol. 171, 2017, p. 20-24.

Simulating and optimizing compound refractive lens-based X-ray microscopes. / Simons, Hugh; Ahl, Sonja Rosenlund; Poulsen, Henning Friis; Detlefs, Carsten. In: Journal of Synchrotron Radiation, Vol. 24, No. 2, 2017, p. 392-401.

SiO₂ Glass Density to Lower-Mantle Pressures. / Petitgirard, Sylvain; Malfait, Wim J.; Journaux, Baptiste; Collings, Ines E.; Jennings, Eleanor S.; Blanchard, Ingrid; Kantor, Innokenty; Kurnosov, Alexander; Cotte, Marine; Dane, Thomas; Burghammer, Manfred; Rubie, David C. In: Physical Review Letters, Vol. 119, No. 21, 215701, 2017.

Spin excitations and quantum criticality in the quasi-one-dimensional Ising-like ferromagnet CoCl₂·2D₂O in a transverse field. / Larsen, J.; Schäffer, T. K.; Hansen, U. B.; Holm, S. L.; Ahl, Sonja Rosenlund; Toft-Petersen, Rasmus; Taylor, J.; Ehlers, G.; Jensen, J.; Rønnow, H. M.; Lefmann, K.; Christensen, Niels Bech. In: Physical Review B, Vol. 96, No. 17, 174424, 2017. (with Niels Bohr Institute)

Spin orientation in solid solution hematite-ilmenite. / Brok, Erik; Frandsen, Cathrine; Lefmann, Kim; McEnroe, Suzanne A.; Robinson, Peter; Burton, Benjamin P.; Hansen, Thomas C.; Harrison, Richard. In: American Mineralogist, Vol. 102, No. 6, 2017, p. 1234-1243. (with Niels Bohr Institute)

Stability of charge-stripe ordered La_{2-x}Sr_xNiO_{4+δ} at one third doping. / Freeman, P.G.; Mole, R.A.; Christensen, Niels Bech; Stunault, A.; Prabhakaran, D. In: Physica B: Condensed Matter, 2017.

Structural stability of naphthyl end-capped oligothiophenes in organic field-effect transistors measured by grazing-incidence X-ray diffraction in operando. / Huss-Hansen, Mathias K.; Lauritzen, Andreas E.; Bikondoa, Oier; Torkkeli, Mika; Tavares, Luciana; Knaapila, Matti; Kjølstrup-Hansen, Jakob. In: Organic Electronics, Vol. 49, 2017, p. 375-381.

The Importance of Surface IrO_x in Stabilizing RuO₂ for Oxygen Evolution. / Escibano, Maria Escudero; Pedersen, Anders Filsøe; Paoli, Elisa Antares; Frydendal, Rasmus; Friebe, Daniel; Malacrida, Paolo; Rossmesl, Jan; Stephens, Ifan E L; Chorkendorff, Ib. In: Journal of Physical Chemistry Part B: Condensed Matter, Materials, Surfaces, Interfaces & Biophysical, 2017.

Time-of-Flight Three Dimensional Neutron Diffraction in Transmission Mode for Mapping Crystal Grain Structures. / Cereser, Alberto; Strobl, Markus; Hall, Stephen A.; Steuwer, Axel; Kiyonagi, Ryoji; Tremsin, Anton S.; Bergbäck Knudsen, Erik; Shinohara, Takenao; Willendrup, Peter Kjær; Bastos da Silva Fanta, Alice; Iyengar, Srinivasan; Larsen, Peter Mahler; Hanashima, Takayasu; Moyoshi, Taketo; Kadletz, Peter M; Krooß, Philipp; Niendorf, Thomas; Sales, Morten; Schmahl, Wolfgang W.; Schmidt, Søren. In: Scientific Reports, Vol. 7, No. 1, 9561, 2017.

Towards identifying the active sites on RuO₂(110) in catalyzing oxygen evolution . / Rao, Reshma R. ; Kolb, Manuel J. ; Halck, Niels Bendtsen; Pedersen, Anders Filsøe; Mehta, Apurva; You, Hoydoo ; Stoerzinger, Kelsey A. ; Feng, Zhenxing ; Hansen, Heine Anton; Zhou, Hua ; Giordano, Livia ; Rossmesl, Jan; Vegge, Tejs; Chorkendorff, Ib; Stephens, Ifan; Shao-Horn, Yang. In: Energy & Environmental Science, Vol. 10, No. 12, 2017, p. 2626-2637.

Ultrafast dynamics of two copper bis-phenanthroline complexes measured by x-ray transient absorption spectroscopy : Paper. / Kelley, Matthew S.; Shelby, Megan L.; Mara, Michael W.; Haldrup, Kristoffer; Hayes, Dugan; Hadt, Ryan G.; Zhang, Xiaoyi; Stickrath, Andrew B.; Ruppert, Romain; Sauvage, Jean-Pierre; Zhu, Diling; Lemke, Henrik T.; Chollet, Matthieu; Schatz, George C.; Chen, Lin X. In: Journal of Physics B: Atomic, Molecular and Optical Physics, Vol. 50, No. 15, 154006, 2017.

Ultra-low-angle boundary networks within recrystallizing grains. / Ahl, Sonja Rosenlund; Simons, Hugh; Zhang, Yubin; Detlefs, C.; Stöhr, Frederik; Jakobsen, Anders Clemen; Juul Jensen, Dorte; Poulsen, Henning Friis. In: Scripta Materialia, Vol. 139, 2017, p. 87-91. (with DTU MEK)

Unique Crystal Orientation of Poly(ethylene oxide) Thin Films by Crystallization Using a Thermal Gradient. / Gbabode, Gabin; Delvaux, Maxime; Schweicher, Guillaume; Andreasen, Jens Wenzel; Nielsen, Martin Meedom; Geerts, Yves H. In: Macromolecules, Vol. 50, No. 15, 2017, p. 5877-5891. (with DTU ENERGY)

X-ray diffraction microscopy based on refractive optics. / Poulsen, Henning Friis; Jakobsen, A. C.; Simons, Hugh; Ahl, Sonja Rosenlund; Cook, P. K.; Detlefs, C. In: Journal of Applied Crystallography, Vol. 50, No. 5, 2017, p. 1441-1456.

DTU Space

Desiree D. Ferreira, Sonny Masahi, Finn E. Christensen, M. Bavdaz, Max Collon, Boris Landgraf, Nis C. Gellert, Jakob Kormann, Paschalis Dalampiras, Ida F. Rasmussen, Ifikratis Kamanidis, Michael Krumrey, Swenja Schreiber, 'Design, Development and performance of X-ray Mirror coatings for the ATHENA mission', SPIE proceedings Vol 10399.

DTU Wind Energy

Xu CL, Zhang YB, Godfrey A, Wu GL, Liu W, Tischler JZ, Liu Q, Juul Jensen D. (2017) "Direct observation of nucleation in the bulk of an opaque sample" Scientific report. 7, 42508.

Zhang YB, Fan GH, (2017) "Review article: Three-dimensional X-ray diffraction technique for metals science" Materials China, 36, 181-187. (In Chinese.)

Ahl SR, Simons H, Zhang YB, Detlefs C, Stohr F, Jakobsen AC, Juul Jensen D, Poulsen HF, (2017) "Ultra low-angle boundary networks within recrystallizing grains" Scripta Mater. 139, 87-91. **(Together with DTU Physics).**

Zhang YB, Budai JD, Tischler JZ, Liu W, Xu R, Homer ER, Godfrey A, Juul Jensen D (2017) "Boundary migration in a 3D deformed microstructure inside an opaque sample" Scientific report. 7, 4423.

Dhar S, Zhang YB, Xu R, Danielsen HK, Juul Jensen D, (2017) "Synchrotron X-Ray measurement of residual stress within the nose of a worn manganese steel railway crossing" IOP Conference Series: Materials Science and Engineering. 219, 012016.

Zhang CL, Zhang YB, Wu G, Liu W, Godfrey A, (2017) "Quantification of deformation microstructure at ultra-low tensile strain in pure Al prepared by spark plasma sintering." IOP Conference Series: Materials Science and Engineering. 219, 012050.

Zhang YB, Andriollo T, Fæster S, Sturlason A, Liu W, Barabash R, (2017) "Synchrotron measurements of local microstructure and thermal residual strains in ductile cast iron" IOP Conference Series: Materials Science and Engineering. 219, 012054. **(Together with DTU MEK).**

Niels Bohr Institute, Copenhagen University

Chernyy, S., Kirkensgaard, J.J.K, Bakke, A., Mortensen, K., Almdal, K. (2017) On the properties of poly(isoprene-*b*-ferrocenylmethyl methacrylate) block copolymers. *Polymers* 122, 129-136. DOI <https://doi.org/10.1016/j.polymer.2017.11.036> .

Christiansen, T., Cotte, M., Loredó-Portales, R., Lindelof, P.E., Mortensen, K., Ryholt, K., Larsen, S. (2017) The nature of ancient Egyptian copper-containing carbon inks is revealed by synchrotron radiation based X-ray microscopy. *Scientific Reports* 7, 15346, 1-8. DOI <http://dx.doi.org/10.1038/s41598-017-15652-7>.

Wingstrand, S., Shen, B., Kornfield, J., Mortensen, K., Parisi, D., Vlassopoulos, D., Hassager, O. (2017) Rheological Link Between Polymer Melts with a High Molecular Weight Tail and Enhanced Formation of Shish-kebabs. *ACS Macro Letters* 6, 1268–1273. DOI <http://dx.doi.org/10.1021/acsmacrolett.7b00718>.

Khaliqi, K., Ghazal, A., Azmi, I.D.M., Amenitsch, H., Mortensen, K., Salentinig, S., Yagmur, A. (2017) Direct Monitoring of Lipid Transfer on Exposure of Citrem Nanoparticles to an Ethanol Solution Containing Soybean Phospholipid by Combining Synchrotron SAXS with Microfluidics. *Analyst* 142, 3118–3126 DOI <http://dx.doi.org/10.1039/C7AN00860K>.

Goldstein, A., Annor, G., Vamadevan, V., Tetlow, I., Kirkensgaard, J.J.K., Mortensen, K., Blennow, A., Hebelstrup, K.H., Bertoft, E. (2017) Influence of diurnal photosynthetic activity on the morphology, structure, and thermal properties of normal and waxy barley starch. *International Journal of Biological Macromolecules* 98, 188–200. DOI <http://dx.doi.org/10.1016/j.ijbiomac.2017.01.118>.

Wingstrand, S.L., van Drongelen, M., Mortensen, K., Graham, R.S., Huang, Q., Hassager, O. (2017) The influence of extensional stress overshoot on crystallization of LDPE. *Macromolecules* 50, 1134-1140 DOI: <http://dx.doi.org/10.1021/acs.macromol.6b02543>.

Chernyy, S., Wang, Z., Kirkensgaard, J.J.K., Bakke, A., Mortensen, K., Ndoni, S., Almdal, K. (2017) Synthesis and Characterization of Ferrocene Containing Block Copolymers. *J. Pol. Sci. A: Pol. Chem.* 55, 495-503. Doi: <http://dx.doi.org/10.1002/pola.28435>.

Runnsjö, A., Kocherbitov, V., Graf, G., Pettigrew, A., Scherer, D., Mortensen, K., Engblom, J. (2017) Semifluorinated Alkanes and Alkanes: A Phase Study of the Perfluorohexyloctane - Tetradecane system, *J. Chem. Thermodynamics* 105, 352-361, 2017. doi: <http://dx.doi.org/10.1016/j.jct.2016.10.032>.

Hansen, S. (2017). DLSanalysis.org - A web interface for analysis of dynamic light scattering data. *Eur. Biophys. J.* DOI 10.1007/s00249-017-1232-8.

Andersson, M., Mattle, D., Sitsel, O., Klymchuk, T., Nielsen, A. M., Møller, L. B., White, S. H., Nissen, P., and Gourdon, P. (2014) Copper-transporting P-type ATPases use a unique ion release pathway, *Nature structural & molecular biology* 21, 43-48.

Bilag 2: Liste over peer-reviewed artikler 2017

Larsen, J., Schäffer, T.K., Hansen, U.B., Holm, S.L., Ahl, S.R., Toft-Petersen, R., Taylor, J. Ehlers, G., Jensen, J., Rønnow, H.M., Lefmann, K., Christensen, N.B. (2017) Spin excitations and quantum criticality in the quasi one-dimensional Ising-like ferromagnet $\text{CoCl}_2 \cdot 2\text{D}_2\text{O}$ in a transverse field, *Physical Review B* 96, 174424. **(Med DTU).**

Ray, P.J., Andersen, N.H., Jensen, T.B.S., Mohottala, H.E., Niedermayer, C., Lefmann, K., Wells, B.O., v. Zimmermann, M., Udby, L. (2017) Staging superstructure in high-Tc Sr/O co-doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, *Physical Review B* 96, 174106. **(Med DTU).**

Brok, E, Lefmann, K., Nilsen, G.J., Kure, M, Frandsen, C. (2017) Off-axis spin orientation in goethite nanoparticles, *Physical Review B* 96, 104426. **(Med DTU).**

Gannon, W.J., Halperin, W.P., Eskildsen, M.R., Dai, P., Hansen, U.B., Lefmann, K., Stunault, A. (2017) Spin susceptibility of the topological superconductor UPt_3 from polarized neutron diffraction, *Physical Review B* 96, 041111(R).

Fedrico, A, Williams, A.R. Strobl, M., Panzner, T., Lefmann, K., Jørgensen, L., Lindelof, P.E., Scherillo, A., Porcher, F., Grazi, F. (2017) Extraction and obstruction of intrinsic archaeological information in metallic artefacts – a neutron diffraction study (on Viking swords), *Journal of Archaeological Science - Reports* 12, 425-436.

Hansen, U.B., Bertelsen, M., Stahn, J., Lefmann, K. (2017) An optional focusing SELENE extension to conventional neutron guides, a case study for the ESS instrument BIFROST, *Nuclear Instruments and Methods A* 852, 46–56.

Brok, E., Frandsen, C., Lefmann, K., McEnroe, S., Robinson, P., Burton, B.P., Hansen, T.C., Harrison, R. (2017) Spin orientation in solid solution hematite-ilmenite, *American Mineralogist* 102, 1234-1243. **(Med DTU).**

Fedrico, A., Strobl, M., Williams, A.R., Lefmann, K., Lindelof, P.E., Jørgensen, L., Pentz, P., Bausenwein, D., Schillinger, B., Kovyakh, A., Grazi, F. (2017) Neutron imaging study of ‘pattern-welded’ swords from the Viking Age, *Archaeological and Anthropological Sciences*, DOI 10.1007/s12520-016-0454-5.

Ignazzi, R., Gates, W. P., Diallo, S. O., Yu, D., Juranyi, F., Natali, F., Bordallo, H. N. (2017) Electric Field Induced Polarization Effects Measured by In Situ Neutron Spectroscopy, *Journal of Physical Chemistry C*, 121, 23582–23591.

Martins, M. L., Eckert, J., Jacobsen, H., dos Santos, E. C., Ignazzi, R., de Araujo, D. R., Bellissent-Funel, M.-C., Natali, F., Koza, M. M., Matic, A., de Paula, E., Bordallo, H. N. (2017) Raman and Infrared spectroscopies and X-ray diffraction data on bupivacaine and ropivacaine complexed with 2-hydroxypropyl- β -cyclodextrin. *Data in Brief*, 15, 25-29.

Gates, W. P., Aldridge, L. P., Guzman, G. G., Mole, R. A., Yu, D., Iles, G. N., Klapproth, A., Bordallo, H. N. (2017) Water desorption and absorption isotherms of sodium montmorillonite: A QENS study. *Applied Clay Science*, 147, 97–104.

Bilag 2: Liste over peer-reviewed artikler 2017

Berg, M. C., Dalby, K. N., Tsapatsaris, N., Okhrimenko, D. V., Sørensen, H. O., Jha, D., Embs, J. P., Stipp, S. L. S., Bordallo, H. N. (2017) Water Mobility in Chalk: A Quasielastic Neutron Scattering Study. *Journal of Physical Chemistry C*, 121, 14088–14095.

Viani, A., Zbiri, M., Bordallo, H. N., Gualtieri, A. F., Mácová P. (2017) Investigation of the Setting Reaction in Magnesium Phosphate Ceramics With Quasielastic Neutron Scattering. *Journal of Physical Chemistry C*, 121, 11355–67.

dos Santos, E. C., Rozynek, Z., Hansen, E. L., Hartmann-Petersen, R., Klitgaard, R. N., Løbner-Olesen, A., Michels, L., Mikkelsen, A., Plivelic, T. S., Bordallo, H. N., Fossum, J. O. (2017) Ciprofloxacin intercalated in fluorohectorite clay: Identical pure drug activity and toxicity with higher adsorption and controlled release rate. *RSC Adv.* 7, 26537–45.

Martins, M. L., Eckert, J., Jacobsen, H., dos Santos, E. C., Ignazzi, R., de Araujo, D. R., Bellissent-Funel, M.-C., Natali, F., Koza, M. M., Matic, A., de Paula, E., Bordallo, H. N. (2017) Probing the dynamics of complexed local anesthetics via neutron scattering spectroscopy and DFT calculations. *Int. J. Pharm.* 524, 397–406.

Kapishnikov, S., Grolimund, D., Schneider, G., Pereiro, E., McNally, J. G., Als-Nielsen, J., Leiserowitz, L. (2017) Unraveling heme detoxification in the malaria parasite by in situ correlative X-ray fluorescence microscopy and soft X-ray tomography, *Scientific Reports*, 7, 7610.

Kapishnikov, S., Leiserowitz, L., Yang, Y., Cloetens, P., Pereiro, E., Awamu Ndonglack, F., Matuschewski, K., Als-Nielsen, J. (2017) Biochemistry of malaria parasite infected red blood cells by X-ray microscopy, *Scientific Reports* 7, 802.

Martins, M. L., Eckert, J., Jacobsen, H., dos Santos, E. C., Ignazzi, R., de Araujo, D. R., Bellissent-Funel, M.-C., Natali, F., Koza, M. M., Matic, A., de Paula, E., Bordallo, H. N. (2017) Raman and Infrared spectroscopies and X-ray diffraction data on bupivacaine and ropivacaine complexed with 2-hydroxypropyl- β -cyclodextrin. *Data in Brief*, 15, 25-29.

dos Santos, E. C., Rozynek, Z., Hansen, E. L., Hartmann-Petersen, R., Klitgaard, R. N., Løbner-Olesen, A., Michels, L., Mikkelsen, A., Plivelic, T. S., Bordallo, H. N., Fossum, J. O. (2017) Ciprofloxacin intercalated in fluorohectorite clay: Identical pure drug activity and toxicity with higher adsorption and controlled release rate. *RSC Adv.* 7, 26537–45.

Martins, M. L., Eckert, J., Jacobsen, H., dos Santos, E. C., Ignazzi, R., de Araujo, D. R., Bellissent-Funel, M.-C., Natali, F., Koza, M. M., Matic, A., de Paula, E., Bordallo, H. N. (2017) Probing the dynamics of complexed local anesthetics via neutron scattering spectroscopy and DFT calculations. *Int. J. Pharm.* 524, 397–406.

Berg, M. C., Dalby, K. N., Tsapatsaris, N., Okhrimenko, D. V., Sørensen, H. O., Jha, D., Embs, J. P., Stipp, S. L. S., Bordallo, H. N. (2017) Water Mobility in Chalk: A Quasielastic Neutron Scattering Study. *Journal of Physical Chemistry C*, 121, 14088–14095.

Bilag 2: Liste over peer-reviewed artikler 2017

Birolo, Leila, Antonella Tomeo, Marco Trifuoggi, Finizia Auriemma, Luigi Paduano, Angela Amoresano, Roberto Vinciguerra, et al. 2017. "A Hypothesis on Different Technological Solutions for Outdoor and Indoor Roman Wall Paintings." *Archaeological and Anthropological Sciences* 9 (4): 591–602. doi:10.1007/s12520-016-0408-y.

Brok, Erik, Cathrine Frandsen, Kim Lefmann, Suzanne McEnroe, Peter Robinson, Benjamin P. Burton, Thomas C. Hansen, and Richard Harrison. 2017. "Spin Orientation in Solid Solution Hematite-Ilmenite." *American Mineralogist* 102 (6): 1234–43. doi:10.2138/am-2017-5792CCBY.

Brok, Erik, Jacob Larsen, Miriam Varón, Thomas Hansen, and Cathrine Frandsen. 2017. "Induced Mesocrystal-Formation, Hydrothermal Growth and Magnetic Properties of α -Fe₂O₃ Nanoparticles in Salt-Rich Aqueous Solutions." *Crystals* 7 (12): 248. doi:10.3390/cryst7080248.

Brok, Erik, Kim Lefmann, Gøran Jan Nilsen, Mathias Kure, and Cathrine Frandsen. 2017. "Off-Axis Spin Orientation in Goethite Nanoparticles." *Physical Review B* 96 (10): 104426. doi:10.1103/PhysRevB.96.104426.

Irace, Carlo, Gabriella Misso, Antonella Capuozzo, Marialuisa Piccolo, Claudia Riccardi, Alessandra Luchini, Michele Caraglia, Luigi Paduano, Daniela Montesarchio, and Rita Santamaria. 2017. "Antiproliferative Effects of Ruthenium-Based Nucleolipidic Nanoaggregates in Human Models of Breast Cancer in Vitro: Insights into Their Mode of Action." *Scientific Reports* 7 (March): 45236. doi:10.1038/srep45236.

Jaiganesh, Avinash, Yoshie Narui, Raul Araya-Secchi, and Marcos Sotomayor. 2017. "Beyond Cell–Cell Adhesion: Sensational Cadherins for Hearing and Balance." *Cold Spring Harbor Perspectives in Biology*, August, a029280. doi:10.1101/cshperspect.a029280.

Lou, Chenguang, Niels Johan Christensen, Manuel C. Martos-Maldonado, Søren Roi Midtgaard, Maria Ejlersen, Peter W. Thulstrup, Kasper K. Sørensen, Knud J. Jensen, and Jesper Wengel. 2017. "Folding Topology of a Short Coiled-Coil Peptide Structure Templated by an Oligonucleotide Triplex." *Chemistry - A European Journal* 23 (39): 9297–9305. doi:10.1002/chem.201700971.

Luchini, Alessandra, Yuri Gerelli, Giovanna Fragneto, Tommy Nylander, Gunnar K Pálsson, Marie-Sousai Appavou, and Luigi Paduano. 2017. "Neutron Reflectometry Reveals the Interaction between Functionalized SPIONs and the Surface of Lipid Bilayers." *Colloids and Surfaces B: Biointerfaces* 151 (March): 76–87. doi:10.1016/j.colsurfb.2016.12.005.

Machoke, Albert Gonche Fortunatus, Benjamin Apeleo Zubiri, Rainer Leonhardt, Venkata Ramana Reddy Marthala, Martin Schmiele, Tobias Unruh, Martin Hartmann, Erdman Spiecker, and Wilhelm Schwieger. 2017. "Densification of Silica Spheres: A New Pathway to Nano-Dimensioned Zeolite-Based Catalysts." *Chemistry - A European Journal* 23 (46): 10983–86. doi:10.1002/chem.201702768.

Marthala, V. R. Reddy, Lynn Urmoneit, Zhou Zhou, Albert G. F. Machoke, Martin Schmiele, Tobias Unruh, Wilhelm Schwieger, and Martin Hartmann. 2017. "Boron-Containing MFI-Type Zeolites with a Hierarchical Nanosheet Assembly for Lipase Immobilization." *Dalton Transactions* 46 (13): 4165–69. doi:10.1039/C7DT00092H.

Mears, Laura L. E., Emily R. Draper, Ana M. Castilla, Hao Su, Zhuola, Bart Dietrich, Michael C. Nolan, et al. 2017. "Drying Affects the Fiber Network in Low Molecular Weight Hydrogels." *Biomacromolecules* 18 (11): 3531–40. doi:10.1021/acs.biomac.7b00823.

North, S. M., E. R. Jones, G. N. Smith, O. O. Mykhaylyk, T. Annable, and S. P. Armes. 2017. "Adsorption of Small Cationic Nanoparticles onto Large Anionic Particles from Aqueous Solution: A Model System for Understanding Pigment Dispersion and the Problem of Effective Particle Density." *Langmuir* 33 (5): 1275–84. doi:10.1021/acs.langmuir.6b04541.

O'Shea, Charlotte, Lasse Staby, Sidsel Krogh Bendsen, Frederik Grønbæk Tidemand, Andreas Redsted, Martin Willemoës, Birthe B. Kragelund, and Karen Skriver. 2017. "Structures and Short Linear Motif of Disordered Transcription Factor Regions Provide Clues to the Interactome of the Cellular Hub Protein Radical-Induced Cell Death1." *Journal of Biological Chemistry* 292 (2): 512–27. doi:10.1074/jbc.M116.753426.

Pedersen, Martin Cramer, and Stephen T. Hyde. 2017. "Hyperbolic Crystallography of Two-Periodic Surfaces and Associated Structures." *Acta Crystallographica Section A Foundations and Advances* 73 (2): 124–34. doi:10.1107/S2053273316019112.

Russo Krauss, Irene, Riccardo Imperatore, Augusta De Santis, Alessandra Luchini, Luigi Paduano, and Gerardino D'Errico. 2017. "Structure and Dynamics of Cetyltrimethylammonium Chloride-Sodium Dodecylsulfate (CTAC-SDS) Catanionic Vesicles: High-Value Nano-Vehicles from Low-Cost Surfactants." *Journal of Colloid and Interface Science* 501 (September): 112–22. doi:10.1016/j.jcis.2017.04.032.

Sander, M., M. Herzog, J. E. Pudell, M. Bargheer, N. Weinkauff, M. Pedersen, G. Newby, et al. 2017. "Spatiotemporal Coherent Control of Thermal Excitations in Solids." *Physical Review Letters* 119 (7): 75901. doi:10.1103/PhysRevLett.119.075901.

Schindler, Torben, Tilo Schmutzler, Martin Schmieles, Wei Lin, Doris Segets, Wolfgang Peukert, Marie-Sousia Appavou, Armin Kriele, Ralph Gilles, and Tobias Unruh. 2017. "Changes within the Stabilizing Layer of ZnO Nanoparticles upon Washing." *Journal of Colloid and Interface Science* 504 (October): 356–62. doi:10.1016/j.jcis.2017.05.059.

Smith, Gregory N., Samuel D. Finlayson, Sarah E. Rogers, Paul Bartlett, and Julian Eastoe. 2017. "Electrolyte-Induced Instability of Colloidal Dispersions in Nonpolar Solvents." *The Journal of Physical Chemistry Letters* 8 (19): 4668–72. doi:10.1021/acs.jpclett.7b01685.

Smith, Gregory N., Silvia Ahualli, Ángel V. Delgado, David A. J. Gillespie, Roger Kemp, Jocelyn Peach, Jonathan C. Pegg, et al. 2017. "Charging Poly(methyl Methacrylate) Latexes in Nonpolar Solvents: Effect of Particle Concentration." *Langmuir* 33 (47): 13543–53. doi:10.1021/acs.langmuir.7b02257.

Smith, Gregory N., James E Hallett, Paul Joseph, Svetlana Tretsiakova-McNally, Tan Zhang, Frank D Blum, and Julian Eastoe. 2017. "Structural Studies of Thermally Stable, Combustion-Resistant Polymer Composites." *Polymer Journal* 49 (10): 711–19. doi:10.1038/pj.2017.44.

Bilag 2: Liste over peer-reviewed artikler 2017

Waldie, Sarah, Tania K. Lind, Kathryn Browning, Martine Moulin, Michael Haertlein, V.

Trevor Forsyth, Alessandra Luchini, et al. 2018. "Localization of Cholesterol within Supported Lipid Bilayers Made of a Natural Extract of Tailor-Deuterated Phosphatidylcholine." *Langmuir* 34 (1): 472–79. doi:10.1021/acs.langmuir.7b02716.

Witteloostuijn, Søren B. van, Louise S. Dalbøge, Gitte Hansen, Søren Roi Midtgaard, Grethe Vestergaard Jensen, Knud J. Jensen, Niels Vrang, Jacob Jelsing, and Søren L. Pedersen. 2017. "GUB06-046, a Novel Secretin/glucagon-like Peptide 1 Co-Agonist, Decreases Food Intake, Improves Glycemic Control, and Preserves Beta Cell Mass in Diabetic Mice." *Journal of Peptide Science* 23 (12): 845–54. doi:10.1002/psc.3048.

Department of Chemistry, University of Copenhagen

S. S. Hakim, M. H. M. Olsson, H. O. Sørensen, N. Bovet, J. Bohr, R. Feidenhans'l, S. L. S. Stipp (2017) Interactions of the Calcite {10.4} Surface with Organic Compounds: Structure and Behaviour at Mineral – Organic Interfaces. *Sci. Rep.* 7, 7592. DOI: 10.1038/s41598-017-06977-4. **Publikation med anden**

DANSCATT gruppe.

E. A. Chavez Panduro, M. Torsæter, K. Gawel, R. Bjørge, A. Gibaud, Y. Yang, S. Bruns, Y. Zheng, H. O. Sørensen, D. W. Breiby (2017) In-situ X-ray tomography study of well cement exposed to CO₂ saturated brine. *Envir. Sci. Techn.* 51, 9344-9351. DOI: 10.1021/acs.est.6b06534. **Publikation med anden**

DANSCATT gruppe.

Y. Yang, S. Bruns, S. L. S. Stipp, H. O. Sørensen (2017) Dissolved CO₂ increases breakthrough in natural porous materials. *Envir. Sci. Techn.* 51(14), 7982–7991. DOI: 10.1021/acs.est.7b02157.

S. Bruns, S. L. S. Stipp, H. O. Sørensen (2017) Statistical Representative Elementary Volumes of Porous Media determined using Greyscale Analysis of 3D Tomograms. *Adv. Water Res.* 107, 32-42. DOI: 10.1016/j.advwatres.2017.06.002.

M.C. Berg, K.N. Dalby, N. Tsapatsaris, D. Okhrimenko, H.O. Sørensen, D. Jha, J. Embs, S.L.S. Stipp, H.N. Bordallo (2017) Water mobility in chalk: A Quasielastic Neutron Scattering study. *J. Phys. Chem. C* 121, 14088–14095. DOI: 10.1021/acs.jpcc.7b01998. **Publikation med anden DANSCATT gruppe.**

S. Bruns, S. L. S. Stipp, H. O. Sørensen (2017) Looking for the Signal: A Guide to Iterative Noise and Artefact Removal in X-ray Tomography Reconstructions of Reservoir Rocks. *Adv. Water Res.* 105, 96-107. DOI: 10.1016/j.advwatres.2017.04.020.

R. Besselink, J.D. Rodriguez-Blanco, T.M. Stawski, L.G. Benning, D.J. Tobler (2017) How short-lived ikaite affects calcite crystallization. *Cryst. Growth Des.* 17 (12), 6224–6230. DOI: 10.1021/acs.cgd.7b00743.

Wood, S.R., Woods, K. N., Plassmeyer, P. N., Marsh, D. A., Johnson, D. W., Page, C. J., Jensen, K. M. Ø., Johnson, D.C. (2017), Same Precursor, Two Different Products: Comparing the Structural Evolution of In–Ga–O “Gel-Derived” Powders and Solution-Cast Films Using Pair Distribution Function Analysis. *Journal of the American Chemical Society*, 139 (15), 5607-5613.

Pedersen, K. S., Woodruff, D. N., Singh, S. K., Tressaud, A., Durand, E., Atanasov, M., Perlepe, P., Ollefs, K., Wilhelm, F., Mathonière, C., Neese, F., Rogalev, A., Bendix, J., and Clérac, R. (2017) [OsF₆]^{x-}: Molecular Models for Spin-Orbit Entangled Phenomena, *Chem. Eur. J.* 23, 11244-11248. **Publikation med anden DANSCATT gruppe.**

Frandsen, K.E.H., Poulsen J-C.N., Tandrup, T., L.Lo Leggio (2017) Unliganded and substrate bound structures of the cellobiosaccharide active lytic polysaccharide monooxygenase LsAA9A at low pH *Carb. Res.* 448, 187-190.

Bilag 2: Liste over peer-reviewed artikler 2017

Frandsen, K.E.H., Poulsen, J.C.N., Tovborg, M., Johansen, K.S. and Lo Leggio, L. (2017) Learning from oligosaccharide soaks of crystals of an AA13 lytic polysaccharide monooxygenase: crystal packing, ligand binding and active site disorder *Acta Cryst D* 73, 64-76.

Simmons, T.J., Frandsen, K.E.H., Ciano, L., Tryfona, T., Lenfant, N., Poulsen, J.C.N., Wilson, L.F.L., Tandrup, T., Tovborg, M., Schnorr, K., Johansen, K.S., Henrissat, B., Walton, P.H., Lo Leggio, L. and Dupree P. (2017) Structural and electronic determinants of lytic polysaccharide monooxygenase reactivity on polysaccharide substrates, *Nature comms.* 8, 1064. doi:10.1038/s41467-017-01247-3.

Christiansen, T., Cotte, M., Loredó-Portales, R., Lindelof, P.E., Mortensen, K., Ryholt, K. & Larsen, S. (2017) The nature of ancient Egyptian copper-containing carbon inks is revealed by synchrotron radiation based X-ray microscopy, *Scientific Reports* 7, 15346 DOI: 10.1038/s41598-017-15652-7.

Publikation med anden DANSCATT gruppe.

Department of Drug Design and Pharmacology, University of Copenhagen

Møllerud, S., Pinto, A., Marconi, L., Frydenvang, K., Thorsen, T. S., Laulumaa, S., Venskutonytė, R., Winther, S., Moral, A. M. C., Tamborini, L., Conti, P., Pickering, D. S., and Kastrup, J. S. (2017) Structure and Affinity of Two Bicyclic Glutamate Analogues at AMPA and Kainate Receptors. *ACS Chem. Neurosci.* 8, 2056-2064.

Larsen, A. P., Fièvre, S., Frydenvang, K., Francotte, P., Pirotte, B., Kastrup, J. S., and Mulle, C. (2017) Identification and Structure-Function Study of Positive Allosteric Modulators of Kainate Receptors. *Mol. Pharmacol.* 91, 576-585.

Krogsgaard-Larsen, N., Delgar, C. G., Koch, K., Brown, P. M., Møller, C., Han, L., Huynh, T. H., Hansen, S. W., Nielsen, B., Bowie, D., Pickering, D. S., Kastrup, J. S., Frydenvang, K., and Bunch, L. (2017). Design and Synthesis of a Series of l-trans-4-Substituted Prolines as Selective Antagonists for the Ionotropic Glutamate Receptors Including Functional and X-ray Crystallographic Studies of New Subtype Selective Kainic Acid Receptor Subtype 1 (GluK1) Antagonist (2S,4R)-4-(2-Carboxyphenoxy)pyrrolidine-2-carboxylic Acid. *J. Med. Chem.* 60, 441-457.

Meno, K. H., Kastrup, J. S., Kuo, I. C., Chua, K. Y., and Gajhede, M. (2017) The structure of the mite allergen Blo t 1 explains the limited antibody cross-reactivity to Der p 1. *Allergy* 72, 665-670.

Møllerud, S., Frydenvang, K., Pickering, D. S., Kastrup, J. S. (2017) Lessons from crystal structures of kainate receptors. *Neuropharmacology* 112, 16-28.

Herranz-Trillo F, Groenning M, van Maarschalkerweerd A, Tauler R, Vestergaard B, Bernadó P. (2017) Structural Analysis of Multi-component Amyloid Systems by Chemometric SAXS Data Decomposition. *Structure* 25, 5-15.

The Novo Nordisk Foundation Center for Protein Research, University of Copenhagen

Reviews:

Stella S., Alcón P., Montoya G. (2017) Class 2 CRISPR-Cas RNA-guided endonucleases: Swiss Army knives of genome editing, *Nature Structural and Molecular Biology* 24(11), 882-892.

Original research articles:

Alba J., Marcaida M.J., Prieto J., Montoya G., Molina R., D'Abramo M. (2017) Structure and dynamics of mesophilic variants from the homing endonuclease I-Dmol, *Journal of Computer-Aided Molecular Design* 31: 1063.

Pitchai G.P., Kaulich M., Bizard A.H., Mesa P., Yao Q., Sarlos K., Streicher W.W., Nigg E.A., Montoya G., Hickson I.D. (2017) A novel TPR-BEN domain interaction mediates PICH-BEND3 association, *Nucleic Acids Research* 19(2), 11413-11424. Open Access: <https://doi.org/10.1093/nar/gkx792>.

Han W., Pan S., López-Méndez B., Montoya G., She Q. (2017) Allosteric regulation of Csx1, a type IIIB-associated CARF domain ribonuclease by RNAs carrying a tetraadenylate tail, *Nucleic Acids Research* 45(18), 10740-10750. Open Access: <https://doi.org/10.1093/nar/gkx726>.

Alcón P., Montoya G., Stella S. (2017) Assembly of *Francisella novicida* Cpf1 endonuclease in complex with guide RNA and target DNA, *Acta Crystallographica Section F: Structural Biology Communications* 73(Pt 7), 409-415.

Stella S., Alcón P., Montoya G. (2017) Structure of the Cpf1 endonuclease R-loop complex after target DNA cleavage, *Nature* 546(7659), 559-563.

Alvarez-Cabrera A.L., Delgado S., Gil-Carton D., Mortuza G.B., Montoya G., Sorzano C.O.S., Tang T.K., Carazo J.M. (2017) Electron microscopy structural insights into CPAP oligomeric behavior: A plausible assembly process of a supramolecular scaffold of the centrosome, *Frontiers in Molecular Biosciences* 4, 17. Open Access: <https://doi.org/10.3389/fmolb.2017.00017>.

Department of Biomedical Sciences, University of Copenhagen

Bjørkskov FB, Krabbe SL, Nurup CN, Missel JW, Spulber M, Bomholt J, Molbaek K, Helix-Nielsen C, Gotfryd K, Gourdon P, Pedersen PA (2017). Purification and functional comparison of nine human Aquaporins produced in *Saccharomyces cerevisiae* for the purpose of biophysical characterization. *Sci Rep.* 7(1):16899.

Erlendsson S, Gotfryd K, Larsen FH, Mortensen JS, Geiger MA, van Rossum BJ, Oschkinat H, Gether U, Teilum K, Loland CJ (2017). Direct assessment of substrate binding to the Neurotransmitter: Sodium Symporter LeuT by solid state NMR. *Elife.* 6. pii: e19314. doi: 10.7554/eLife.19314.

Skjørringe T, Amstrup Pedersen P, Salling Thorborg S, Nissen P, Gourdon P, Birk Møller L (2017). Characterization of ATP7A missense mutants suggests a correlation between intracellular trafficking and severity of Menkes disease. *Sci Rep.* 7(1):757.

Department of Pharmacy, University of Copenhagen

Yaghmur, A., Al-Hosayni, S., Amenitsch, H., and Salentinig, S. (2017) Structural investigation of bulk and dispersed inverse lyotropic hexagonal liquid crystalline phases of eicosapentaenoic acid monoglyceride, *Langmuir* 33, 14045–14057.

Khaliqi, K., Ghazal, A., Azmi, I. D. M., Amenitsch, H., Mortensen, K., Salentinig, S., and Yaghmur, A. (2017) Direct monitoring of lipid transfer on exposure of citrem nanoparticles to an ethanol solution containing soybean phospholipid by combining synchrotron SAXS with microfluidics, *Analyst* 142, 3118-3126. **Co-published with another DANSCATT institution (Niels Bohr Institute).**

Ghazal, A., Gontsarik, M., Kutter, J., Lafleur, J., Ahmadvand, D., Labrador, A., and Yaghmur, A. (2017) Microfluidic platform for the continuous production and characterization of multilamellar vesicles: A synchrotron small-angle X-ray scattering (SAXS) study. *Journal of Physical Chemistry Letters* 8, 73-79.

Department of Science and Environment, Roskilde University

Posselt, D., Zhang, J., Smilgies, D.-M., Berezkin, A., Potemkin, I. , Papadakis, C.M. (2017) Restructuring in Block Copolymer Thin Films: In-Situ GISAXS Investigations During Solvent Vapor Annealing, *Prog. Polym. Sci.* 66, 80–115.

Berezkin, A.V, Jung, F., Posselt, D., Smilgies, D.-M., and Papadakis, C.M. (2017) Vertical vs Lateral Macrophase Separation in Thin Films of Block Copolymer Mixtures: Computer Simulations and GISAXS Experiments, *ACS Appl. Mater. Interfaces*, 9, 31291–31301.

Hansen, H. W., Frick, B., Hecksher, T., Dyre, J. C., and Niss, K. (2017) Connection between fragility, mean-squared displacement, and shear modulus in two van der Waals bonded glass-forming liquids. *Physical Review B* 95, 104202.

Jubeli, E.; Maginty, A. B.; Khalique, N. A.; Raju, L.; Nicholson, D. G.; Larsen, H.; Pungente, M. D.; and Goldring, W. P.D. (2017) Cationic lipids bearing succinic-based, acyclic and macrocyclic hydrophobic domains: Synthetic studies and in vitro gene transfer. *Eur. J. Med. Chem.*, 125, 225-232.

Zeth K, Sancho-Vaello E. (2017) The Human Antimicrobial Peptides Dermcidin and LL-37 Show Novel Distinct Pathways in Membrane Interactions. *Front Chem.* 5, 86.

Sancho-Vaello E, François P, Bonetti EJ, Lilie H, Finger S, Gil-Ortiz F, Gil-Carton D, Zeth K. (2017) Structural remodeling and oligomerization of human cathelicidin on membranes suggest fibril-like structures as active species., *Sci Rep.* 7, 15371.

Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

L.B. Staal, S.C.C. Pushparaj, C. Forano, V. Prevot, D. Ravnsbæk, M. Bjerring, and U.G. Nielsen, Competitive reactions during the synthesis of zinc aluminum layered double hydroxides by thermal decomposition of urea, *Journal of Materials Chemistry A*, 2017, 5, 21795-21806.

P. Huen, F. Peru, G. Charalambopoulou, T. Steriotis, T. R. Jensen, D. B. Ravnsbæk, Nanoconfined NaAlH₄ Conversion Electrodes for Li Batteries, *ACS Omega* 2017, 2, 1956–1967. **Co-authored w. T. R. Jensen, AU.**

Huss-Hansen, M. K., Lauritzen, A. E., Bikondoa, O., Torkkeli, M., Tavares, L., Knaapila, M., and Kjelstrup-Hansen, J. (2017) Structural stability of naphthyl end-capped oligothiophenes in organic field-effect transistors measured by grazing-incidence X-ray diffraction in operando, *Organic Electronics*, 49, 375-381. **Co-authored w. Matti Knaapila, DTU.**

P. Huen, D. B. Ravnsbæk, Insight into Poor Cycling Stability of MgH₂ Anodes, *J. Electrochem. Soc.* 2017, 164, A3138-A3143.

B. Richter, D. B. Ravnsbæk, M. Sharma, A. Spyratou, H. Hagemann, T. R. Jensen, Fluoride substitution in LiBH₄, destabilization and decomposition, *Phys. Chem. Chem. Phys.* 2017, 19, 30157-30165. **Co-authored w. T. R. Jensen, AU.**

Risterucci, P., Renault, O., Zborowski, C., Bertrand, D., Torres, A., Rueff, J.-P., Grenet, G., Tougaard, S., Effective inelastic scattering cross-sections for background analysis in HAXPES of deeply buried layers, *Applied surface science* vol 402, 78-85, 2017.

Haldor Topsoe A/S

Andersen C. W., Borfecchia E., Bremholm M., Jørgensen M. R. V., Vennestrøm P. N. R., Lamberti C., Lundegaard L. F., and Iversen B. B. (2017) Redox-Driven Migration of Copper Ions in the Cu-CHA Zeolite as Shown by the In Situ PXRD/XANES Technique, *Angew. Chem. Int. Ed.*, 56, 10367–10372. **Artiklen er skrevet sammen med Bo Brummerstedts gruppe i Århus.**

Bilag 3: DANSCATT ph.d.-projekter 2017

Department of Chemistry, Aarhus University

Anders BankBlichfeld, *Zinc Antimonides and Copper Chalcogenides as Thermoelectric Materials*

Cecilia Granados-Miralles, *Exchange-Coupling and Nano-Structuring As a Means to Improve the Magnetic Performance of Ferrite Nanoparticles: In Situ and Ex Situ Powder Diffraction Studies*

Elisabeth Grube (Borg), *Materials for hydrogen and heat storage*

Kasper Trans Møller, *Complex Metal Hydrides: Synthesis, Characterisation and High-Pressure Studies*

Maika Klemmer, *Continuous Biomass Conversion via Hydrothermal Liquefaction*

Maja Krüger Thomsen, *Electron Density Studies of Molecular Compounds*

Matilde Saura-Múzquiz, *Optimizing the Performance of Hexaferrite Magnets by Bottom-Up Nanostructuring: An X-Ray and Neutron Powder Diffraction Study*

Mattia Sist, *Crystallographic studies of anharmonicity and disorder in IV-VI semiconductors and caesium halides*

Priscilla Huen, *Metal Hydrides for Electrochemical Energy Storage*

SeyedHosein Payandeh GharibDoust, *Complex Metal Hydrides for hydrogen storage and solid-state ion conductors*

Steinar Birgisson, *Real time observations of materials chemistry in batteries*

Mie Elholm Birkbak, *Multimodal X-ray Imaging of Hierarchical Materials*

Department of Molecular Biology, Aarhus University

Xin Jie Jeryl Cheng: Structural and Biochemical Characterisation of LysM Receptor-like Kinases

Casper Larsen: Structural and functional studies of cobalamin uptake and transport

DTU Chemical Engineering

Trine Marie Hartmann Dabros [formerly Arndal], *Hydrodeoxygenation of Biomass Pyrolysis Vapor Model Compounds over MoS₂ Based Catalysts*, DTU Kemiteknik

DTU Cen

Sine E. Olsen

DTU Chemistry

Kasper Tidemand

Structure and function of the regulatory domain in tryptophanhydroxylase

PhD thesis DTU Chemistry, afleveret August 2017

DTU Energy

Salvatore De Angelis, *Tracking Solid Oxide Cell Microstructure Evolution by High Resolution 3D Nano-Tomography*

DTU Mechanical Engineering

Andriollo, Tito, Graphite nodules and local residual stresses in ductile iron: Thermo-mechanical modeling and experimental validation

Bjerre, Mathis Karsten, In situ observations of graphite formation during solidification of cast iron

Juul, Nicolai Ytterdal, Characterisation and modelling at the grain scale during plastic deformation, DTU Mechanical Engineering

DTU Physics

Advanced Neutron Moderators for the ESS. / Schönfeldt, Troels; Lauritzen, Bent (Main supervisor); Willendrup, Peter Kjær (Supervisor); Zanini, Luca (Supervisor). DTU Nutech, 2016. 158 p.

Standard Structural Analysis Algorithms for Nanomaterials. / Larsen, Peter Mahler; Schiøtz, Jakob (Main supervisor); Schmidt, Søren (Supervisor). Department of Physics, Technical University of Denmark, 2017. 151 p.

DTU Wind Energy

Xu, Chaoling: Nucleation of recrystallization at selected sites in deformed fcc metals

Niels Bohr Institute, University of Copenhagen

Aghiad Ghazal, Combination of Microfluidics with SAXS for the Investigation of Pharmaceutical Formulations. Niels Bohr Institute. February 17, 2017. (Supervisor: Mortensen, K.)

Éverton Carvalho dos Santos, Physical capture and release of drug molecules, water and cations by a smectite clay Double degree: Department of Physics, Norwegian University of Science and Technology, Trondheim – Norway & Niels Bohr Institute, University of Copenhagen, Copenhagen – Denmark (Supervisor; Bordallo, H. N.)

N.S. Nazer Operandu Imaging and Diffraction studies of commercial Li-Ion Batteries, Norwegian University of Science and Technology, Trondheim – Norway & ESS, Lund – Sweden (Supervisor: Strobl, M.)

Department of Drug Design and Pharmacology, University of Copenhagen

Anja Probst Larsen: Investigations of the Molecular Basis for Positive Allosteric Modulation of Ionotropic Glutamate Receptors. Department of Drug Design and Pharmacology, Faculty of Health and Medical Sciences, University of Copenhagen, March 31

Nils Helge Skovgaard Andersen: Structural characterization of alpha-synuclein fibrils. Department of Drug Design and Pharmacology, Faculty of Health and Medical Sciences, University of Copenhagen, December 11

The Novo Nordisk Foundation Center for Protein Research, University of Copenhagen

Pablo Alcon, Structural studies on chromatin recognition

Department of Science and Environment, Roskilde University

Mikkel Hartmann Jensen, 'Structure and Dynamics of Hydrogen-Bonded Liquids', vejledt af Kristine Niss og Tina Hecksher (RUC) og Christiane Alba-Simionesco (LLB, Paris)

Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

Priscilla Huen, Metal Hydrides for Electrochemical Energy Storage, Aarhus University. **Co-supervised by Dorthe B. Ravnsbæk, SDU**

Bilag 3: DANSCATT ph.d.-projekter 2017

David Poulsen de Sousa , New catalysts for oxidation reactions

Bilag 4: DANSCATT outreach, kurser, studenterafhandlinger, publikationer mv. 2017

Department of Chemistry, Aarhus University

Bidrag til konferencer og kongresser:

Materials Chemistry and Structural Studies at High Pressure

Periode: May 2017

Martin Bremholm (Foredragsholder)

Invited colloquium speaker at Institute for Molecules and Materials, Radboud University, Holland

High pressure studies of perovskites and related structures

Periode: March 2017

Martin Bremholm (Foredragsholder)

Invited seminar speaker at Center for Science at Extreme Conditions, Edinburgh, UK.

Using neutrons to determine spin density and local susceptibility tensors

Periode: 22 nov. 2017 → 29 nov. 2017

Emil Andreasen Klahn, Emil Damgaard-Møller (Foredragsholdere)

Network meeting with IITB, Mumbai, India

Materials for Clean Energy Technologies

Periode: 21 nov. 2017 → 22 nov. 2017

Mogens Christensen (Foredragsholder)

European Spallat Source ESS AB, SE-22100, Lund, Sverige

DanMAX - In situ materials studies in the 15-35 keV range using powder X-ray diffraction and full field imaging

Periode: 14 nov. 2017

Mads Ry Vogel Jørgensen (Oplægsholder)

CMPC Group meeting - Photon Science - deutsches elektronen-synchrotron (DESY), Hamburg, Tyskland

Size and structure of magnetic spinel ferrites (Præsentation)

Periode: 06/10/2017 → 08/10/2017

Henrik Lyder Andersen (Foredragsholder)

iNANO Autumn School 2017, Interdisciplinary Nanoscience Center - iNANO-Kemi, Langelandsgade, Aarhus, Denmark

Improving permanent magnets through nanostructuring

Periode: 5 nov. 2017 → 7 nov. 2017

Mogens Christensen (Foredragsholder)

SurfMat 11th Meeting, Turku, Finland

Structure-property investigations of 2D materials for photocatalysis

Periode: 3 jul. 2017

Nina Lock (Foredragsholder)

European Inorganic Chemistry Conference, University of Copenhagen, Denmark

Liquid-like Li-ion Conduction in Lithium amide-borohydrides

Periode: 18 sep. 2017 → 21 sep. 2017

Yigang Yan (Foredragsholder)

European Materials Research Society, E-MRS Fall Meeting 2017, Warsaw, Polen

Core electron deformation in silicon from powder X-ray diffraction

Periode: 11/09/2017 → 13/09/2017

Kasper Tolborg (Foredragsholder)

Crystallography for Materials Science: French-Danish workshop, Nancy, Frankrig

Magnetic anisotropy in molecular magnets measured with polarized neutron diffraction

Periode: 11/09/2017 → 13/09/2017

Emil Andreasen Klahn (Foredragsholder)

Crystallography for Materials Science: French-Danish workshop, Nancy, Frankrig

Structure solution from powder diffraction data

Periode: 11/09/2017 → 13/09/2017

Mathias Jørgensen (Foredragsholder)

Crystallography for Materials Science: French-Danish workshop, Nancy, Frankrig

Nanostructuring of magnetic materials

Periode: 11 sep. 2017 → 13 sep. 2017

Henrik Lyder Andersen (Foredragsholder)

Crystallography for Materials Science: French-Danish workshop, Université de Lorraine, SRSMC, Vandoeuvre-les-Nancy, Frankrig

Accurate Charge Densities from Powder X-Ray Diffraction

Periode: 21/08/2017 → 28/08/2017

Mads Ry Vogel Jørgensen (Oplægsholder)

XXIV IUCr Congress and General Assembly, Hyderabad, Indien

Magnetic anisotropy in Dy-based SIMs – X-ray and polarized neutron results

Periode: 21/08/2017 → 28/08/2017

Jacob Overgaard (Foredragsholder)

XXIV IUCr Congress and General Assembly, Hyderabad, Indien

High-Pressure X-ray Diffraction and Mössbauer Spectroscopy Study of Fe_{1.087}Te

Periode: 21/08/2017 → 28/08/2017

Jens-Erik Jørgensen (Foredragsholder)

XXIV IUCr Congress and General Assembly, Hyderabad, Indien

Core electron deformation in silicon from powder X-ray diffraction

Periode: 21/08/2017 → 28/08/2017

Kasper Tolborg (Foredragsholder)

XXIV IUCr Congress and General Assembly, Hyderabad, Indien

3D-magnetic difference-PDF analysis of magnetic frustrations in Bixbyite

Periode: 21/08/2017 → 28/08/2017

Nikolaj Roth (Foredragsholder)

XXIV IUCr Congress and General Assembly, Hyderabad, Indien

Designing Layered Thermoelectric Materials Through Orbital Engineering and Carrier Pocket Engineering

Periode: 30/07/2017 → 03/08/2017

Jiawei Zhang (Foredragsholder)

36th International Conference on Thermoelectrics - ICT2017, Pasadena, USA

Enhanced thermoelectric performance in p-type $\text{Mg}_{3-x}\text{Ag}_x\text{Sb}_2$ Zintl compounds by tuning carrier density

Periode: 30/07/2017 → 03/08/2017

Lirong Song (Foredragsholder)

36th International Conference on Thermoelectrics - ICT2017, Pasadena, USA

HEIMDAL@ESS A thermal Neutron Powder Diffractometer Combined with SANS and Imaging

Periode: 9 jul. 2017 → 13 jul. 2017

Mogens Christensen (Foredragsholder)

International Conference on Neutron Scattering 2017, Daejeon, Sydkorea

Magnetic anisotropy in single molecule magnets determined using neutron and X-ray diffraction

Periode: 15 jun. 2017

Jacob Overgaard (Foredragsholder)

Kemisk forenings årsmøde 2017, Odense, Danmark

DanMAX – In situ materials studies in the 15-35 keV range using powder X-ray diffraction and full field imaging

Periode: 01/06/2017 → 02/06/2017

Mads Ry Vogel Jørgensen (Oplægsholder)

Danscatt 2017, Odense, Danmark

Size and structure of magnetic spinel ferrite nanocrystallites

Periode: 29/05/2017 → 02/06/2017

Henrik Lyder Andersen (Foredragsholder)

To.Sca.Lake 2.0: Total Scattering for Nanotechnology on the Como Lake, Como, Italien

Beyond Hydrogen Storage, Complex Hydrides as Solid Electrolyte for Battery

Periode: 1 jun. 2017 → 2 jun. 2017

Yigang Yan (Foredragsholder)

Danscatt 2017, Odense, Danmark

Materials for Energy Applications through Neutron and X-Ray Eyes

Periode: 22 maj 2017 → 23 maj 2017

Cecilia Granados-Miralles (Deltager)

Mogens Christensen (Arrangør)

Jakob Ahlburg (Deltager)

Frederik Gjørup (Deltager)

Mathias Mørch (Deltager)

Jennifer Hoelscher (Deltager)

Materials for Energy Applications through Neutron and X-Ray Eyes, Göteborg, Sverige

Oplæg på kemilærerforeningens årsmøde - Strukturkemi i gymnasiet

Periode: 15/03/2017 → 17/03/2017

Jacob Overgaard (Foredragsholder)

kemilærerforeningens årsmøde 2017, Horsens, Danmark

Halogenated Sodium Closo-Dodecaboranes

Periode: 26/02/2017 → 03/03/2017

Mathias Jørgensen (Foredragsholder)

11th International Symposium on Hydrogen Energy, Waikoloa Beach, USA

Energy storage materials and nanoconfinement

Periode: 23 jan. 2017

Torben René Jensen (Foredragsholder)

University of Hamburg, Hamburg, Tyskland

Beyond Hydrogen Storage, Complex Hydrides as Solid Electrolyte for Future Safe Battery

Periode: 13 jan. 2017

Yigang Yan (Foredragsholder)

CMC meeting, Göttingen, Tyskland

In operando study of layered $\text{NaXNi}_0.3\text{Mn}_0.7\text{O}_2$ cathode material for sodium ion batteries

Periode: 13 jan. 2017

Solveig Kjeldgaard (Foredragsholder)

CMC Meeting, Göttingen, Tyskland

Multi-functional energy storage materials

Periode: 13 jan. 2017

Torben René Jensen (Foredragsholder)

South China University of Technology, Kina

Multi-functional energy storage materials

Periode: 10 jan. 2017

Torben René Jensen (Foredragsholder)

Wuhan university of Technology, Wuhan, Kina

Bone microstructure revealed by sub-micron resolution Diffraction Scattering Computed Tomography

Periode: 29/05/2017 → 02/06/2017

Nina Kjøln Wittig (Foredragsholder)

To.Sca.Lake 2.0: Total Scattering for Nanotechnology on the Como Lake, Como, Italien

Designs and structures of biological and bioinspired materials

Periode: 22/03/2017 → 24/03/2017

Henrik Birkedal (Foredragsholder)

KAIST/Aarhus University Bilateral Workshop, Daejeon, Sydkorea

Insights into hierarchical materials from Diffraction Scattering Computed Tomography; Invited talk

Periode: 13/02/2017 → 15/02/2017

Henrik Birkedal (Foredragsholder)

X-rays at Ultra-Low Emittance Sources, Hamburg, Tyskland

Biological and Bioinspired Materials; Invited talk

Periode: 9 feb. 2017

Henrik Birkedal (Foredragsholder)

Sine Larsen Symposium, København, Danmark

Posters:

Anisotropy in thermoelectric materials

Forfattere: Færch Fischer, K. F., Iversen, B. B.

Udgivelsesår: 30 jul. 2017

Begivenhed: Poster session præsenteret ved 2017ICT - 36TH International Conference on Thermoelectrics, Pasadena, USA.

Anisotropic magnetoresistivity from van der Pauw measurements on LaSb₂

Forfattere: Færch Fischer, K. F., Iversen, B. B.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Danscatt 2017, Odense, Danmark.

Synthesis of Halide- and Solvent Free Metal Borohydrides

Forfattere: Grinderslev, J., Jensen, T. R., Møller, K. T., Richter, B.

Udgivelsesår: 15 jul. 2017

Begivenhed: Poster session præsenteret ved Gordon Research Conference - Metal hydrogen systems (2017)

Superconducting Topological Materials by Doping of Bi₂Se₃

Forfattere: Munkholm Kevy, S., Bremholm, M.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Danscatt 2017, Odense, Danmark.

Spin density measurement of water-bridged Co-dimer using polarized neutrons

Forfattere: Damgaard-Møller, E., Overgaard, J., Chilton, N., Walsh, J., Stunault, A., Fabelo, O., Hathwar, V. R., Thomsen, M.

Udgivelsesår: 2 jun. 2017

Begivenhed: Poster session præsenteret ved Danscatt 2017, Odense, Danmark.

Group 13 metal oxide formation, transformation and pre-nucleation: A study of the indium oxide system

Forfattere: Nielsen, I., Sommer, S., Iversen, B. B.

Udgivelsesår: 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

Size and structure of hydrothermally synthesized magnetic spinel ferrite nanocrystallites

Forfattere: Andersen, H. L., Granados-Mirallas, C., Saura-Múzquiz, M., Stingaciu, M., Søndergaard-Pedersen, F. M., Ahlburg, J., Christensen, M.

Udgivelsesår: 9 jul. 2017

Begivenhed: Poster session præsenteret ved International Conference on Neutron Scattering 2017, Daejeon, Sydkorea.

Pair distribution function analysis of Jahn-Teller fluctuation in copper Tutton's salt

Forfattere: Mikkelsen, J., Iversen, B. B.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

Optimization of spring exchange coupled ferrites, studied by in situ neutron diffraction.

Forfattere: Ahlburg, J., Christensen, M., Granados-Mirallas, C., Andersen, H. L., Garbus, P. G.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

Optimization of spring exchange coupled ferrites, studied by in situ neutron diffraction.

Forfattere: Ahlburg, J., Christensen, M., Granados-Mirallas, C., Andersen, H. L., Garbus, P. G.

Udgivelsesår: 22 maj 2017

Begivenhed: Poster session præsenteret ved Materials for Energy Applications through Neutron and X-Ray Eyes, Göteborg, Sverige.

Optimization of spring exchange coupled ferrites, studied by in situ neutron diffraction.

Forfattere: Ahlburg, J., Christensen, M., Granados-Mirallas, C., Garbus, P. G., Andersen, H. L.

Udgivelsesår: 11 jul. 2017

Begivenhed: Poster session præsenteret ved International Conference on Neutron Scattering 2017, Daejeon, Sydkorea.

Enhancement of the magnetic properties of SrFe₁₂O₁₉ bulk magnets by controlling the dimensions of the constituent nanocrystallites

Forfattere: Eikeland, A., Stingaciu, M., Christensen, M.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

Accurate charge densities from powder X-ray diffraction

Forfattere: Tolborg, K., Jørgensen, M. R. V., Kasai, H., Becker, J., Dippel, A., Als-Nielsen, J., Iversen, B. B.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

Site susceptibilities in single ion magnets by single crystal polarized neutron diffraction

Forfattere: Klahn, E. A., Overgaard, J., Gillon, B., Jiang, S. D.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

High Pressure Studies of SrGeO₃ Polymorphs

Forfattere: Kronbo, C. H., Eikeland, E. Z., Bremholm, M.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

High Pressure Studies of SrGeO₃ Polymorphs

Forfattere: Kronbo, C. H., Eikeland, E. Z., Bremholm, M.

Udgivelsesår: 2 jul. 2017

Begivenhed: Poster session præsenteret ved 4th European Crystallography School, Warsaw, Polen.

Thermal energy storage materials in hydrogen storage

Forfattere: Borg, E., Jensen, T. R.

Udgivelsesår: jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

A Potassium and Aluminium based Amidoborane

Forfattere: Møller, K. T., Andreasen, J. G., Jørgensen, M., Skibsted, J., Łodziana, Z., Filinchuk, Y., Jensen, T. R.

Udgivelsesår: 11 jan. 2017

Begivenhed: Poster session præsenteret ved iNano Annual Meeting 2017, Aarhus, Danmark.

Potassium Tetraamidoboranealuminate, K[Al(NH₂BH₃)₄]: Synthesis, Characterization and Thermal Decomposition.

Forfattere: Møller, K. T., Jørgensen, M., Andreasen, J. G., Skibsted, J., Łodziana, Z., Filinchuk, Y., Jensen, T. R.

Udgivelsesår: 18 jul. 2017

Begivenhed: Poster session præsenteret ved Hydrogen-Metal Systems Gordon Research Conference 2017, Eastern, USA.

Examining lead vacancies in lead chalcogenides and their effect on thermoelectric performance

Forfattere: Zeuthen, C. B., Thorup, P. S., Iversen, B. B.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

A NaAlH₄-Ca(BH₄)₂ Composite System for Hydrogen Storage

Forfattere: Møller, K. T., Grinderslev, J., Jensen, T. R.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

Neutrons for multi-functional hydrides - FunHy

Forfattere: Grinderslev, J., Jensen, T. R., Sahlberg, M., Häussermann, U., Karlsson, M., Nygård, M., Hauback, B., Sørby, M., Ek, G.

Udgivelsesår: maj 2017

Begivenhed: Poster session præsenteret ved SNSS meeting, Uppsala, Sverige.

Synthesis of halide- and solvent free metal borohydrides

Forfattere: Grinderslev, J., Møller, K. T., Richter, B., Jensen, T. R.

Udgivelsesår: maj 2017

Begivenhed: Poster session præsenteret ved Danscatt 2017, Odense, Danmark.

Bio-oil production in a continuous-flow reactor: What could possibly go wrong?

Forfattere: Klemmer, M., Iversen, B. B.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Danscatt 2017, Odense, Danmark.

Magnetic Short Range Ordering in Frustrated Magnets

Forfattere: Roth, N., Iversen, B. B.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Danscatt 2017, Odense, Danmark.

Combined In Situ and Ex Situ Powder Diffraction Study on the Crystallization of Magnetic SrFe₁₂O₁₉ Nanocrystallites by the Hydrothermal Method

Forfattere: Granados-Miralles, C., Saura-Múzquiz, M., Bøjesen, E. D., Jensen, K. M. Ø., Andersen, H. L., Christensen, M.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Danscatt 2017, Odense, Danmark.

High pressure structural studies of two SrIrO₃ perovskite polymorphs

Organisationer: European Synchrotron Radiation Facility ESRF, Grenoble

Forfattere: Kronbo, C. H., Nielsen, M. B., Munkholm Kevy, S., Parisiades, P., Bremholm, M.

Udgivelsesår: 12 jan. 2017

Begivenhed: Poster session præsenteret ved 12th USPEX workshop, Poitiers, Frankrig.

Solid state lithium ion conductors LiLa(BH₄)₃X, X=Cl, Br, I

Forfattere: Payandeh GharibDoust, S., Brighi, M., Sadikin, Y., Ravnsbæk, D. B., Jensen, T. R.

Udgivelsesår: 11 jan. 2017

Begivenhed: Poster session præsenteret ved 15th iNANO Annual Meeting, Aarhus, Danmark.

Tailoring density, band gap and thermal diffusivity of phase pure nanostructured ZnAl₂O₄ by direct spark plasma sintering: Justerbar densitet, båndgab og termisk diffusivitet af faserent, nano ZnAl₂O₄ ved direkte spark plasma sintering

Organisationer: European Synchrotron Radiation Facility ESRF, Grenoble

Forfattere: Sommer, S., Iversen, B. B., Bøjesen, E. D., Blichfeld, A. B.

Udgivelsesår: mar. 2017

Begivenhed: HERCULES 2017: Higher European Research Course for Users of Large Experimental SSysytems, Grenoble, Frankrig.

Dialing in the Ratio of Covalent and Coordination Cross-links in Self-healing Hydrogels

Forfattere: Andersen, A., Krogsgaard, M., Birkedal, H.

Udgivelsesår: 6 mar. 2017

Begivenhed: Poster session præsenteret ved Fifth International Conference on Multifunctional, Hybrid and Nanomaterials, Lisbon, Portugal.

Bone Microstructure Revealed by Combined Sub-micron Resolution Diffraction and Fluorescence Tomography

Forfattere: Wittig, N., Frølich, S., Birkbak, M. E., Palle, J., Østergaard, M., Spiers, K., Garrevoet, J., Birkedal, H.

Udgivelsesår: 15 maj 2017

Begivenhed: Poster session præsenteret ved ESRF: Hercules Specialized Course HSC1 9 Quantitative Imaging using X- rays and Neutrons, Grenoble, Schweiz.

High pressure structural studies of two SrIrO₃ perovskite polymorphs

Forfattere: Kronbo, C. H., Nielsen, M. B., Munkholm Kevy, S., Parisiades, P., Bremholm, M.

Udgivelsesår: 12 jan. 2017

Begivenhed: Poster session præsenteret ved 12th USPEX workshop, Poitiers, Frankrig.

In situ and Ex situ Annealing Studies of Hydrothermally Synthesized SrFe₁₂O₁₉ Nano Platelets.

Forfattere: Gjørup, Frederik; Saura-Múzquiz, Matilde; Ahlburg, Jakob; Christensen, Mogens.

Udgivelsesår: 5. okt. 2017

Begivenhed: Poster session presented at Advanced Powder Diffraction Workshop, Uppsala, Sweden.

In situ and Ex situ Annealing Studies of Hydrothermally Synthesized SrFe₁₂O₁₉ Nano Platelets.

Forfattere: Gjørup, Frederik; Saura-Múzquiz, Matilde; Ahlburg, Jakob; Christensen, Mogens.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Danscatt 2017, Odense, Danmark.

In situ and Ex situ Annealing Studies of Hydrothermally Synthesized SrFe₁₂O₁₉ Nano Platelets.

Forfattere: Gjørup, Frederik; Saura-Múzquiz, Matilde; Ahlburg, Jakob; Christensen, Mogens.

Udgivelsesår: 22 maj 2017

Begivenhed: Poster session præsenteret ved Materials for Energy Applications through Neutron and X-Ray Eyes, Göteborg, Sverige.

Metal boranes as solid-state electrolytes.

Forfattere: Jensen, Steffen; Humphries, Terry D.; Jensen, Torben René; Buckley, Craig E. ; Paskevicius, Mark.

Udgivelsesår: 10th nov. 2017

Begivenhed: 4th WA Synchrotron Symposium, Curtin University, Australia

M(AlH₄)₂- xNH₃ compounds (M = Mg and Ca).

Forfattere: Jensen, Steffen; Jensen, Torben René.

Udgivelsesår: 18 jul. 2017

Begivenhed: Poster session præsenteret ved Hydrogen-Metal Systems Gordon Research Conference 2017, Eastern, USA.

Investigation of NH₃ containing alanates.

Forfattere: Jensen, Steffen; Jensen, Torben René.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

Hydrogenation of M₂B₁₀H₁₀ and M₂B₁₂H₁₂ with MH (M = Li and Na).

Forfattere: Jensen, Steffen; R. S. Hansen, Bjarne; Paskevicius, Mark; Jakobsen, Anders Svarre; Jensen, Torben René.

Udgivelsesår: 11 jan. 2017

Begivenhed: Poster session præsenteret ved 15th iNANO Annual Meeting, Aarhus, Danmark.

Effect of precursor choice and sintering conditions for W hexaferrite formation.

Forfattere: Mørch, Mathias; Eikeland, Anna; Christensen, Mogens.

Udgivelsesår: 1 jun. 2017

Begivenhed: Poster session præsenteret ved Dancatt 2017, Odense, Danmark.

Tailoring metal-organic frameworks: Connecting Co₄O₄ cubane complexes with the right organic linker

Forfattere: Mads Folkjær, Claire Deville, and Nina Lock

Udgivelsesår: 1 jun. 2017 → 2 jun. 2017

Begivenhed: Dancatt 2017, Odense, Danmark

Tailoring metal-organic frameworks: Connecting Co₄O₄ cubane complexes with the right organic linker

Forfattere: Mads Folkjær, Claire Deville, and Nina Lock

Udgivelsesår: 3 jul. 2017

Begivenhed: European Inorganic Chemistry Conference, University of Copenhagen

Direct growth of HKUST-1/graphene composite films on glassy carbon

Forfattere: Paolo Lamagni, Birgitte Lodberg Pedersen, Xinming Hu, Steen Uttrup Pedersen, Kim Daasbjerg, Nina Lock

Udgivelsesår: 1 jun. 2017 → 2 jun. 2017

Begivenhed: Dancatt 2017, Odense, Danmark

Direct growth of HKUST-1/graphene composite films on glassy carbon

Forfattere: Paolo Lamagni, Birgitte Lodberg Pedersen, Xinming Hu, Steen Uttrup Pedersen, Kim Daasbjerg, Nina Lock

Udgivelsesår: 3 jul. 2017

Begivenhed: European Inorganic Chemistry Conference, University of Copenhagen

Anden formidling/outreach, m.v. (tv, radio, kronikker, foredrag, osv.):

NXS Grads Seek Atomistic Insights Into Ferroelectric Materials

Mads Ry Vogel Jørgensen

22/05/2017

OAK Ridge National Laboratory, Neutron Sciences (International), USA, Internet

<https://neutrons.ornl.gov/content/nxs-grads-seek-atomistic-insights-ferroelectric-materials>

Young scientists: Interview with Hazel Reardon

Hazel Reardon

27/04/2017

Author: Kristina Sandberg Hrbinic

Link: <http://www.scienceandsociety.eu/2017/04/27/young-scientists-interview-with-hazel-reardon/>

Undervisning og kurser (Ph.d.-skoler og –kurser, sommerskoler, andet):

To.sca.lake 2.0: Total Scattering for Nanotechnology on the Como Lake

Periode: 29 maj 2017 → 2 jun. 2017

Deltagere: Lasse Rabøl Jørgensen, Pelle Garbus, Hazel Reardon, Nils Lau Nyborg Broge, Martin

Roelsgaard, Frederik Søndergaard-Pedersen, Henrik Lyder Andersen, Nina Wittig

Lake Como School of Advanced Studies

Research stay at ChemMatCars at APS

Periode: 28 jun. 2017 → 18 aug. 2017

Nikolaj Roth (Deltager)

Argonne National Laboratory, Argonne, USA

Advanced Measuring Techniques for LFA Systems

Periode: 19 maj 2017

Karl Frederik Færch Fischer (Deltager)

Advanced Measuring Techniques for LFA Systems, Stockholm, Sverige

NNSP/SwedNess Neutron School

Periode: 11 sep. 2017 → 22 sep. 2017

Anna Zink Mortensen (Deltager)

NNSP/SwedNess Neutron School, Taru, Estland

Navne på MSc kandidater og BSc (afsluttede):

MSc (afsluttede; Student name, Project title, Supervisor):

Ida Gjerlevsen Nielsen, Indium oxides - Precursor clusters and reaction pathways. A group 13 Metal Oxide Study, Bo Brummerstedt Iversen

Jakob Ahlborg, A Tale of Neutrons and Magnets and Ingenuity, Mogens Christensen

Pelle Gorm Garbus, Synthesis & Reduction of Iron Oxides - A Case Study of α - And γ -Iron Oxides Reduction Observed By Neutron Diffraction, Mogens Christensen

Mathias Jørgensen, Complex Metal Hydrides for Energy Storage, Torben Rene Jensen

Martin Bondesgaard, A new approach for characterization of nanoparticle systems by merging inorganic and organic methods, Bo Brummerstedt Iversen

Sanna Sommer, Formation and Growth of Nanoparticles by Multitechnique Studies, Bo Brummerstedt Iversen

Solveig Kjeldgaard, Structural and electrochemical investigation of battery materials, Bo Brummerstedt Iversen

Steffan Schmidt, Exploration of Synthesis Strategies for Perovskites at Ambient and High Pressure, Torben Rene Jensen

Anders Svarre Jakobsen, Synthesis and Characterisation of Metal closo-dodecaboranes and Metal closo-decaboranes as solid state electrolytes, Torben Rene Jensen

Svend Lemming Jacobsen, Undersøgelse af metalhydrider og deres reaktion med CO₂, Torben Rene Jensen

Karl Frederik Færch Fischer, Anisotropy in thermoelectric materials & furthering the characterization hereof, Bo Brummerstedt Iversen

Niklas Durhuus Vichairat, Synthesis and Characterization of Soft Magnetic Materials, Henrik Birkedal

Amanda Andersen, Self-Healing Materials Based On Catechol Analogues, Henrik Birkedal

BSc: (Student name, supervisor)

Louise Ring Jensen, Martin Bremholm

Sarah Ursula Stenner Mortensen, Martin Bremholm

Christina Breth Nielsen, Martin Bremholm

Andreas Munch Thiel, Martin Bremholm

Laura Wollesen, Martin Bremholm

Ida Wivel Holm, Bo Brummerstedt Iversen

Tenna Lisborg Frydenberg, Bo Brummerstedt Iversen

Maja Østergaard, Henrik Birkedal

Mads Fonager Hansen, Martin Bremholm

Peter Skjøtt Thorup, Bo Brummerstedt Iversen

Mathias Mørch, Mogens Christensen

Mads Folkjær, Martin Bremholm

Awards:

DANSCATT 2017 – Best Poster prize

Anna Zink Mortensen (Modtager)

2017 ITS Goldsmid Award

Jiawei Zhang (Modtager)

Tildelingsdato: 2 aug. 2017

Grad af anerkendelse: International

Tildelende organisationer: International Thermoelectric Society

Event: 36th International Conference on Thermoelectrics - ICT2017

Department of Molecular Biology, Aarhus University

Forside fra tidsskrifter:

Protein Science (2017): 26(8),



Bidrag til konferencer og kongresser:

Structural basis for a novel immune deficiency. MAX IV user meeting 2017 (GRA)

Structural basis for eculizumab mediated inhibition of the complement terminal pathway. 6th International Conference "HUS & related diseases" in Innsbruck from 11th - 13th of June 2017. (GRA)

ASBMB 2017 Annual Meeting, Chicago: Discrete Structural Dynamics of Pseudo-Palindromic Motifs Control DNA Binding of Bacterial Toxin-Antitoxin Complexes, Brodersen, D. E., Bendtsen, K. L., Xu, K., Luckmann, M., Winther, K., Shah, S. A. & Pedersen, C. N. S. Apr 2017 In : F A S E B Journal. 31, No. 1 supplement, 1 p., 777.2

Invited speaker (BPP) 18-19. May 2017 "The Novo Nordisk Prize Symposium 2017. PUMPS - PUMPKin and beyond", Aarhus University, Denmark. Organizer: Poul Nissen.

Seminar/Invited speaker (BPP) 6. Apr. 2017 "Pumping Potassium through Channels", Seminar, University of Regensburg, Germany. Invited by Ulrich Hammes.

Structural and Functional Studies of Biomembranes, Univ. Copenhagen, inaugural lecture, affiliated professor, February 2, 2017, Poul Nissen

How do membrane transporters switch sides and get away with it? EMBO Workshop - Towards Novel Therapies: Emerging Insights from Structural and Molecular Biology, Groningen, Netherlands, March 8, 2017, Poul Nissen

PUMPS AND CIRCUMSTANCES, Novo Nordisk Prize Lecture, Aarhus University, March 10, 2017, Poul Nissen

Bilag 4: DANSCATT outreach, kurser, studenterafhandlinger, publikationer mv. 2017

PUMPS AND CIRCUMSTANCES, Novo Nordisk Prize Ceremony, Novo Nordisk Bagsværd, March 17, 2017, Poul Nissen

How do membrane transporters switch sides? ETH, Dept. Biochemistry, Zürich, Switzerland, March 30, 2017, Poul Nissen

Membrane transporters in the brain. Erice International School of Crystallography, June 5th, 2017, Poul Nissen

Snapshots and dynamics of membrane proteins and biomembranes. Neutrons in Structural Biology 2017, Grenoble, June 9th, 2017, Poul Nissen

Can we bridge between different levels of neuroscience? Annual Meeting, Dept. Molecular Biology and Genetics, AU, June 16th, 2017, Poul Nissen

Structure and mechanism of membrane transporters studied through protein engineering. Benzon Symposium no. 63 - New Paradigms of Protein Engineering, Aug. 24th, 2017, Poul Nissen

DANDRITE – Danish Research Institute of Translational Neuroscience , director's overview, Sep. 5th, 2017, Poul Nissen

Structure and Mechanism of P-type ATPase transporters. Dynamics of Membrane Systems - CRC 1208 Conference, Düsseldorf, Sep. 15th 2017, Poul Nissen

The Structure and Mechanism of P-type ATPases. The 15th International Conference on Na, K-ATPase and Related Transport ATPases, Lake Biwa Otsu, Japan, Sep 25th, 2017, Poul Nissen

The evil twin and other translations. CoLuAa 2017, Copenhagen, Oct. 30th, 2017, Poul Nissen

Structural biology using neutrons. Nordic-EMBL-ESS workshop on structural biology, Nov. 7-8th, 2017, Poul Nissen (organizer)

Maintaining a leading position within Life Science. The Danish Academy of the Technical Sciences, Annual Meeting, Nov, 9th, 2017, Poul Nissen (session chair)

Structure and mechanism of membrane transport proteins. Univ. Copenhagen, Dept. Chemistry, Nov 10th, 2017, Poul Nissen

Structure and mechanism of membrane transporters of the P-type ATPase family The 4th ShanghaiTech SIAIS Bioforum, Nov. 15th, 2017, Poul Nissen

The use of advanced neutron and X-ray technologies in structural biology. Annual meeting of LINX, Dec. 11th, 2017 Poul Nissen

The use of advanced neutron and X-ray technologies in drug discovery. LINX meeting at Leo Pharma A/S, Dec. 20th, 2017, Poul Nissen

Anden formidling/outreach, m.v. (tv, radio, kronikker, foredrag, osv.):

LAMAER KAN HJÆLPE OS TIL UDVIKLING AF NYE LÆGEMIDLER. Populærvidenskabeligt foredrag, forskningens dag. (GRA)

Forskningens døgn AU april 2017 (foredrag og showcase) (PN)

Folkeuniversitet AU-Emdrup September 2017 (foredrag 2 timer) (PN)

Folkeuniversitet AU-Aarhus, November 2017 (foredrag 2 timer) (PN)

Undervisning og kurser (Ph.d.-skoler og –kurser, sommerskoler, andet):

Speaker (DEB) in Protein.DTU 16th workshop, 22 May 2017

Speaker (SST) in phd-course: Receptor Structure and Function, Drug Research Academy, KU, May 15 –19, 2017

Speaker (SST) in phd-course: Bionanotools, AU, 14-18 August 2017

Teacher (CBFA) Ph.d course: “Proteins”, Health, AU

MAX4ESSFUN summer school ” Data collection and structure determination in macromolecular crystallography”. Aarhus University 28-8 to 2-9 2017. 24 participants. GRA organized the entire summer school.

Erice International School of Crystallography, June 5th, 2017, Poul Nissen

Navne på MSc kandidater og BSc (afsluttede):

Jeppe Achton Nielsen (MSc)

Farrokh Alicehajic (BSc)

Regitze Foged Bertelsen (BSc)

Simon B Hansen (BSc)

Thea G. Birkefeldt (BSc)

Jakob Moesbo (BSc)

Gustav Alexander Poulsgaard (BSc)

Sofia Mazarakis (BSc)

Sara Basse (MSc)

Line Marie Christensen (BSc)

DTU Cen

Bidrag til konferencer og kongresser:

Combining X-ray and Electron Based in situ Characterization of Catalysts. Invited speaker Christian Danvad Damsgaard. 23. september 2017, Trieste, Italien.

DTU Chemistry

Bidrag til konferencer og kongresser:

K.B. Møller, invited talk

Ultrafast electronic and nuclear dynamics in photo-excited transition-metal complexes.

International Workshop on Molecular Quantum Dynamics and Kinetics on 18th-21st April 2017 at ETH Zürich, Switzerland.

G. Levi, oral presentation

Ultrafast direct dynamics simulations of transition metal complexes for solar energy conversion.

22nd International Symposium on Photochemistry and Photophysics of Coordination Compounds (ISPPCC) on 9th-14th July 2017 at St. Catherine's College, Oxford, UK.

Sujata Mahapatra, Werner W. Streicher, Allan Nørgaard, Günther H.J. Peters, Pernille Harris

Poster: Effect of molecular crowding in protein formulation.

PEGS Europe: Protein & Antibody Engineering Summit, 16-17 November 2017, Lisbon, PT.

Christin Pohl, Allan Nørgaard, Werner W. Streicher, Sowmya Indrakumar, Günther H.J. Peters, Pernille Harris

Poster: *"Characterization of protein solution structure using light scattering techniques and SAXS"*

PEGS Europe: Protein & Antibody Engineering Summit, 16-17 November 2017, Lisbon, PT.

Alina Kulakova, Werner W. Streicher, Günther H.J. Peters, Pernille Harris

Poster: *Stability study on Human Serum Transferrin*

PEGS Europe: Protein & Antibody Engineering Summit, 16-17 November 2017, Lisbon, PT.

Line Abildgaard Ryberg, Pernille Sønderby, Pernille Harris, Jens T. Bukrinski, Fabian B. Garcia and Günther H. Peters

Poster: Detemir - albumin interactions studied by small-angle X-ray scattering and in-silico modelling.

Recent Breakthroughs and New Perspectives of Protein Aggregation (BioProNET), 13 February 2017, UoM, UK.

Anden formidling/outreach, m.v. (tv, radio, kronikker, foredrag, osv.):

Pernille Harris

PIPPI – Protein-excipient Interactions and Protein-Protein Interactions in formulation – ERC

Science Impact 8, 75-77, 2017

DOI: <https://doi.org/10.21820/23987073.2017.8.75>

Undervisning og kurser (Ph.d.-skoler og –kurser, sommerskoler, andet):

Applications of X-ray and neutron scattering in biology, chemistry and physics.

DTU and KU, three week summer school August 2017

DTU Chemical Engineering

Bidrag til konferencer og kongresser:

Arndal, T. M. H., Høj, M., Gaur, A., Prüssmann, T., Pintos, D. G., Studt, F., Gabrielsen, J., Grunwaldt, J.-D., Hansen, T. W., Jensen, A. D. (2017). Influence of Promotor, H₂O and H₂S on the Hydrodeoxygenation of Biomass Pyrolysis Vapor over MoS₂ Catalysts. *Abstract from 25th North American Catalysis Society Meeting*, Denver, United States.

Arndal, T. M. H., Høj, M., Gaur, A., Prüssmann, T., Pintos, D. G., Studt, F., Gabrielsen, J., Grunwaldt, J.-D., Hansen, T. W., Jensen, A. D. (2017). Influence of Promotor, H₂O and H₂S on the Hydrodeoxygenation of Biomass Pyrolysis Vapor over MoS₂ Catalysts. *Abstract from 13th European Congress on Catalysis (EUROPACAT 2017)*, Florence, Italy.

DTU Energy

Collaboration with other DANSCATT institutions marked by *

Bidrag til konferencer og kongresser:

Kuhn, L. Theil, In situ Multiscale Analysis by Neutrons and Electrons of Electrode Materials for Solid Oxide Electrochemical Cells, *AnalytiX-2017, 22-24 March 2017, Fukuoka, Japan*.

*Sales, M. , Strobl, M., Shinohara, T., Tremsin, A., Kuhn, L. Theil, Lionheart, W. R. B., Desai, n. M., Dahl, A. Bjorholm, Schmidt, S., Three Dimensional Polarimetric Neutron Tomography of Magnetic Fields, *9th Workshop on Neutron Wavelength Dependent Imaging (NEUWAVE- 9) 11-14 June 2017, NIST, USA*.

*Lacatusu, M.-E., Kuhn, L. Theil, Schmidt S., Strobl, M., Makowska, M., Phase distribution visualization in Solid Oxide Fuel Cells by monochromatic neutron Bragg-edge tomography, *3rd International Conference on Tomography of Materials and Structures, 26–30 June 2017, Lund, Sweden*

*Strobl, M., Makowska, M., Frandsen, H. L., De Angelis, S., Schmidt S., Lacatusu, M.-E., Kabra, S., Kockelmann, W., Morgano, M., Trtik, P., Kai T., Shinohara T., Tremsin, A. S., Kuhn, L. Theil, In-Situ Observation of Redox Behavior in Ni-YSZ Solid Oxide Fuel Cell Electrodes, *International Conference on Neutron scattering 2017, 3-13. July 2017, Korea*

*Sierra J.X., Jørgensen P. S., Poulsen H. F., Detlefs C., Cook P., Simons H., Bowen J. R. (2017) In operando studies of an yttria stabilized zirconia electrolyte supported symmetric solid oxide cell by Dark field X-ray Microscopy at ID06, *ESRF Annual User Meeting 6-8 February 2017 Grenoble, France*. Poster presentation

*Sierra J.X., Poulsen H. F., Jørgensen P. S., Detlefs C., Cook P., Simons H., Yildirim C., Ahl S. R., Jakobsen A. C., Kantor I., Bowen J. R. (2017) In operando studies of ScYSZ electrolyte supported symmetric solid oxide cell by X-ray Diffraction at ESRF, ID06 Beamline, *3rd International Conference on Tomography of Materials and Structures (ICTMS2017) 26-30 June 2017, Lund Sweden*. Poster presentation

Lefevr, J., Das, S., Blanchard, D. (2017) X-Ray and Raman studies on all-solid-state Li-S batteries built around LiBH₄ solid electrolyte, *2nd Conference on Lithium Sulfur: Mechanisms, Modelling & Materials (LI-SM3 2017), April 26-27, 2017, London*.

http://orbit.dtu.dk/files/130797813/X_Ray_and_Raman_studies_on_all_solid_state_Li_S_batteries_built_around_LiBH4_solid_electrolyte.pdf

Lefevr, J., Blanchard, D. (2017) X-Ray microtomography studies on all-solid-state Li-S batteries built around LiBH₄ solid electrolyte. *DANSCATT Annual meeting 2017, Odense*

Blanchard, D., Garðarsson M. J. S., Sveinbjörnsson, D. Þ., Vegge, T. (2017) Quasi-Elastic Neutron Scattering Studies on Solid Electrolytes for solid state Lithium Batteries, *21st International Conference on Solid State Ionics, June 2017, Padova*

Ramos, T., Jørgensen, J. S., & Andreasen, J. W. (2017). Automated tomographic alignment of translational and rotation uncertainties and application to phase-contrast tomography, *DESY Photon Science Users's Meeting, January, 25-27, Hamburg*

Fevola, G., Ramos, T., Lucas, M. M., Rein, C., Andreasen, J. W. (2017). First Combined Scattering and Fluorescence Scanning Transmission Microscopy at the NanoMAX Beam Line at MAX IV, *DESY Photon Science Users's Meeting, January, 25-27, Hamburg*

Ramos, T., Fevola, G., Lucas, M. M., Rein, C., & Andreasen, J. W. (2017) Combined Scattering and Fluorescence Mapping of Kesterite Precursors at the NanoMAX Beamline, *29th MAX IV Laboratory User Meeting, March 13-15, Lund*

Fevola, G., Ramos, T., Lucas, M. M., Rein, C., Andreasen, J. W. (2017). First Combined Scattering and Fluorescence Scanning Transmission Microscopy at the NanoMAX Beam Line at MAX IV, *29th MAX IV Laboratory User Meeting, March 13-15, Lund, Oral presentation*

Ramos, T., Jørgensen, J. S., & Andreasen, J. W. (2017). Flexible 3D tomographic Alignment and Reconstruction of Phase-Contrast Projection Data, *Vision Day, May 9, Lyngby*

Ramos, T., Jørgensen, J. S., & Andreasen, J. W. (2017). Flexible 3D tomographic Alignment and Reconstruction of Phase-Contrast Projection Data, *Danscatt Annual meeting 2017, June 1-2, Odense*

Ramos, T., Fevola, G., Lucas, M. M., Rein, C., Andreasen, J. W. (2017) Combined Scattering and Fluorescence Mapping of Kesterite Precursors at the NanoMAX Beamline, *Danscatt Annual meeting 2017, June 1-2, Odense*

Ramos, T., Jørgensen, J. S., & Andreasen, J. W. (2017). Flexible 3D tomographic Alignment and Reconstruction of Phase-Contrast Projection Data, *Materials for Energy Applications through Neutron and X-Ray Eyes, Interreg Workshop, May 22-23, Göteborg*

Ramos, T., Fevola, G., Lucas, M. M., Rein, C., Andreasen, J. W. (2017) Combined Scattering and Fluorescence Mapping of Kesterite Precursors at the NanoMAX Beamline, *Materials for Energy Applications through Neutron and X-Ray Eyes, Interreg Workshop, May 22-23, Göteborg*

De Angelis, S., Jørgensen, P.S., Esposito, V., Tsai, E.H.R., Holler, M., Kreka, K., Abdellahi, E., Bowen, J.R. (2017) Ex-Situ 3D Nano-Ptychography of Ni-YSZ SOFC Anode during Redox Cycling, *Materials for Energy Applications through Neutron and X-Ray Eyes, Interreg Workshop, May 22-23, Göteborg, Oral presentation*

Ramos, T., Jørgensen, J. S., & Andreasen, J. W. (2017). Flexible 3D tomographic Alignment and Reconstruction of Phase-Contrast Projection Data, *3rd International Conference on Tomography of Materials and Structure, June 26-30, Lund*

Andreasen, J. W. (2017) Imaging structure formation in polymer solar cells by high resolution tomography and *in situ* X-ray scattering, *3rd International Conference on Tomography of Materials and Structure, June 26-30, Lund, Oral presentation*

De Angelis, S., Jørgensen, P.S., Esposito, V., Tsai, E.H.R., Holler, M., Kreka, K., Abdellahi, E., Bowen, J.R. (2017), 3D microstructural evolution of a solid oxide cell during a redox cycle by high resolution ptychographic tomography, *3rd International Conference on Tomography of Materials and Structure, June 26-30, Lund, Oral presentation*

Jørgensen, P. S. (2017) Quantitative transport network comparison of different locations in a tested solid oxide electrolysis cell, *3rd International Conference on Tomography of Materials and Structure, June 26-30, Lund*

Andreasen, J. W. (2017) Disruptive X-ray methods for a new generation of materials science, *FiMPART - Frontiers in Materials Processing Applications, Research and Technology, July 9-12, Bordeaux, Oral presentation*

Jørgensen, P. S., Bowen, J. R. & Chen, M. (2017) Spatial comparison of the quality of the three dimensional transport networks in a solid oxide electrolysis cell, *FiMPART - Frontiers in Materials Processing Applications, Research and Technology, July 9-12, Bordeaux, Oral presentation*

*Mar Lucas, M., Rein, C., Lauridsen, E., Poulsen, H.F., Andreasen, J. W. (2017) 3D crystallography of kesterite absorber layers, *DESY Photon Science Users's Meeting, January, 25-27, Hamburg*

Jørgensen, P. S., Fevola, G., Ramos, T., Rein, C., Small, C., Stingelin, N. and Andreasen, J. W. (2017) Resonant X-ray ptychographic Tomography of P3HS solar cells, *DESY Photon Science Users's Meeting, January, 25-27, Hamburg*

*Mar Lucas, M., Rein, C., Oddershede, J., Lyckegaard, A., Poulsen, H. F., Andreasen, J. W. (2017) 3D crystallography of kesterite absorber layers, *29th MAX IV Laboratory User Meeting, March 13-15, Lund*

Norby, P., *In situ diffraction studies of batteries using high energy synchrotron X-ray radiation*, Workshop at PETRA IV: Research with High Energy X-Rays at Ultra-Low Emittance Sources", Feb. 13-15 2017, Hamburg, Germany, Invited talk

Norby, P. *The Hi-C project: Novel in situ and in operando techniques for characterization of interfaces in electrochemical storage systems*, European workshop on nanotechnologies & advanced materials for batteries, Feb. 23-24 2017, Umicore Headquarters, Brussels, Belgium, Invited talk

Mathiesen, J.K., Jensen, K. M. Ø. and Norby, P. *Understanding the Mechanism of Sodium Insertion in Hard Carbon through Ex Situ Pair Distribution Function*, DanScatt Annual Meeting June 1-2 2017 Odense, Denmark, Poster

Norby, P., *New insight from X-ray diffraction studies of energy materials under operative conditions*, Materials for Energy Applications through Neutron and X-Ray Eyes, May 22-23 2017, Göteborg, Sweden, Invited talk

Johnsen, R.E. & Norby, P. *Capillary-Based Micro-Battery Cells for Operando X-Ray Diffraction Studies of Electrode Materials in Working Li-Ion Batteries*. 232nd ECS Meeting, A04 Li-ion Batteries, National Harbor, MD, United States, 1-5 October 2017.

Johnsen, R.E. & Norby, P. (Invited). *Operando X-ray diffraction studies of high-capacity electrode materials using capillary based micro-battery cells*. E-MRS 2017 Spring Meeting, G - Materials for improving energy storage battery technologies, Strasbourg, France, 22 - 26 May 2017.

*Bowen J. R. Jørgensen P. S., Poulsen H. F., De Angelis .S, Trujillo . J. X. S., Chatzichristodoulou C., Frandsen H. L., Simmons H., Schmidt S., Gundlach C., Oddershede J., Villanova J., Wright J., Cook P., Detlefs C., Tsai E. H. R. (2017) Imaging and diffraction studies of solid oxide cell components with

synchrotron radiation (Poster), *Workshop Materials for Energy Applications through Neutron and X-Ray Eyes, Göteborg, 22-23 May 2017*

Andreasen, J. W. (2017) CINEMAXe – workflow for 3D Modelling and Imaging of Material Microstructure, *CoNext, Nov 16, Niels Bohr Institute, Copenhagen, Oral presentation*

Andreasen, J. W. (2017) CINEMA - the alliance for imaging and modelling of energy applications, *Materials for Energy Applications through Neutron and X-Ray Eyes, MAX4ESSFUN Interreg workshop, May 22-23, Chalmers, Göteborg, Oral presentation*

Anden formidling/outreach, m.v. (tv, radio, kronikker, foredrag, osv.):

<https://europeanspallationsource.se/article/eu-supports-local-neutron-researchers-interview-malgorzata-makowska>

<http://www.scienceandsociety.eu/2017/02/02/young-scientists-interview-with-malgorzata-makowska/>

Undervisning og kurser (Ph.d.-skoler og –kurser, sommerskoler, andet):

Kuhn, L. Theil, co-organizer and lecturer on neutron imaging at NNSP-SwedNess Neutron School 2017, 9-21 Sept. 2017, Tartu, Estonia.

Blanchard, D. (2017) Lecture on: Quasi Elastic Neutron Scattering - Application to battery materials. *Applications of neutrons and synchrotron radiation in nanoscience. UCPH Summer School in Nano-Science June 2017*

*Norby, P., co-organizer and lecturer on DTU Course 10209 X-ray and Neutron Experiments at International Research Facilities, June 2017

*Andreasen, J. W., co-organizer and lecturer on DTU Course 10209 X-ray and Neutron Experiments at International Research Facilities, June 2017

*Andreasen, J. W., Organizer, CINEMAX III: Summer School in 3D Imaging and Modeling, International PhD Summer School, Aug 28-Sep 1, Fuglsang, Denmark

Navne på MSc kandidater og BSc (afsluttede):

MSc. Jette Katja Mathiesen, Sodium-ion Battery Electrode Materials; In Situ Analysis of Structural and microstructural Properties

MSc. Mariana Mar Lucas, Identification and 3D Mapping of Crystal Structures and secondary phases in Cu₂ZnSnS₄ thin films for photovoltaic applications, TU Berlin

Contributions to scientific books

Andreasen, J. W. (2017) High Throughput *in situ* Scattering of Roll-To-Roll Coated Functional Polymer Films, *Conjugated Polymers and Oligomers, Structural and Soft Matter Aspects, Materials and Energy vol. 9 (ed. Matti Knaapila), 159-174, World Scientific*

DTU Mechanical Engineering

Bidrag til konferencer og kongresser:

Das, C. R., and Hald, J. (2017) Microstructural evolution in advanced 12Cr steels during creep, 14th International Conference on Creep and Fracture of Engineering Materials and Structures, Creep 2017, Saint Petersburg, Russia (oral presentation).

Diederichs, A. M., Thiel, F., Fischer, T., Lienert, U., and Pantleon, W. (2017), Monitoring microstructural evolution in-situ during cyclic deformation by high resolution reciprocal space mapping, Fatigue Fracture & Wear (FFW2017), Porto, Portugal (oral presentation)

Diederichs, A. M., Thiel, F., Lienert, U., and Pantleon, W. (2017). In-situ investigations of structural changes during cyclic loading by high resolution reciprocal space mapping. International Symposium on Fatigue Design and Material Defects, Lecco, Italy (oral presentation)

Juul, N.Y., Oddershede J., Winther G. (2017), Comparison of measured lattice rotations of individual grains with crystal plasticity simulations, ICOTOM18, Saint George, USA (oral presentation)

Lienert, U., Gábor; R., Tamas, U., Wejdemann, C., and Pantleon, W. (2017) High-Resolution Single-Grain Diffraction of Polycrystalline Materials. *Synchrotron Radiation News*, 30, 35-40.

Niessen, F., Grumsen, F.B., Hald, J., and Somers, M.A.J. (2017) Formation and stabilization of reversed austenite in supermartensitic stainless steel, 24th IFHTSE Congress, Nice, France (oral presentation)

Pantleon, K. (2017), Exciting possibilities, Decisive support, Distinct methods, Intense weeks for materials research on steels – thanks to EDDI, BESSY EDDI Workshop, Berlin, Germany (invited presentation)

Pantleon, K. (2017), Surface Engineering of metallic materials – small changes give a huge effect, Colloquium at University of Saarland, Saarbrücken, Germany (invited presentation)

Pantleon, W. (2017), Evolving deformation structures: high-resolution reciprocal space mapping and orientation distribution of individual grains, ICOTOM18, Saint George, USA (plenary presentation)

Pantleon, W. (2017), Monitoring the elastic response of individual subgrains of a dislocation structure during small changes in the imposed strain, 2017 MRS Spring Meeting, Phoenix, USA (invited presentation)

Winther, G., Juul, N.Y., Oddershede, J. (2017), Measured resolved shear stresses and active slip systems in austenitic steel, ICOTOM18, Saint George, USA (invited presentation)

Winther, G. (2017), Parallel evolution of deformation textures and dislocation boundaries, 27th International Workshop on Computational Mechanics of Materials (IWCMM-27), Leuven, Belgium (oral presentation)

Winther, G. (2017), Hierarchical microstructures in metals due to dislocation-mediated plasticity, Symposium on Multiscale Computational Analysis of Complex Materials, Lyngby, Denmark (invited presentation)

Anden formidling/outreach, m.v. (tv, radio, kronikker, foredrag, osv.):

F. Nießen, DTU Press News <http://www.oilgas.dtu.dk/english/press/nyhedsbase/Nyhed?id={CA0339B0-010A-4C31-89E7-D29D29A609E3}>

K. Pantleon, Member of the HZB (BESSY) Scientific Selection Panel for Material Sciences and Hard Condensed Matter

W. Pantleon, Member of the DESY (PETRA) Project Review Panel for Engineering Materials Science

Undervisning og kurser (Ph.d.-skoler og –kurser, sommerskoler, andet):

41691 Ph.D. course on application of x-ray diffraction in materials science (5 ECTS)

Navne på MSc kandidater og BSc (afsluttede):

M.Sc. thesis, Chloe B.E. Devos, Cryotreatment of Tool Steels

M.Sc. thesis, Yichen Meng, Cryogenic treatment of titanium alloys

M.Sc. thesis, Chiara Tibollo, Carbide transformations in centrifugally cast high temperature steels

DTU Physics

Patenter:

High precision computed tomography for metrology, WO2017186804, H. F. Poulsen, C. Gundlach.

A method of security scanning of carry-on items, and a carry-on items security scanning system, WO2017005757, H. F. Poulsen, U. L. Olsen, J. Kehres.

A method of security scanning of carry-on items, and a security scanning system of carry-on items, EP20150175560, H. F. Poulsen, U. L. Olsen.

Conference articles and articles in proceedings

McXtrace 1.4: latest developments in the new release. / Knudsen, Erik B.; Willendrup, Peter Kjær; Garde, Jakob; Jørgensen, Mads R. V.; Kantor, Innokenty. In: Proceedings of S P I E - International Society for Optical Engineering, Vol. 10388, 1038809, 2017.(with AU CHEM)

Spectral correction algorithm for multispectral CdTe x-ray detectors. / Christensen, Erik D.; Kehres, Jan; Gu, Yun; Feidenhans'l, Robert ; Olsen, Ulrik Lund. In: Proceedings of S P I E - International Society for Optical Engineering, Vol. 10391, 103930H, 2017.(with Niels Bohr Institute)

A Monte Carlo simulation of scattering reduction in spectral x-ray computed tomography. / Busi, Matteo; Olsen, Ulrik Lund; Bergbäck Knudsen, Erik; Frisvad, Jeppe Revall; Kehres, Jan; Christensen, Erik D.; Khalil, Mohamad; Haldrup, Kristoffer. Advances in Computational Methods for X-Ray Optics IV. ed. / Oleg Chubar; Kawal Sawhney. Vol. 10388 SPIE - International Society for Optical Engineering, 2017. 103880P (Proceedings of S P I E - International Society for Optical Engineering).

Femtosecond X-ray absorption and emission spectroscopy on zno nanoparticles in solution. / Penfold, Thomas J.; Szlachetko, Jakub; Gawelda, Wojciech; Santomauro, Fabio G.; Britz, Alexander; Brandt van Driel, Tim; Sala, Leonardo; Ebner, Simon; Southworth, Stephen H.; Doumy, Gilles; March, Anne Marie; Lehmann, Carl S.; Katayama, Tetsuo; Mucke, Melanie; Iablonskyi, Denis; Kumagai, Yoshiaki; Knopp, Gregor; Motomura, Koji; Togashi, Tadashi; Owada, Shigeki; Yabashi, Makina; Rittmann, Jochen; Nielsen, Martin Meedom; Pajek, Marek; Ueda, Kiyoshi; Chergui, Majed; Abela, Rafael; Milne, Christopher J. International Conference on Ultrafast Phenomena. Vol. 2016 OSA, 2016. (Optics Infobase Conference Papers).

Oral presentations

S. Schmidt, 3D Neutron Diffraction (3DND) Methodology – second generation algorithms, Neuwave 9, June 11-14 2017, NIST, USA

M. Sales, 3D Polarimetric Neutron Tomography of Magnetic Fields, Neuwave 9, June 11-14 2017, NIST, USA

S. Schmidt, Novel Neutron Imaging Modalities for Materials Characterization, The 1st International Symposium on Advanced Structural Materials – Design Characterization and Processing, November 13-15 2017, Chongqing, China

Matti Knaapila, Neutron Scattering Assisted Quantitative Design of High Pressure Synthesized Polymer Hydrogels Dedicated to Antibiotics Carriers The 4th Annual International Workshop on Soft & Complex Matter, Norwegian Academy of Science and Letters, October 29-30, 2017, Oslo, Norway.

Niels Bech Christensen, Magnetic phase diagram of strongly magnetoelectric LiCoPO_4 , foredrag på 9th joint BER II and BESSY II user meeting", December 13-15, 2017.

K. Haldrup, " Sub-picosecond tracking of the coupled electronic, structural and solvation dynamics in metal-centered complexes utilizing multi-modal XFEL experiments", Banff Meeting on Ultrafast Dynamics, February 2017

K. Kjær, " Manipulating the excited state cascade of iron coordination compounds with through ligand- and solvent substitution", LCLS User's Meeting, SLAC, Stanford, September 2017

K. Kjær, LCLS User's Meeting, Young Scientist Award talk, SLAC, Stanford, September 2017

E. Biasin, Femtosecond structural dynamics of solvated metal complexes with anisotropy-enhanced X-ray scattering", Banff Meeting on Ultrafast Dynamics, February 2017

Martin M. Nielsen, "The most powerful X-ray laser in the World - the European XFEL" ", Annual Meeting of the Danish Physical Society, [Middelfart](#) 2017

Martin M. Nielsen, "XFEL experiments on metal complexes", DANSCATT Annual Meeting, [Odense](#) 2017

Martin M. Nielsen, "Opening address at the European XFEL Users meeting", Hamburg, 2017

Martin M. Nielsen, "The most powerful X-ray laser in the World - the European XFEL" ", Annual Meeting of the Danish Optical Society, [Lyngby](#) 2017

Martin M. Nielsen, "XFEL probes for Solvation", LCLS II High Energy Upgrade workshop, SLAC, Stanford, July 2017

Lise Sandberg, "Ultrafast dynamics of photo-excited iron complexes", Annual Meeting of the Danish Physical Society 2017

Mads Laursen, "Breaking Structural Correlations with high-energy TR-WAXS ", Annual Meeting of the Danish Physical Society 2017

Hugh Simons, IUCR (21-28 august 2017), "Multi-scale 3D Characterization with DarkField X-Ray Microscopy"

Hanna Leemreize, MECA SENS (19-21 september 2017). Poster: Hanna Leemreize, Per Sigaard Christensen,

Nikolaj Zangenberg, Henning Friis Poulsen, "Multiscale residual stress analysis on metallic wind mill components by combined neutron, x-ray and electron diffraction"

Henning Friis Poulsen, ICTMS (26-30 juni 2017) Keynote: "X-ray diffraction microscopy"

Henning Friis Poulsen, IUCR (21-28 august 2017), "X-ray diffraction microscopy"

Anders Filsøe Pedersen, Danscatt årsmøde (1-2 juni 2017). Poster: Anders Filsøe Pedersen, Hugh Simons, Carsten Detlefs, Henning Friis Poulsen, "Fractional Fourier transform for X-ray wavefront propagation simulation"

Anders Filsøe Pedersen, SSRL and LCLS user meeting (27-29 september 2017). Præsentation: Anders Filsøe Pedersen, Maria Escudero-Escribano, Elisabeth Ulrikkeholm, Apurva Mehta, Ifan E. L. Stephens, Anders Nilsson, Ib Chorkendorff, "(Surface) XRD structure of the catalytically active overlayer on Pt_xGd and Pt_xY"

Jin Zhang, ICTMS (26-30 juni 2017), "Measuring Material Parameters by Comparing Phase-Field Simulations with 4D Tomography"

Sonja Ahl, DFS årsmøde (22-23 maj 2017). Poster: "Recovery and Recrystallization study by Dark field x-ray microscopy"

Sonja Ahl, Danscatt årsmøde (1-2 juni 2017). Poster: "Recovery and Recrystallization study by Dark field x-ray microscopy".

Anden formidling/outreach, m.v. (tv, radio, kronikker, foredrag, osv.):

Peter Willendrup, Rasmus Toft-Petersen: ESS - European Spallation Source - Ny neutronkilde i Skandinavien (Foredrag i ingeniørforeningen, IDA)

Rasmus Toft-Petersen (interview på IDA's hjemmeside ifm ovenstående):

<https://universe.ida.dk/artikel/verdens-stoerste-neutronkilde-skal-give-superledere-til-folket-54612/>

Niels Bech Christensen: foredrag for Dansk Magnetisk Forening ifm dennes besøg på ESS.

Kristoffer Haldrup, "Verdens kraftigste røntgenlasere - hvordan og hvorfor", IDA fyraftensforedrag, marts 2017

Carsten Gundlach præsentationer:

27/2	'CT -scanning knitting & wool fibres'. ATOMS at SAXO institut, København
9/3	Industry day at LUND
30/3-1/4	SINE2020 workshop, Munchen, Tyskland
16/5	'3D imaging center at DTU', IPAC2017, København
1/6	Danscatt årsmøde, Odense
21/9	'3D Imaging center', High tech summit 2017, Lyngby
15-17/11	'DTU and LINX, input to ESS', Sitges, Spanien
20-22/11	XEN meeting, London, England
27/11	'3D Imaging', DMN workshop, Århus
17/1	Møde på Carlsberg om LINX og 3D Imaging Center
21/3	Fysikaften på DTU

Undervisning og kurser (Ph.d.-skoler og –kurser, sommerskoler, andet):

S. Schmidt & N.B. Nielsen, 10200 Materialers struktur og dynamik studeret med røntgen og neutroner

Matti Knaapila, kursus 10220 "Physics of Soft Materials".

S. Schmidt, PhD school, UCPH Summer School in Nano-Science, July 27th 2017

Peter Willendrup, Erik Knudsen: ISIS STFC McStas Training April 26th-28th 2017

(<http://april2017.mcstas.org>)

Rasmus Toft-Petersen, Niels Bech Christensen: Foredrag om neutronspektroskopi ifm sommerskole på KU/DTU Applications of X-ray and neutron scattering in biology, chemistry and physics

10209 X-ray and Neutron Experiments at International Research Facilities (Undervisere: Niels Bech Christensen, Matti Knaapila, Henning Friis Poulsen, Carsten Gundlach, Martin Meedom Nielsen + folk fra DTU Energi)

10200 The structure and dynamics of materials studied with X-rays and neutrons (Undervisere: Primært Niels Bech Christensen og Søren Schmidt. Enkeltforedrag af Peter Willendrup + Matti Knaapila)

K. Haldrup, " Ultrafast time-resolved X-ray scattering with XFEL sources - Methods, Challenges and Opportunities " , Modern light Sources and their applications, Szeged, Hungary, December 2017

K. Haldrup, " X-ray investigations of ultrafast materials dynamics using synchrotrons and XFELs" , forelæsning i kurset "Modern Physics" for Phd-studerende v. DTU Fysiks PhD-skole

K. Haldrup, "Super-intens røntgenstråling - Hvad er det, og hvad kan man bruge det til?", erhvervspraktikanter på DTU Fysik Feb. 2017

Carsten Gundlach, enkeltforedrag, Scientific Computing for X-Ray Computed Tomography (CT) (02946) 3/1

Carsten Gundlach, enkeltforedrag, Røntgen- og neutroneksperimenter ved internationale forskningsanlæg (10209) 2/6

Carsten Gundlach, enkeltforedrag, 'CT -scanning knitting & wool fibres'. ATOMS at SAXO institut, 3/8

Carsten Gundlach, enkeltforedrag, Anvendelse af røntgen og neutron-spredning i biologi, kemi og fysik (26265) 18/8

Henning Friis Poulsen, 41680: Introduction to cyber materials.

Henning Friis Poulsen, 10209: X-ray and Neutron Experiments at International Research Facilities.

MSc kandidater og BSc (afsluttede):

Søren Schmidt, "Imaging with polarised neutrons", Michael Korning Sørensen (MSc)

Matti Knaapila, "Surfactant treated organic field-effect transistors: Simulation, preparation and structural and electrical characterization", Andreas E. Lauritzen (MSc)

Kristoffer Haldrup, "Ultrafast Dynamics in Photoexcited Iron-Carbene Molecules – an X-ray Study", Lise Sandberg (MSc with KU)

Carsten Gundlach (medvejleder), "Response of single fibers to pullout forces at different embedment angles", Vlad Chiriac og Vasile Daniel Mois (DTU Byg)(MSc)

Carsten Gundlach (medvejleder), "Creep behavior of Fiber Reinforced Concrete", Robert Havlik og Ivan Galik (DTU Byg)(MSc)

Matti Knaapila, "Simulation of interface structures in oil-in-water microemulsions", Jakob Thorsbro (BSc)

Niels Bech Christensen, "Magnetism and entanglement in small spin clusters", Frederik Werner Isaksen (BSc)

Niels Bech Christensen, "Probing the magnetic phase diagram of TbNi₂B₂C", Steffen Sloth (BSc)

Niels Bech Christensen, "Monte Carlo simulations of mixed-anisotropy spin systems", Rasmus Eilker Hansen (BSc)

Kristoffer Haldrup, "Analysis and comparison of the ultrafast structural dynamics of TI-PtPOP studied with X-ray scattering data acquired at LCLS", Asbjørn Moltke (BSc)

Kristoffer Haldrup, "Fourier Transformations of Time Resolved X-ray Scattering", Aksel Obdrup (BSc)

Carsten Gundlach (medvejleder), "Complex 3D Fiber Segmentation and Characterization", Benjamin Cordes (DTU Compute)(BSc)

Carsten Gundlach (medvejleder), "Complex 3D Fiber Characterization", Patrick Møller Jensen (DTU Compute)(BSc)

Niels Bohr Institute, Copenhagen University

Bidrag til konferencer og kongresser:

INVITED

Mortensen, K. (2017) Danish Neutron User Community and ESS. BrightnESS. Canadian Neutron Science at ESS. Copenhagen, Denmark November 21-23

Mortensen, K. (2017) Establishment of ESS in the Øresund region. Det Unge Akademi (DUA) Copenhagen November 11.

Mortensen, K., Kirkensgaard, J., Borger, A., Hassager, O., Almdal, K., Huang, Q., Dorokhin, A., Garvey, C.J. (2017) Complex Structured Polymers in Extensional Flow – Rheology and Small-Angle Neutron Scattering. *ICNS-2017*, Daejeon Korea, July 9-13.

Mortensen, K. (2017) DANSCATT – PSI collaboration with Denmark. *Paul Scherrer Institut 20 years SINQ*. Villigen, Switzerland April 18.

Lefmann, K. Unexpected suppression of magnetic stripes by field in the underdoped superconductor LSCO – SNSS annual Meeting, Uppsala (May 2017)

Lefmann, K. Quantum Materials, Invited lecture, DANSCATT Annual Meeting, Odense (June 2017)

Lefmann, K. On the nature of magnetic stripes in superconductors, NNSP Workshop on correlated electron systems, Lund (July 2017)

Lefmann K. Magnetic ground state and magnon-phonon interaction in multiferroic h- YMnO_3 , International Conference on Neutron Scattering, Daejeon South Korea (July 2017)

Bordallo, H.: “Microscopic view of hydrogen motion from neutron scattering”, Institute of Theoretical and Applied Mechanics ASCR, Centre of Excellence Telč, Telč, Czech Republic

Bordallo, H.: “Filling in the gaps: improving our quality of life by understanding hydrogen bonds”, Neutrons for Health, Bad Reichenhall, Germany (June 2017)

Bordallo, H.: “Hints on how to design and setup a robust and reliable experiment: Tips and Tricks”, Danish Research Centre for Magnetic Resonance, Hvidovre Hospital, Hvidovre, Denmark (August 2017)

Bordallo, H.: “Microscopic view of hydrogen motion from neutron scattering”, Center for Molecular Biophysics Seminar, Oak Ridge National Laboratory, USA (September 2017)

Bordallo, H.: “Biophysics in drug development: impact, challenges and opportunities opened by neutron scattering”, Annual Meeting of the Brazilian Biophysics Society, Santos, Brazil (October 2017)

Kapishnikov, S.: Danish Bio-imaging Society Meeting, *Copenhagen*, Denmark (November 2017)

Kapishnikov, S.: Danish Research Centre for Magnetic Resonance, Hvidovre Hospital, *Hvidovre*, Denmark (August 2017)

Kapishnikov, S.: Brookhaven National Lab, NSLS-II, *Upton*, NY, USA (March 2017)

Kapishnikov, S.: MAX IV, *Lund*, Sweden (February 2017)

Santos, E. C. D.: “A synthetic smectite, fluorohectorite, as a promising carrier for controlled drug delivery”, 4th Annual International Workshop on Soft & Complex Matter, Norwegian Academy of Science and Letters, Oslo, Norway. (October 2017)

Santos, E. C. D.: “Argila sintética Fluorohectorita: um material promissor para drug delivery”, Local Seminar, Institute of Chemistry, University of São Paulo State, Araraquara, Brazil. (May 2017)

Santos, E. C. D.: “Intercalation of ciprofloxacin into lithium-fluorohectorite at different pHs”, Nordic Workshop on Scattering From Soft & Biological Materials, University of Oslo, Oslo, Norway. (January 2017)

Pereira, J. E. M.: Hydrogen bonds in enantiomers: The alanine paradigm – International Conference on Neutron Scattering 2017 (ICNS 2017), Daejeon (Korea). (July 2017)

Pereira, J. E. M.: Hydrogen bond dynamics in antipsychotics by neutron spectroscopy and density functional theory – MLZ conference: Neutrons for Health 2017, Bad Reichenhall (Germany). (June 2017)

Pereira, J. E. M.: Hydrogen bond dynamics, conformational flexibility and polymorphism in antipsychotics - The Annual Condensed Matter and Materials Meeting 2017, Wagga Wagga (Australia) (January 2017)

Strobl, M.: “Neutron Imaging and Engineering Diffraction at PSI”, EPFL Seminar, Neuchatel, Switzerland. (November 2017)

Strobl, M.: “Novel Neutron Imaging Techniques and Processing Requirements at ESS”, CoNEXT Symposium, Copenhagen, Denmark. (November 2017)

CONTRIBUTED

Wingstrand, S. L, Mortensen, K., Huang, Q. Shen, B., Kornfield, J. A., Imperiali, L., Stepanyan R. and O. Hassager. (2017) Extensional rheology and flow-induced crystallization of polyethylene above T_m. *The Society of Rheology 89th Annual Meeting*. Denver, Colorado, October 8-12.

Jakubauskas, D., Rudowska, L., Mortensen, K., Jensen, P.E., Kirkensgaard, J. (2017) Applying small angle scattering to investigate thylakoid membranes. SEBiology Annual Meeting, Gothenburg Sweden. July 3–6.

Borger, A., Mortensen, K., Kirkensgaard, J., Hassager, O., Huang, Q. (2017) Will Wide Angle X-ray Scattering (SAXS) reveal the molecular alignment of polystyrene stretched in its melted state. *Danish Physical Society Annual Meeting*, Middelfart, May 22.-23.

Wingstrand, S.L., van Drongelen, K., Mortensen, K., Graham, R.S., Huang, Q. (2017) Extensional rheology and final morphology of LDPE fibers. *Society of Rheology 88th Annual Meeting*. Tampa Florida, February 12-16.

Wingstrand, S.L., van Drongelen, M., Mortensen, K., Graham, R.S., Huang, Q., Shen, B., Kornfield, J.A., Hassager, O. (2017) Crystallinity of polyethylene in uni-axial extensional flow. *European Rheology Conference 2017*. Copenhagen, April 3-6.

* H. Jacobsen, S. L. Holm, M.-E. Lăcătușu, A. T. Rømer, M. Bertelsen, M. Boehm, R. Toft-Petersen, J.-C. Grivel, S. B. Emery, L. Udby, B. O. Wells, and K. Lefmann, *Distinct Nature of Static and Dynamic Magnetic Stripes in Cuprate Superconductors*, Phys. Rev. Lett. 120, 037003 (2018)

* P. J. Ray, N. H. Andersen, T. B. S. Jensen, H. E. Mohottala, Ch. Niedermayer, ... & L. Udby, *Staging superstructures in high- T_c Sr/O codoped $La_{2-x}Sr_xCuO_{4+y}$* , Phys. Rev B 96, 174106 (2017)

* J. H. Overgard, J. Bruun, M. May, & L. Udby, *Virtual neutron scattering experiments : Training and preparing students for large-scale facility experiments*, Læring og Medier 16 (9) (2017)

L. Udby & N.C. Petersen, *Wikis for textbooks, online collaboration and course presentation*, Læring og Medier 16 (9) (2017)

Berg, M: Poster: International Conference on Neutron Scattering: Understanding the dynamics of aqueous solutions in dental cements, Daejeon, Republic of Korea. (2017)

Rasmussen, Martin K.: Poster: "Localization of Hepatitis B in SBA-15", Annual DANSCATT meeting, University of Southern Denmark, Odense, DK) (June 2017)

Larsen, Simon R.: Poster: Dynamical analysis of Ciprofloxacin intercalated in fluorohectorite", Annual DANSCATT meeting, University of Southern Denmark, Odense, DK) (June 2017)

Magkos, Sotirios: Poster: *X-ray and neutron tomography of charred cereal grains from archaeological site in southern Sweden*", Annual DANSCATT meeting (June 2017) University of Southern Denmark, Odense, DK)

Anden formidling/outreach, m.v. (tv, radio, kronikker, foredrag, osv.):

A large number of public news articles on the Papyrus study, which include DANSCATT members from KU-NBI and KU-Chem:

Newsweek, 03 Dec 2017. *The Indian Express*, 13 Nov 2017. *Mining.com*, 15 Nov 2017. *Science Newsline*, 13 Nov 2017. *International Business Times*, 13 Nov 2017. *Eurasia Review*, 13 Nov 2017. *MSN*, 12 Nov 2017. *Newsweek*, 11 Nov 2017. *IANS Live*, 11 Nov 2017. *Times of India*, 11 Nov 2017. *Business Standard*, 11 Nov 2017. *Millenium Post*, 11 Nov 2017. *Business Standard*, 11 Nov 2017. *Daijiworld.com*, 11 Nov 2017. *Yahoo! News*, 11 Nov 2017. *ANI News*, 11 Nov 2017. *Laboratory Equipment*, 10 Nov 2017.

Bilag 4: DANSCATT outreach, kurser, studenterafhandlinger, publikationer mv. 2017

UPI.com, 10 Nov 2017. *Phys.Org*, 10 Nov 2017. *Business Standard*, 10 Nov 2017. *Breitbart News Network*, 10 Nov 2017. *EurekAlert*, 10 Nov 2017.

Bordallo, H.: “Solving materials challenges using neutron vision” - Kick off meeting at the Niels Bohr Institute, University of Copenhagen, Copenhagen – Denmark

Bordallo, H.: “Does Superman really have X-rays Vision?” - Kulturnat 2017 - Copenhagen, Denmark

Bordallo, H.: “Kræftbehandling uden bivirkninger or Cancer treatment without side effects” - Temadag 2017 - Niels Bohr Institute, University of Copenhagen, Copenhagen – Denmark

Bordallo, H.: “Press releases by the European Spallation Source:

<https://europeanspallationsource.se/article/research-neutrons-opens-new-paths-predict-behaviour-local-anesthetics>

Synchrotron research highlights:

Kapishnikov, S.: “Biochemistry of the malaria parasite by X-ray microscopy”, ESRF Highlights 2017 (*In Press*)

Kapishnikov, S.: “New Insights about Malaria Parasite's Infection Mechanisms”, ALBA Synchrotron Light Source news article from 10/2017 (<https://www.albasynchrotron.es/en/media/news/new-insights-about-malaria-parasites-infection-mechanisms>)

Press releases:

Kapishnikov, S.: 08/2017 “Spying on malaria parasites at -196 Celsius.” Niels Bohr Institute – University of Copenhagen. *Press release*. <http://www.nbi.ku.dk/english/news/news17/spying-on-malaria-parasites-at-196-celsius/>

Kapishnikov, S.: 04/2017 “An important step towards new malaria medicine.” Niels Bohr Institute – University of Copenhagen. *Press release*. <http://www.nbi.ku.dk/english/news/news17/an-important-step-towards-new-malaria-medicine/>

Pereira, J. E. M: “Be Filter – Research Work Experience” at the Australian Nuclear Science and Technology Organization (ANSTO).

Strobl, M: “Perspectives of quantitative neutron time-of-flight dark-field imaging”, XNPIG, Zurich, Switzerland. (September 2017)

Strobl, M.: “In-situ observation of redox behavior in Ni-YSZ Solid Oxide Cell electrodes” – International Conference on Neutron Scattering 2017 (ICNS 2017), Daejeon, Korea. (July 2017)

Strobl, M.: “Dark-field neutron imaging”. NeuWave. Gaithersburg, USA. (June 2017)

Bilag 4: DANSCATT outreach, kurser, studenterafhandlinger, publikationer mv. 2017

* P.J. Ray, *Superstructures in LSCO+O*, poster. Won the prize for best poster at ICNS 2017 in South Korea

T.B Tejsner, Phonon anomaly in LSCO+O, poster ICNS2017 South Korea and SCES2017 in Prague.

Midtgaard, S. R. Brok, E. "Land of milk and neutrons." Physics World, October 2017

Undervisning og kurser (Ph.d.-skoler og –kurser, sommerskoler, andet):

Mortensen, K.: Experimental X-ray Physics. 7.5 ECTS MSc/PhD course KU

Mortensen, K.: Polymer Physics. 5 ECTS PhD course, DTU+KU

Bordallo, H.: Lecturer at the Geilo School, March 2017, Geilo-Norway

Bordallo, H.: Contribution 1: Neutrons: the key to understanding hydrogen bonds and improving our quality of life

Bordallo, H.: Contribution 2: Working with the world's biggest microscope

Bordallo, H.: Co-organizer of the 1st SPSLNX: "São Paulo School on Scattering: Diffraction and Imaging using Light, Neutrons and X-rays, July 17th - 21st 2017, São Paulo, Brazil

Bordallo, H.: Contribution: Filling in the gaps: from instrumentation to real systems

Bordallo, H.: Lecturer at the neutron course

Bordallo, H.: Responsible for the Course NFYK12004E: Applications of X-ray and neutron scattering in biology, chemistry and physics offered by the Niels Bohr Institute, University of Copenhagen, Copenhagen – Denmark, 7.5 ECTS

Berg, M: Atomistic Modeling for Neutron Scattering, Oak Ridge, USA, 7-9 June, 2017, organized by Oak Ridge National Laboratory.

Pereira, J. E. M: 08/2017 Teaching Assistant in the course: NFYK12004U - Applications of X-ray and Neutron Scattering in Biology, Chemistry and Physics, Niels Bohr Institute, University of Copenhagen, Copenhagen – Denmark.

Udby, L.: SwedNESS-NNSP Phd school on neutron scattering. E-learning material.

Navne på MSc kandidater og BSc (afsluttede):

BSc

Nikoline Lyk Pedersen, BSc (2017) (Lefmann, K.)
Rasmus Tang, BSc (2017) (Lefmann, K.)
Helle Kogsbøll Leerberg, BSc (2017) (Lefmann, K.)
Magnus Bøggild, BSc (2017) (Lefmann, K.)
Mariam Ahmad, Bsc (2017) (Udby, L.)
Gidega Vijayakumar
Malene Backenhaus
Julie Klepstad
Chastine F. Munk

MSc

Anders Bakke, MsC (2017) (Mortensen, K.)
Jakob Lass, MSc (2017) (Lefmann, K.)
Ana-Elena Tutueanu, MSc (2017) (Lefmann, K.)
Lise Ørdu Sandberg, MSc (2017) (Lefmann, K.)
Sofie Janas, MSc (2017) (Lefmann, K.)
Christopher Røhl Andersen, MSc (2017) (Lefmann, K.)
Henrik Hoffmann Carlsen, MSc (2017) (Lefmann, K.)
Magnus Aagren Jensen, MSc (2017) (Lefmann, K.)
Simon R. Larsen (2017) (Bordallo, H. + Santos, E. C. D.)
Martin K. Rasmussen (2017) (Bordallo, H.)

Department of Chemistry, University of Copenhagen

Bidrag til konferencer og kongresser:

Oral presentations:

1. *PETRA IV: Research with High Energy X-Rays at Ultra-Low Emittance Sources workshop*. 16. Februar 2017. Title: High energy X-ray scattering for nanostructure analysis, DESY, Hamburg, Germany. Presenter: Kirsten M. Ø. Jensen
2. *Oxford Solid State Research Seminar*. June 2nd 2017. Title: New Nanostructure from X-ray total scattering. University of Oxford, UK. Presenter: Kirsten M. Ø. Jensen
3. *EICC 2017*. July 4th 2017. Title: New Nanostructure from X-ray total scattering. Copenhagen. Presenter: Kirsten M. Ø. Jensen
4. *APS User Science Seminar*. July 12th 2017. Title: New Nanostructure from X-ray total scattering. APS, Chicago, USA. Presenter: Kirsten M. Ø. Jensen
5. *Chemistry Science at SRS Beamlines: Status and Future Challenges Workshop*. July 17th 2017. Title: Live tapings of nanoparticle formation and growth. APS, Chicago, USA. Presenter: Kirsten M. Ø. Jensen
6. Sept. 4-7, 2017, Porto Venere, Italy, 4th JVS workshop on Electronic Structure and Molecular Magnetism, Jesper Bendix; Lanthanide Single Molecule Magnets by Design
7. Sept. 4-7, 2017, Porto Venere, Italy, 4th JVS workshop on Electronic Structure and Molecular Magnetism, Mikkel A. Sørensen; Muon spin spectroscopy and its application to molecular magnetism
8. H. O. Sørensen, Y. Yang, S. L. S. Stipp, The 4th International Symposium on "Application of NanoGeosciences in Petroleum Engineering", The University of Tokyo, Tokyo, Japan, 20-21 November 2017 *What are the Potential Consequences of Storing CO₂ in Chalk: A Fine Grained Carbonate?* (keynote)
9. H. O. Sørensen, S. Bruns, K. N. Dalby, D. Mütter, K. Uesugi, S. L. S. Stipp, Goldschmidt 2017, Paris, France, 13-18 August 2017 *Predicting Macroscale Properties of Rocks from Nanoscale Data*
10. Y. Yang, S. L. S. Stipp, H. O. Sørensen, Goldschmidt 2017, Paris, France, 13-18 August 2017, *Direct Observation of Geochemical and Geomechanical Coupling in Chalk*
11. L. Voigt, K. Dideriksen, S. H. J. Eiby, C. M. van Genuchten, C. Frandsen, K. M. Ø. Jensen, S. L. S. Stipp, D. J. Tobler, Goldschmidt 2017, Paris, France, 13-18 August 2017, *The Effect of Aluminium on Green Rust Sulphate Structure and Reactivity*
12. S. Eiby, D. J. Tobler, L. Voigt, Z. Yin, C. M. van Genuchten, K. Jensen, T. Stawski, R. Wirth, L. G. Benning, H. C. B. Hansen, S. L. S. Stipp, K. Dideriksen, Goldschmidt 2017, Paris, France, 13-18 August 2017, *Solid State Transformation of Green Rust in Response to Oxidation*
13. Leila Lo Leggio, Open Day Annual CCC Symposium, Location Hampshire Plaza Hotel Groningen, 21 April 2017. *Lytic polysaccharide monooxygenases: a crystallographer's view* (invited)
14. Leila Lo Leggio, Carbohydrate Bioengineering Meeting 12, Vienna, Austria, 23-26 April 2017 *Fungal LPMOs and their interactions with ligands: what have we learned from structures?* (oral presentation)
15. Leila Lo Leggio, Gordon Research Conference "Cellulases & Other Carbohydrate-Active Enzymes", Andover, US 23-28 July 2017 *Recent progress in structural characterization of LPMOs* (invited talk).
16. Tobias Tandrup, CoLuAa XXV 2017, Copenhagen, Denmark, 30 October 2017, *Lytic Polysaccharide Monooxygenases interactions with substrate*

17. Anders Kokkenborg Varming, CoLuAa XXV 2017, Copenhagen, Denmark, 30 October 2017, *Structural Biology of the Genetic Switch From Bacteriophage TP901-1 – Focusing on the CI Repressor*
18. Tobias Tandrup, 3rd satellite workshop before CBM12, Danish Technical University, Kgs. Lyngby, Denmark, 21 April, 2017, Unravelling the structural features of the first engineered arabinofuranose-transferring enzymes
19. Kim Krighaar Rasmussen. Danscatt Annual meeting 2017, Odense, Denmark, June 2017. *Integrative structural biology of the genetic switch of TP901-1.*

Posters:

1. *EICC 2017*. July 4th 2017. Title: Small Box Modelling of Complex Molybdenum Oxide Nanostructures. Presenter: Troels Lindahl Christiansen
2. *EICC 2017*. July 4th 2017. Title: Determining Structures and defects in WOx nanostructures. Presenter: Mikkel Juelsholt.
3. *Danscatt annual meeting, SDU, June 2017*: Synthesis and characterization of CuCrO₂ delafossite nanoplatelets. Presenter: Emil Thyge Skaaning Kjær
4. *Danscatt annual meeting, SDU, June 2017*: Mechanisms for NiO nanoparticle formation in organic solvents. Presenter: Emil Rössing Elholm
5. *Danscatt annual meeting, SDU, June 2017*: PDF Modelling of Complex Molybdenum Oxide Nanostructures. Presenter: Troels Lindahl Christiansen
6. *Danscatt annual meeting, SDU, June 2017*: Structural Developments in Molybdenum based Catalysts: From Precursor to Final Catalyst. Presenter: Jette K. Mathiesen
7. *Danscatt annual meeting, SDU, June 2017*: Title: Determining Structures and defects in WOx nanostructures. Presenter: Mikkel Juelsholt.
8. *Danscatt annual meeting, SDU, June 2017*. Title: *Understanding the Mechanism of Sodium Insertion in Hard Carbon through Ex Situ Pair Distribution Function Analysis*. Presenter: Triana Wulandari.
9. HERCULES, February 2017: Title: How do we design new materials using polyoxometalate building blocks: Total Scattering studies of Molybdenum Oxide Nanostructures.
10. July 1-5, 2017, Copenhagen, 4th European Inorganic Chemistry Conference, Andreas Konstantatos; Lanthanide coordination complexes framed by alkali-metal ions and their magnetic behavior
11. July 1-5, 2017, Copenhagen, 4th European Inorganic Chemistry Conference, Mikkel A. Sørensen; Platinum-based metalloligands as versatile tools for the design of high-symmetry f-element complexes
12. July 1-5, 2017, Copenhagen, 4th European Inorganic Chemistry Conference, Emil Hansen; Lanthanide complexes with metallophilic exteriors.
13. July 1-5, 2017, Copenhagen, 4th European Inorganic Chemistry Conference, Stergios Piligkos; Towards Molecular 4f Single-Ion Magnet Qubits
14. July 1-5, 2017, Copenhagen, 4th European Inorganic Chemistry Conference, Morten G. Vinum; Influence of Ligand Field Distortions in a family of tetragonal MII-ReIV single chain magnets
15. July 1-5, 2017, Copenhagen, 4th European Inorganic Chemistry Conference, Kenneth Wärnmark, Jesper Bendix; Fe N-Heterocyclic Carbene Complexes as Promising Photosensitizers
16. D. Tobler, H. O. Sørensen, S. Bruns, D. Jha, Y. Yang, S. L. S. Stipp, Goldschmidt 2017, Paris, France. 13-18 August 2017, *Visualising Individual Microbial Cells Inside Rock Pores*

17. S. Bruns, K. Dalby, D. Mütter, F. Engstrøm, S. Stipp, H. O. Sørensen, 3rd International Conference on Tomography of Materials and Structures, Lund, Sweden, 26-30 June 2017, *Automated Analysis of Petrophysical Parameters*
18. D. Mütter, K. Dalby, S. Bruns, J. Oddershede, K. Uesugi, H. O. Sørensen, 3rd International Conference on Tomography of Materials and Structures, Lund, Sweden, 26-30 June 2017, *Multiscale Mechanical Modelling of Chalk*
19. Thomas J. Simmons, Kristian E. H. Frandsen, Luisa Ciano, Theodora Tryfona, Nicolas Lenfant, Jens-Christian N. Poulsen, Louis F.L. Wilson, Tobias Tandrup, Morten Tovborg, Kirk Schnorr, Katja S. Johansen, Bernard Henrissat, Paul H. Walton, Leila Lo Leggio, Paul Dupree, CoLuAa XXV 2017, Copenhagen, 30 October 2017, *Lytic Polysaccharide Monoxygenases interactions with substrate* (Poster prize)
20. Tobias Tandrup, Jens-Christian N. Poulsen, Bastien Bissaro, Claire Dumon, Michael O'Donohue, Régis Fauré, and Leila Lo Leggio, 1st ISBUC conference, Copenhagen, Denmark, 15 September, 2017, *Unravelling the structural features of the first engineered arabinofuranose-transferring enzymes*
21. Tobias Tandrup, Jens-Christian N. Poulsen, Bastien Bissaro, Claire Dumon, Pierre Monsan, Julien Durand, Michael O'Donohue, Régis Fauré, and Leila Lo Leggio, MAX4ESSFUN summer school, Aarhus University, Denmark, 28 August – 2 September, 2017, *Unravelling the structural features of the first engineered arabinofuranose-transferring enzymes*
22. Tobias Tandrup, Jens-Christian N. Poulsen, Bastien Bissaro, Claire Dumon, Pierre Monsan, Julien Durand, Michael O'Donohue, Régis Fauré, and Leila Lo Leggio, MAXIV User Meeting 17, MAXIV, Lund, Sweden, 13-15 March, 2017, *Unravelling the structural features of the first engineered arabinofuranose-transferring enzymes*
23. H. A. Ernst, L.J. Jørgensen, K. Piontek, C. Bukh, L. H. Østergaard, S. Larsen, M. J. Bjerrum, DanScatt Annual Meeting, Odense, June 2017 *Structure of Myceliophthora thermophila laccase*
24. R. M. Knudsen, J-C. N Poulsen. S. Mazurkewich, J. Larsbrink, J. A. Bååth, L. L. Leggio, CoLuAa XXV 2017 Conference, Copenhagen, October 30-31 *Structural characterization of a Glucuronoyl Esterase found in Oritatus terrae*
25. Z. Fábrián, E. Németh, E. Hermann, B. Gyurcsik, H. A. Ernst, S. Larsen, H. E. M. Christensen, 25th CoLuAa Conference, Copenhagen, October 2017 *Structural activation of NCoIE7-based artificial metallonucleases*
26. R. M. Knudsen, J-C. N Poulsen. S. Mazurkewich, J. Larsbrink, J. A. Bååth, L. L. Leggio, The Protein.DTU & Linderstrøm-Lang Symposium 'Current topics in protein chemistry', Copenhagen, November 17 *Structural characterization of a Glucuronoyl Esterase found in Oritatus terrae*
27. Anders K. Varming, Kim K. Rasmussen, Kristian H. Frandsen, Malene R. Jensen, Karin Hammer, Margit Pedersen, Peter W. Thulstrup, Jens-Christian N. Poulsen and Leila Lo Leggio. MAXIV User Meeting 17, MAXIV, Lund, Sweden, 13-15 March, 2017, *Structural Characterization of the Lactococcal Bacteriophage TP901-1 CI Repressor Protein*
28. Anders K. Varming, Kim K. Rasmussen, Kristian H. Frandsen, Malene R. Jensen, Karin Hammer, Margit Pedersen, Peter W. Thulstrup, Jens-Christian N. Poulsen and Leila Lo Leggio. 1st ISBUC conference, University of Copenhagen, Denmark, 15 September, 2017, *Structural Characterization of the Lactococcal Bacteriophage TP901-1 CI Repressor Protein*

29. Anders K. Varming, Kim K. Rasmussen, Kristian H. Frandsen, E. B. Erba, Margit Pedersen, Mogens Kistrup, Karin Hammer, Peter W. Thulstrup, Jens-Christian N. Poulsen, Malene R. Jensen and Leila Lo Leggio. CoLuAa XXV 2017, Copenhagen, Denmark, 30 October 2017, *Structural Biology of the Genetic Switch From Bacteriophage TP901-1 – Focusing on the CI Repressor*
30. Anders K. Varming, Kim K. Rasmussen, Kristian H. Frandsen, E. B. Erba, Margit Pedersen, Mogens Kistrup, Karin Hammer, Peter W. Thulstrup, Jens-Christian N. Poulsen, Malene R. Jensen and Leila Lo Leggio. The Protein.DTU & Linderstrøm-Lang Symposium "Current topics in protein chemistry", Copenhagen, 17 November 2017, *Structural Biology of the Genetic Switch From Bacteriophage TP901-1 – Focusing on the CI Repressor Poster*
31. Janina Sprenger, Jannette Carey, Sara S. Linse, Leila Lo Leggio, CoLuAa XXV 2017, Copenhagen, 30 October 2017, *Towards a universal crystal host method.*
32. Kim Krighaar Rasmussen, Kristian E.H. Frandsen, Elisabetta Boeri Erba, Margit Pedersen, Anders K. Varming, Mogens Kistrup, Karin Hammer, Peter W. Thulstrup, Malene Ringkjøbing Jensen, Leila Lo Leggio. CoLuAa XXV meeting, University of Copenhagen, Copenhagen November 2017. *Structural Biology of the Genetic Switch from Bacteriophage TP901-1.*
33. Kim Krighaar Rasmussen, Kristian E.H. Frandsen, Elisabetta Boeri Erba, Margit Pedersen, Anders K. Varming, Mogens Kistrup, Karin Hammer, Peter W. Thulstrup, Malene Ringkjøbing Jensen, Leila Lo Leggio. The Protein.DTU & Linderstrøm-Lang Symposium "Current topics in protein chemistry" University of Copenhagen, Copenhagen November 2017. *Structural Biology of the Genetic Switch from Bacteriophage TP901-1.*
34. Kim Krighaar Rasmussen, Kristian E.H. Frandsen, Elisabetta Boeri Erba, Margit Pedersen, Anders K. Varming, Mogens Kistrup, Karin Hammer, Peter W. Thulstrup, Malene Ringkjøbing Jensen, Leila Lo Leggio. ISBUC Conference, University of Copenhagen, Copenhagen September 2017. *Structural Biology of the Genetic Switch from Bacteriophage TP901-1.*
35. Kim Krighaar Rasmussen, Kristian E.H. Frandsen, Elisabetta Boeri Erba, Margit Pedersen, Anders K. Varming, Mogens Kistrup, Karin Hammer, Peter W. Thulstrup, Malene Ringkjøbing Jensen, Leila Lo Leggio. FEMS Conference, Valencia, Spain, Juli 2017 (FEMS grant) *Structural Biology of the Genetic Switch from Bacteriophage TP901-1.*

Anden formidling/outreach, m.v. (tv, radio, kronikker, foredrag, osv.):

1. *Materialekemi på atomar skala*. Foredrag i Videnskabernes selskab, 5. december 2017. Presenter: Kirsten M. Ø. Jensen
2. *Nanoscience* og nye materialer. Foredrag til gymnasielærerdag, Københavns Universitet, 2. februar 2017
3. *Materialekemi på atomar skala*. 5 foredrag for besøgende gymnasieklasser på Nanoscience, Københavns Universitet, 2017
4. D. Müter, S. Bruns, Y. Yang, H. O. Sørensen, *Numerical derivation of material properties using tomography data, Topical Day on Bridging experiments and continuum scale modelling of physical-chemical processes at the pore scale*, Mol, Belgium, 16 November 2017, invited talk.

Undervisning og kurser (Ph.d.-skoler og –kurser, sommerskoler, andet):

1. Teaching at "Advanced Powder Diffraction Workshop", Uppsala October 4-6th 2017. Title of seminar and tutorial: Pair Distribution Function Analysis of nanomaterials. Presenter: Kirsten M. Ø. Jensen
2. Teaching at "UCPH Summer School in Nano-Science", Magleås June 26th-30th. Title of seminar and tutorial: Powder Diffraction and Pair Distribution Function Analysis of nanomaterials. Presenter: Kirsten M. Ø. Jensen
3. UCPH Summer School in Nano-Science, Applications of neutrons and synchrotron radiation in nanoscience, Magleås Conference Center, Høsterkøb, Denmark, 26-30 June 2017. Responsible Henning O. Sørensen
4. Crystallography-B.Sc. (7.5 ECTS), Crystallography-MSc (7.5 ECTS), Proteins:structure and function (7.5 ECTS), ansvarlig: Leila Lo Leggio; Structural tools in nano-science (7.5 ECTS) ansvarlig: Nicolas Bovet; Materials Chemistry (7.5 ECTS) ansvarlige: Henning O. Sørensen og Kirsten M. Ø. Jensen. Kurser udbudt af Kemisk Institut, København Universitet

Navne på MSc kandidater og BSc (afsluttede):

BSc:

1. Christina Basse Riel (vejleder Kirsten M. Ø. Jensen)
2. Mathias Helmsøe-Zinck (vejleder Kirsten M. Ø. Jensen)
3. Emil Thyge Skaaning Kjær (vejleder Kirsten M. Ø. Jensen)
4. Sebastian Jannick Munderspach: *Structural Studies of the Lytic Polysaccharide MonoOxygenase AoAA13* (vejleder Leila Lo Leggio)

MSc:

1. Emil Rössing Elholm (vejleder Kirsten M. Ø. Jensen)
2. Emil Hansen
3. Svend H. C. Weihe, *Hematite reduction by Shewanella oneidensis MR-1 under conditions mimicking natural environments.*
4. Tobias Tandrup: *Structure determination of carbohydrate active enzymes: Arabinofuranosidase and Lytic Polysaccharide MonoOxygenase* (vejleder Leila Lo Leggio)
5. Anders K. Varming: *Characterization of the TP901-1 CI repressor: Structural Study of the Flexible Linker and C-Terminal Domain* (vejleder Leila Lo Leggio)

Department of Drug Design and Pharmacology, University of Copenhagen

Bidrag til konferencer og kongresser:

Rasmussen, D., Larsen, A. P., Laulumaa, S. K., and Kastrup, J. S. Activating GluD2 Lurcher with D-serine by introducing GluN1 hinge and point mutation. Dancatt Annual meeting, University of Southern Denmark June 1-2 (poster)

Larsen, A. P., Fièvre, S., Frydenvang, K., Francotte, P., Pirotte, B., Kastrup, J. S., and Mulle, C. Identification and structure-function study of positive allosteric modulators of kainate receptors. Dancatt Annual meeting, University of Southern Denmark June 1-2 (poster)

Laulumaa S, Kastrup J. S., Exploring the ligand binding site of ionotropic glutamate receptor using neutron crystallography. Dancatt Annual meeting, University of Southern Denmark June 1-2 (poster)

Nikolajsen, L. F., Peng, Y., Munk, C, Harpsøe, K., Liu, Z., Stevens, R., Gajhede, M., Kastrup, J. S., and Gloriam, D. GPCR Crystallography. CoLuAa XXV 2017 Conference, University of Copenhagen, October 30-31 (poster)

Kastrup, J. S. Dramatic motions in ionotropic glutamate receptors. CoNeXT Magleås meeting October 23 (lecture)

Maria Rafiq, Insights into the structurally engineered cytochrome P450 BM3 in complex with NSAIDs. CoLuAa XXV 2017 Conference, University of Copenhagen, October 30-31

Kirstine Louise Bendtsen, Understanding protein-protein interactions relevant for neuronal spreading of alphasynuclein. CoLuAa XXV 2017 Conference, University of Copenhagen, October 30-31

Dilip Narayanan, Jakob Staun Pallesen, Sara Solbak, Kim Tai Tran, Michael Gajhede, and Anders Bach. Targeting Keap1 by fragment-based drug discovery (FBDD) and X-ray crystallography. CoLuAa XXV 2017 Conference, University of Copenhagen, October 30-31 (poster)

Bente Vestergaard, Invited speaker at EMBO conference: Molecular Machines – Integrative Structural and Molecular Biology, Heidelberg, DE Nov 20-23, 2016

Saskia Bucciarelli, Presentation at the MAX IV user meeting, March 13-15 2017, Lund, SE

Dancatt meeting June 1-2, Odense, DK (Folmer Fredslund & Kirstine Bendtsen (w posters), Line Koch Skaaning & Annette Langkilde (participants))

6th Amyloid Disease Annual Meeting, Sept 6-8, Linköping, SE Line Koch Skaaning (poster)

6th Amyloid Disease Annual Meeting, Sept 6-8, Linköping, SE Kirstine Bendtsen (poster)

CoLuAa meeting, October 30-31, Copenhagen, DK (Kirstine Bendtsen (oral presentation), Folmer Fredslund (poster), Line Koch Skaaning, Annette (participants))

Annette Langkilde Invited speaker Nordic-EMBL-ESS workshop on neutron scattering studies in structural biology, Nov 7-8 2017, Lund, SE

Annette Langkilde, Invited speaker EUCALL Workshop: Biology at Advanced Laser Light Sources, Nov 30-Dec 1 2017, Hamburg, DE

Anden formidling/outreach, m.v. (tv, radio, kronikker, foredrag, osv.):

Kastrup, J. S.: Lægemidler mod hjernens sygdomme. Foredrag for gymnasieklasser

Nielsen, L. og Kastrup, J.S. Krystallisation af lysozym og analyse af proteinstrukturer ved hjælp af programmet PyMOL. Praktik d. 24. november i forbindelse med SRP opgave for gymnasieelev.

DanScatt symposium: Sine Larsen Symposium, University of Copenhagen, Feb. 9th (several organizers from Biostructural Research)

Book contributions

Marasini C., Vestergaard B. (2017) SAS-Based Studies of Protein Fibrillation. In: Chaudhuri B., Muñoz I., Qian S., Urban V. (eds) Biological Small Angle Scattering: Techniques, Strategies and Tips. *Advances in Experimental Medicine and Biology*, vol 1009 (book chapter)

Undervisning og kurser (Ph.d.-skoler og -kurser, sommerskoler, andet):

Kastrup, J. S.: Receptor Structure and Function. PhD course (course responsible and teacher)

Navne på MSc kandidater (afsluttede):

Silvia Barbateskovic
Daniel Rasmussen
Nicklas Hjortshøj Scheyer
Adrianna Laruba
Daniel Schacht
Liv Sofia Elinor Damgaard

The Novo Nordisk Foundation Center for Protein Research, University of Copenhagen

Patents:

Tailored assembly of a modular bud polypeptide, WO2018001858A1 (Guillermo Montoya, Stefano Stella)
<https://patents.google.com/patent/WO2018001858A1/en>

Contributions to conferences and congresses:

Poster presentation	EMBO Conference: The DNA damage response in cell physiology and disease (Greece)	Diana Kowalik
Poster Prize	Best Poster at the Instruct Biennial (Brno 2017)	Pablo Alcón
Invited speaker	NNF DNA Stalling Processes (Denmark)	Pablo Alcón
Poster presentation	Protein Signalling - NovoNordisk Foundation (Denmark)	Bhargav Prabhakar
Poster presentation	CoLuAa (Denmark)	Nicholas Egholm Sofos
Conference participation	2017 International Conference on Structural Biology, China	Danyang Wang
Conference participation	Macromolecular Crystallography School-MCS2017, Spain	Danyang Wang
Conference participation	International School of Biological Crystallisation, Spain	Danyang Wang
Conference participation	AIC International School 2017, Italy	Danyang Wang
Conference participation	The 1st European PhD and Postdoc symposium "Breaking Down Complexity: Innovative Models and Techniques in Biomedicine"	Danyang Wang
Conference participation	Scipion-Facilities Meeting, July 27th-28th, 2017, Madrid	Pablo Mesa
invited speaker	Erice 2017 - Integrative Structural Biology. Erice, Italy, 2 -11 June 2017	Stefano Stella
Poster presentation	The FEBS Congress 2017, FROM MOLECULES TO CELLS AND BACK - Jerusalem, Israel.	Stefano Stella
Poster presentation	Cell Symposium: CRISPR: From Biology to Technology and Novel Therapeutics. Sitges (Spain)	Stefano Stella
invited speaker	Precise Genome Editing Technologies August 24-25, 2017 Copenhagen (DK)	Stefano Stella
Organizer	CoLuAa 2017	Guillermo Montoya
Invited speaker	ENABLE 2017	Guillermo Montoya
Invited speaker	CNAF2017, China Canton	Guillermo Montoya

Bilag 4: DANSCATT outreach, kurser, studenterafhandler, publikationer mv. 2017

Invited speaker	EMBL Conference:Revolutions in Structural Biology	Guillermo Montoya
Invited speaker	Structural biology conference, Beijing	Guillermo Montoya
Invited speaker	Invited lecture scilifelab, Stockholm	Guillermo Montoya
Invited speaker	Chaperones meeting CNIO, Madrid	Guillermo Montoya
Invited speaker	Invited speaker, Santander	Guillermo Montoya
Invited speaker	Invited speaker IQFR CSIC, Madrid	Guillermo Montoya

Other communication / outreach

Radio interviews (two) (Guillermo Montoya) <https://www.altmetric.com/details/20733877/news>
<https://www.altmetric.com/details/27515902/news>

Education and courses

Organizer of the Cryo-EM workshop, 20-21 November 2017 (Guillermo Montoya)

Department of Biomedical Sciences, University of Copenhagen

Contributions to conferences/ Congresses

Kamil Gotfryd

Inaugural lecture for XXV CoLuAa conference (30/10-17): New structural insights into the regulation of human aquaporin

Qiaxia Hu

Poster for the 15th international conference on Na, K-ATPase and related transport ATPases. Title: Functional studies of P1B4-ATPases

Elena Longhin

Poster at The 15th International Conference on Na,K-ATPase and Related Transport ATPases, Otsu (JP). September 24-30, 2017

Christina Gronberg

Talk at The 15th International Conference on Na,K-ATPase and Related Transport ATPases, Otsu (JP). September 24-30, 2017, with the title: Ion-binding to purified and functional human copper transporting P-type ATPase ATP7B; Tällberg 2017: Towards the first crystal structure of a PIB-4-ATPase

Tamim Al-Jubair

Poster at the 22nd Swedish Conference on Macromolecular Structure and Function, Structural studies of Co(II)-transporting PIB-4 ATPases

Annette Duelli

Poster at the 22nd Swedish Conference on macromolecular Structure and Function and The 15th International Conference on Na,K-ATPase and Related Transport ATPases, Otsu (JP): Structural studies of a metal-bound zinc-transporting P1B-type ATPase

Julie Winkel Missel

Tällberg: Towards structural and functional characterization of the human aqua-ammonia porin; BMI day: New structural insights into the regulation of human aquaporins; CoLuAa: New structural insights into the regulation of human aquaporins

Anders Drabaeck Wiuf

Tällberg 2017 Unzipping the ZIPs. Towards functional and structural characterization of bacterial zinc transporters

Education and courses (PhD schools and courses, summer schools, other)

Elena Longhin

Teaching: Kidney physiology course

Julie Winkel Missel

Teaching: Human Biology (cell biology and human metabolism) at SUND, UCPH

Anders Drabaeck Wiuf

Class teacher Human Biology Course autumn 2017

Names of MSc candidates and BSc (completed)

Martina Tamburello, Erasmus traineeship

Alba Ferrer Pérez, Erasmus traineeship

Sunniva Holm Poulsen, molecular biomedicine;

Christian Sigvald Breinholt, biochemistry

Department of Pharmacy, University of Copenhagen

Doctoral dissertations 2017:

Name: Christa Nilsson

Title: Cubosomes and Hexosomes as Theranostic Nanocarriers

Affiliation: Department of Pharmacy, Faculty of Health and Medical Sciences (Copenhagen University)

Contributions to conferences and congresses in 2017:

Yaghmur, A. Cubosomes and Hexosomes as Versatile Platforms for Drug Delivery, Danish Cancer Society Research Center (Invited Talk).

Yaghmur, A., Al-Hosayni, S., Bor, G., Shao, X., Amenitsch, H., and Salentinig, S. Self-assemblies based on the new omega-3 lipid eicosapentaenoic acid monoglyceride, Workshop on Synchrotron X-ray and Neutron application to Food Science and Technology, Lund, Sweden (Talk).

Ghazal, A., Gontsarik, M., Kutter, J., Lafleur, J., Labrador, A., Mortensen, K., and Yaghmur, A. Combination of X-ray techniques with microfluidics for continuous production and characterization of nanoparticles, Workshop on microfluidics and micro/nanoparticles, Faculty of Health and Medical Sciences, University of Copenhagen (Talk).

Yaghmur, A. Cubosomes and Hexosomes as Versatile Platforms for Drug Delivery, Danish Chemical Society (Talk).

Names of MSc candidates and BSc (completed):

Master Students completed their studies: Umar Asghar, Hasan Akram, Wael Alhallaq, and Firas

Department of Science and Environment, Roskilde University

Bidrag til konferencer og kongresser 2017:

Dorthe Posselt:

Nordic workshop on Scattering from Soft and Biological Matter, Oslo University, January 12-13
'Restructuring in block copolymer thin films: in-situ GISAXS investigations during solvent vapor annealing'

19th IUPAB congress and 11th EBSA congress, Edinburgh, July 16-20, 'Dynamics of Biological Membranes - Quasi Elastic Neutron Scattering Studies of Model Membranes'

Kristine Niss:

'Experimental support of the Isomorph Theory', The 8th International Discussion Meeting on Relaxations in Complex Systems, Wisla, Poland, 23.-29.7.2017

'Dynamics of glass-forming liquids — from picosecond to kilosecond', Danish Physical Society, Annual Meeting, Nyborg, Denmark, 22.7.-23.5.2017

Henriette Wase Hansen:

8th International Discussion Meeting on Relaxations in Complex Systems, 23-28 July, Wisla, Poland,
"Isochronal study with combined neutron and dielectric spectroscopy"

International Conference on Neutron Scattering, 9-13 July, Daejeon, Korea:
"Isomorphs in glass-forming liquids"

DanScatt Annual meeting, 1-2 June, Odense, Denmark:
"Dynamics in glass-forming liquids under pressure from second to picosecond"

Danish Physical Society, 22-23 May, Fænø Sund, Denmark:
"High-pressure neutron experiments on glass-forming liquids"

Dynamics of Glass-forming Liquids: Will Theory and Experiment Ever Meet? 5-7 April 2017, Carlsberg Academy, Copenhagen, Denmark:
"Isochronal superposition on second and picosecond timescales"

Anden formidling/outreach, m.v. (tv, radio, kronikker, foredrag, osv.):

Alejandro Sanz: Member of the college 6 (Structure and dynamics of liquids and glasses) for evaluating proposals at the ILL.

Dorthe Posselt: SYNKNØYT panel - Det Norske Forskningsråd.

Undervisning og kurser (Ph.d.-skoler og –kurser, sommerskoler, andet):

Dorthe Posselt: Cross-institutional Mastercourse: Applications of X-ray and neutron scattering in biology, chemistry and physics, August 2017

Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

Bidrag til konferencer og kongresser:

Competitive reactions during the synthesis of layered double hydroxides by the urea method, Ulla Gro Nielsen, 16th International Clay Conference, Granada, Spain, July 2017.

Solving structural ambiguities in layered double hydroxides by solid state NMR in combination with other experimental techniques, Ulla Gro Nielsen, 10th Alpine Conference on Solid State NMR, Chamonix-Mt Blanc, September 2017.

Power at the atomic scale – Designing new materials for rechargeable batteries, Dorthe B. Ravnsbæk, Kemisk Forenings Årsmøde 2017, Syddansk Universitet, Odense, Denmark, 15. Juni 2017.

Battery research at SDU, Dorthe B. Ravnsbæk, Danish Battery Society Annual Meeting 2017, Syddansk Universitet, Odense, Denmark, 6. Marts 2017.

A Biomimetic Circular Atom Economy, Christine McKenzie, Plenary Annual Danish Chemistry Society meeting, Odense, Denmark, June 15, 2017.

Halogen Bonding Traps an Iron Catalyst-Hypervalent Iodine Adduct, Annual DANSCATT meeting, Odense, Denmark, May 2, 2017.

O. Renault, C. Zborowski, P. Risterucci, G. Grenet, S. Tougaard, QUANTITATIVE HAXPES FROM INELASTICALLY-SCATTERED PHOTOELECTRONS INVESTIGATIONS OF DEEPLY BURIED INTERFACES IN NANO-ELECTRONIC DEVICES, American Vacuum Society meeting AVS 64 October 29th – November 3rd, 2017 in Tampa, Florida.

C. Zborowski, O. Renault, A. Torres, C. Guedj, Y. Yamashita, G. Grenet, S. Tougaard, INELASTIC BACKGROUND ANALYSIS IN HAXPES USING A REFERENCE SAMPLE, ECASIA 2017 (17th European Conference on Applications of Surface and Interface Analysis), 24-29/9 in Montpellier, France.

Undervisning og kurser (Ph.d.-skoler og –kurser, sommerskoler, andet):

Looking inside running batteries – Operando X-ray diffraction of future electrode materials, Dorthe B. Ravnsbæk, Materials for Energy Applications through Neutron and X-Ray Eyes, Workshop by Interreg project MAX4ESSFUN and the Nordforsk Neutron Network on Functional Materials, Göteborg 22nd-23rd of May 2017 at Chalmers University of Technology, Göteborg, Sweden

Navne på MSc kandidater og BSc (afsluttede):

MSc: Jonas Hyldahl Christensen, Christian Henriksen

BSc: Martin Aaskov Karlsen, Anders Kring Clausen, Christian Lund Jakobsen