

# Rapport skema

Styrelsen for Forskning og Innovation  
Bredgade 40  
1260 København K



Dato:

Formålet med denne faglige rapportering er: 1) at vurdere bevillingen i forhold til ansøgningen, herunder vurdere ressourcernes anvendelse i forhold til bevillingens resultater, 2) at give mulighed for at afslutte bevillingen med godkendelse.

Angiv det relevante faglige råd eller den relevante programkomite

## 1. Grundoplysninger

Bevillingens titel:

Sagsnr. (fx 09-012345)

Bevillingshavers navn og stilling

Arbejdsplads (adresse, telefon og email)

Bevillingens hjemmeside hvis relevant

Virkemiddel

## 2. Bevillingsperiode

Oprindelig bevillingsperiode Fra:  Til:

Seneste godkendte bevillingsperiode Fra:  Til:

Årsager til eventuelle væsentlige ændringer i bevillingsperioden

### 3. Partnere/ledelse

Deltagende partnere, f.eks. universiteter, virksomheder og offentlige institutioner, herunder internationale partnere. Angiv oprindelige partnere og forklar evt. senere væsentlige ændringer i deltagerkredsens sammensætning:

Se Bilag 1 for en fuldstændig liste over personer der i 2016 har deltaget i aktiviteter med relation til DANSCATT.

DANSCATT har i 2016 haft følgende deltagende partnere:

DTU, KU, AU, RUC, SDU, Haldor Topsøe A/S.

DANSCATTs bestyrelse har fra 1 januar 2017 følgende medlemmer:

Formand Henning Friis Poulsen, DTU Fysik  
Næstformand Kell Mortensen, KU Niels Bohr Institutet  
Niels Bech Christensen, DTU Fysik  
Michael Gajhede, KU Lægemedeldesign og Farmakologi  
Pernille Harris, DTU Kemi  
Bo Brummerstedt Iversen, AU Kemi  
Sine Larsen, KU Kemi  
Kim Lefmann, KU Niels Bohr Institutet  
Alfons Molenbroek, Haldor Topsøe A/S  
Martin Meedom Nielsen, DTU Fysik  
Søren Thirup, AU Molekylærbiologi og Genetik  
Dorthe B. Ravnsbæk, SDU Fysik, Kemi, Farmaci  
Dorthe Posselt, RUC Institut for Naturvidenskab og Miljø  
Jimmy Binderup Andersen, Foreningen LINX  
Morten Scharff, Repræsentant for Uddannelses- og forskningsministeriet

Anfør væsentlige ændringer i bevillingens ledelse, herunder personer, struktur og proces.

Ved udgangen af 2016 udtræder Robert Feidenhans'1 af bestyrelsen. Fra 2017 indtræder 4 nye medlemmer i bestyrelsen:

Dorthe B. Ravnsbæk, SDU Fysik, Kemi, Farmaci  
Dorthe Posselt, RUC Institut for Naturvidenskab og Miljø  
Jimmy Binderup Andersen, Foreningen LINX  
Morten Scharff, Repræsentant for Uddannelses- og forskningsministeriet

### 4. Økonomi

Oprindeligt bevilget beløb (kr.)

Ekskl. overhead:

4.000.000

Inkl. overhead:

4.000.000

Eventuel tillægsbevilling (kr.)

Ekskl. overhead:

Inkl. overhead:

Forklar væsentlige afvigelser mellem budget og regnskab og i givet fald årsagerne hertil

Eventuel medfinansiering - fra arbejdssted eller anden side (kr.)

### 5. Kvalitativ afrapportering ved bevilling fra Det Frie Forskningsråd

Skriv i feltet herunder en kort beskrivelse af projektførløbet. Beskrivelsen skal være på ca. 2.000 anslag og indeholde:

- projektets formål (inkl. hypotese, teori, metoder og data)
- en redegørelse for eventuelle videnskabelige afvigelser fra den oprindelige projektplan samt en forklaring på disse
- en beskrivelse af de væsentligste resultater og hvordan de bidrog til realiseringen af projektets formål/ testede projektets hypoteser
- en redegørelse for eventuelle nye, videnskabelige spørgsmål projektets resultater medfører, eller om du har identificeret nye forskningsbehov i løbet af projektet.

The Danish community of users of large scale X-ray and Neutron facilities are organized within the instrument centre DANSCATT. The user community span from Biology, Chemistry, Physics, materials science over food science and pharmacy to industrial applications, including several companies. The main activity of DANSCATT is to facilitate access to the international large scale facilities with beamtime granted via peer review. A substantial part of the funding is hence directly targeted to support travel cost.

DANSCATT is also supporting training of younger scientists at the PSI in Switzerland, in order to assure preferred access for Danish user groups to this facility. The access is essential for the Danish user groups to be at the forefront of science and to allow the building up of capacity and competence of the users community towards the spallation source ESS in Lund and the X-ray free-electron laser E-XFEL in Hamburg.

DANSCATT organizes and structures the community and is enabling interdisciplinary projects via its network activities. Denmark is a member of the facilities ESRF and ILL in Grenoble and European XFEL in Hamburg. The board of DANSCATT acts as a supervisory board of the Danish participation in order to maximize the impact. The DANSCATT board also interacts closely with the Danish Ministry concerning issues related to the facilities.

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## **5. Kvalitativ afrapportering ved bevilling fra Det Strategiske Forskningsråd**

Rapporteres i et separat bilag med mulighed for indsættelse af figurer, mm. (max 5 sider).

Den kvalitative afrapportering bør som minimum beskrive og vurdere den gennemførte aktivitet inden for følgende områder:

- Forskningsmæssige resultater
- Erhvervs-mæssige-samfundsmæssige resultater
- Forskeruddannelse
- Samarbejde, herunder tværinstitutionelt, tværdisciplinært og internationalt samarbejde

## Kvantitativ afrapportering (Du anbefales for hver rubrik at afrapportere i punktopstilling)

### 6. Stipendier

Ph.d.-stipendier/grader og postdocstipendier (navne, cpr-nr, arbejdsplads, antal måneder finansieret af bevillingen, nationalitet, køn (M/K))

Ved samfinansiering med EU CoFUND-midler er der i 2016 finansieret to postdocs af bevillingen:  
Postdoc Jonas Okkels Birk (M, Danmark, cpr. 160480-2799), Paul Scherrer Institutet, 12 måneder  
Postdoc Emmanuel Canevet (M, Frankrig, fødselsdato 15.03.1983), Paul Scherrer Institutet, 12 måneder

### 7. Publikationer affødt af det finansierede projekt

Vejledning:

Oversigten er udarbejdet i overensstemmelse med universiteternes registreringssystem for publikationer og følger samme definitioner af publikationstyper. Kun de publikationstyper, som er væsentligst for Det Frie Forskningsråd/Det Strategiske Forskningsråd, er omfattet. For hver publikationstype skal angives forfatter, titel, sideantal, evt. tidsskrift og årstal. Desuden skal der for hver publikation angives evt. publicering i Open Acces (OA), samt hvor stor andel af publikationen, der skønsmæssigt er finansieret af bevillingen i procent (X %).

#### Videnskabelig formidling

Artikler, peer reviewed

Se Bilag 2 (indeholder 270 peer-reviewede artikler; estimeret til 240 når sampublikationer mellem institutioner fraregnes)

Artikler, ikke peer reviewed

Doktordisputatser

Ph.d.-afhandlinger

Se Bilag 3.

Videnskabelige bøger/antologier

Videnskabelige rapporter

Se Bilag 4.

Bidrag til bøger/antologier/rapporter

Working papers/arbejdsrapporter/preprints

Konferenceartikler, peer reviewed

Se Bilag 4.

Konferenceartikler, ikke peer reviewed

Patenter, patentansøgninger

The crystal structure of dopamine  $\beta$ -hydroxylase; European patent application No. 16164227.7 filed on 7th April 2016, DTU Kemi

Datasæt (x hvis afleveret til Dansk Data Arkiv)

Planlagte publikationer (angiv type)

#### Anden formidling

Fx forskningsformidlende bøger/antologier, kronikker, tv, mm.

Se Bilag 4 for flere formidlingsaktiviteter.

Lo Leggio, L., Tovborg, M., Johansen, K.S. (2016) Enzymatisk nedbrydning af polysaccharider, Dansk Kemi 97, 23-25 (in danish).

Kirsten M. Ø. Jensen: Udtalelse til artikel i Weekendavisen: Til Lysfest i Lund, 24. juni 2016.

Kirsten M. Ø. Jensen: Foredrag ved 'Senioruniversitetet Værløse', 21 og 24 November, 2016. 2 foredrag af 90 minutter.

Interview til Weekendavisen vedr. MAX-IV (Til lysfest i Lund af Annette K. Nielsen) 29-06-2016.

Magneter, Mogens Chrisensen, High school visit, Deutches Gymnasium Aabenraa, AU

Materialeforskning ved verdens kraftigste neutronkilde, Mogens Christensen, Forsknings Døgn 2016

Ekspllosivstoffer: Om eksplosivstofferne kemi, virkemåde og kulturhistorie, Peter Hald, UNF Odense: Eksplosivstoffer

Et nyt energisystem, Torben René Jensen, Gymnasieforedrag, Teknisk Gymnasium Viby J

Dorthe B. Ravnsbæk, "Bedre og billigere batteries", Folkeuniversitet, Aarhus 12. October 2016 and Emdrup 17. November 2016

Interview on TV2 News, 8 minutes on scientific breakthrough,  
<http://livsstil.tv2.dk/sundhed/2016-04-08-danske-og-engelske-forskere-finder-enzym-kan-behandle-depressioner-og-adhd>, DTU Kemi

Videnskabs Verden DR P1, Danish radio broadcast, half hour interview and feature, <http://www.dr.dk/radio/ondemand/p1/videnskabs-verden-2016-05-10#!/>, DTU Kemi

News radio broadcast, DR P1 and P4, in Danish.  
ScienceNordic.com, featured research,  
<http://sciencenordic.com/breakthrough-depression-schizophrenia-and-high-blood-pressure>.

Videnskab.dk, featured research, in Danish,  
<http://videnskab.dk/krop-sundhed/gennembrud-adhd-skizofreni-og-forhojet-blodtryk>.

Martin Meedom Nielsen, 6. oktober 2016, interview med Die Zeit: <http://www.zeit.de/2016/42/photovoltaik-roentgen-laser-european-xfel-probebetrieb>

Kristoffer Haldrup, 15. oktober 2016, interview med Kristeligt Dagblad: <https://www.kristeligt-dagblad.dk/viden-forskning/et-skridt-mod-endoloese-maengder-af-gratis-energi>

Kristoffer Haldrup, Interview på DR2 21. juni 2016, om åbningen af MaxIV.

Carsten Gundlach, 26/8-2016: 'Røntgen mikrotomografi', Foredrag hos Odense By museer

## Rådgivning

Fx artikler, videnskabelige rapporter, mm.

Se Bilag 4

## Undervisning

Fx lærebøger, kompendier, kurser, kandidatuddannelser

DANSCATT bidrager til at en lang række studerende på ph.d.-, kandidat- og bachelorniveau kan deltage i måletidsrejser.

Der er blevet uddannet mere end 76 MSc og BSc inden for DANSCATTs område i 2016 (ikke alle er oplyst).

DANSCATT har desuden bidraget til ph.d.-kurser og flere kurser, også på kandidat- og bachelorniveau. Se Bilag 4:

Cross-institutional Mastercourse: Applications of X-ray and neutron scattering in biology, chemistry and physics, August 2016, RUC

Cross-institutional PhD course: Molecular Biophysics, October 2016, RUC

Christine McKenzie, KE810 Bioinorganic Chemistry (PhD course at SDU where synchrotron methods are covered), SDU

Christine McKenzie, Training School EPR and Mössbauer Spectroscopy, Max Planck Institute, Mülheim, Germany, 14-16 December, 2016, SDU

Applications of X-ray and neutron scattering in biology, chemistry and physics. (KU & DTU), DTU Kemi

## 8. Andre resultater/spin off affødt af projektet

Nye samarbejder nationalt og internationalt

Nye ansøgninger, der er direkte afledt af bevillingens resultater

Ny finansiering, baseret på bevillingens resultater

Nye teknologier, metoder, processer, mv. baseret på bevillingens resultater

Nye produkter, baseret på bevillingens resultater

Nye virksomheder, baseret på bevillingens resultater

## 9. Formidlingseget sammenfatning egnet til offentliggørelse på [www.fi.dk](http://www.fi.dk) (udfyldes kun, når skemaet bruges til faglig slutrapportering)

Vejledning:

Beskriv på en enkel og forståelig måde det gennemførte forskningsprojekt 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](http://www.fi.dk). Beskrivelsen bør tage udgangspunkt i følgende spørgsmål:

- Hvad handler dit forskningsprojekt om?
- Hvad er formålet med dit projekt?
- Har dit projekt ført til interessant ny viden?
- Hvad er de vigtigste problemstillinger i projektet?
- Hvilke spændende perspektiver ser du i dit projekt?
- Vil dit projekt kunne få en samfundsmæssig betydning?
- Fører dit projekt til nye forskningsprojekter?

Formidlingseget præsentation på både dansk og engelsk (se vejledning herover):

Fremtidens avancerede materialer og lægemidler vil kræve større forståelse af materialer og biologiske systemer på nanometer og molekylær skala. Røntgen- og neutronstråling er to vigtige redskaber, som kan give os denne information. Målingerne foretages i dag ikke længere i laboratoriet, men ved store internationale forskningsfaciliteter. Apparatet og opstillingerne er blevet så store og avancerede, at de enkelte forskergrupper ikke længere har mulighederne for selv at anskaffe dem. DANSCATT's hovedformål er at sikre danske brugergrupper adgang til de bedste faciliteter ved bl.a. at støtte målrejser til disse faciliteter. Danmark er p.t. medlem af faciliteterne ESRF og ILL i Grenoble og European XFEL i Hamborg. Danmark er desuden medvært ved den Europæiske Spallationskilde ESS i Lund. DANSCATT sikrer den langsigtede danske kompetence inden for området, som vil give størst gennemslagskraft for danske grupper, inklusiv virksomheder, ved de nye faciliteter.

Detailed structural information on the molecular and atomic level is a prerequisite to develop new functional materials or

pharmaceutical products. Synchrotron X-ray and neutron radiation are unique techniques to provide this information. The equipment has become so advanced - and expensive - that individual research groups cannot acquire nor run such facilities. DANSCATT ensures access and supports beamtime travels to international facilities. Denmark is currently a member of the facilities ESRF and ILL in Grenoble and the European XFEL in Hamburg. Furthermore, Denmark is co-hosting the European Spallation Source (ESS) in Lund. DANSCATT serve to maximize the impact of Danish research groups and companies at these facilities and to ensure that qualifications and know-how in this area remain at an internationally leading position.

Maks. 5 vigtigste publikationer

1. Larsen, Andreas N.; Sørensen, Kasper K.; Johansen, Nicolai T.; Martel, Anne; Kirkensgaard, Jacob J. K.; Jensen, Knud J.; Arleth, Lise; Midtgaard, Søren Roi. Dimeric peptides with three different linkers self-assemble with phospholipids to form peptide nanodiscs that stabilize membrane proteins. *SOFT MATTER* 12, 27, 5937-5949, 2016. DOI <http://dx.doi.org/10.1039/c6sm00495d>
2. Tim B. van Driel, Kasper S. Kjær, Robert Hartsock, Asmus O. Dohn, Tobias Harlang, Matthieu Chollet, Morten Christensen, Wojciech Gawelda, Niels E. Henriksen, Jong Goo Kim, Kristoffer Haldrup, Kyung Hwan Kim, Hyotcherl Ihee, Jeongho Kim Henrik Lemke, Zheng Sun, Villy Sundstrom, Wenkai Zhang, Diling Zhu, Klaus B. Møller, Martin M. Nielsen\* and Kelly J. Gaffney\*, Atomistic characterization of the active-site solvation dynamics of a model photocatalyst, *Nature Comm*, 13678 (2016), DOI: 10.1038/ncomms13678.
3. Trine V. Vendelboe, Pernille Harris, Yuguang Zhao, Thomas S. Walter, Karl Harlos, Kamel El Omari, and Hans E. M. Christensen The crystal structure of human dopamine  $\beta$ -hydroxylase at 2.9 Å resolution *Sci Adv.* 2016 Apr; 2(4): e1500980.
4. Zhang, J., Song, L., Madsen, G. K. H., Fischer, K. F. F., Zhang, W., Shi, X. and Iversen, B. B. (2016) Designing high-performance layered thermoelectric materials through orbital engineering, *Nature Commun.* 7, 10892, doi: 10.1038/ncomms10892
5. Malinauskaite, L., Said, S., Sahin, C., Grouleff, J., Shahsavari, A., Bjerregaard, H., Noer, P., Severinsen, K., Boesen, T., Schiott, B., Sinning, S., and Nissen, P. (2016) A conserved leucine occupies the empty substrate site of LeuT in the Na(+)-free return state, *Nature communications* 7, 11673.

Andre væsentlige resultater

Gem som

Reset Form

Bilag 1: DANSCATT personoversigt 2016

<b>Groupleader</b>	<b>VIP's (Professors, Senior scientists etc.)</b>	<b>Postdocs / assistant professors</b>	<b>PhD students</b>	<b>Students</b>	<b>TAP's (Technicians, Administrative staff etc.) and Scientific assistants</b>
<p><b>Søren S. Thirup</b> Dept. of Molecular Biology, Aarhus University</p>	<p>Ditlev E. Brodersen C. B. F. Andersen Gregers R. Andersen Lasse B. Jenner Poul Nissen Rune Hartmann Søren S. Thirup Thomas Boesen</p>	<p>Andreas Bøggild Antoni Kowalski Azadeh Shahsavar B.P.Pedersen Claus Olesen Dovile Janulienė Hans Henrik Gad Henriette E. Autzen Ingrid Dach Jacob L. Andersen Jakob Mikkelsen Jonas L. Gregersen Joseph Lyons Kasper R. Andersen Kasper Runager Kira Gysel Kristian Stødkilde Maja H. Nielsen Manuela Gorgel Meriem Senissar Nick S. Laursen Peter Paulsen Prasad Kasaragod Rune Kidmose</p>	<p>Alessandro Zarantonello Aljona Kotsubei Andreas Holleufer Caroline Neumann Casper Larsen Dennis V. Pedersen Dorota Focht Ewa Terczynska-Dyla Goran Bajic Hao Zhou Helle Gotfred-Rasmussen Jacob Ulstrup Janus A. Schatz-Jacobsen Jaslyn M. Wong Jeryl X.J. Cheng Joachim Vilstrup Josephine Nissen Marlene Sørensen Mateusz Dyla Melek Cemre Manav Mikael Winkler Milena Laban Rasmus K. Jensen Rasmus Kock Flygaard Sigrid T. Larsen S. Sirotkina Tania Custodio Trine Gadeberg</p>	<p>Aljona Kotsubei Jeppe A. Nielsen Mette Berendtsen Sara Basse Simon B. Hansen</p>	<p>Anne Marie Nielsen Dorthe J. Strandbygaard Jesper L. Karlsen K. M. Nielsen Lan B. Van Lotte T. Pedersen Tetyana Klymchuk</p>



Bilag 1: DANSCATT personoversigt 2016

<p><b>Bo Brummerstedt Iversen,</b> Dept. of Chemistry, Aarhus University</p>	<p>Bo Brummerstedt Iversen Hai-Wen Li Henrik Birkedal Hidetaka Kasai Jacob Overgaard Jens-Erik Jørgensen Martin Bremholm Mogens Christensen Torben R. Jensen</p>	<p>Alberto Biancoli Ann-Christin Dippel Bjarne R. S. Hansen Chen Gao Dipankar Saha Espen D. Bøjesen Espen Eikeland Fiona Bach-Gansmo Hao Yin Hazel Reardon Lars H. Jepsen Mads Ry Jørgensen Marian Stingaciu Mark Paskevicius Mattia Sist Mette S. Filsø Mie Birkbak Morten B. Nielsen Nina Kølln-Wittig Peter Nørby Samera Siddiqui Sebastian Christensen Simon Frølich Simone Sanna Tan-Phat Huynh Venkatesha Hathwar Yigang Yan</p>	<p>Casper W. Andersen Casper Ibsen Cecilia Granados Miralles Christian Zeuthen Elisabeth Grube Ellen Jensen Elsa Roedern Emil Damgaard-Møller Erika Dematteis Fillippo Peru Henriette Ravn Henrik Hellstern Henrik L. Andersen Hosein Payandeh Jakob Ahlburg Jiawei Zhang Karl F. Fischer Kasper Møller Kasper Tolborg Lirong Song Maika Klemmer Maja Krüger Thomsen Martin Bondesgaard Martin Roelsgaard Mathias Jørgensen Matilde Saura Nanna Wahlberg Nils Lau Nyborg Broge Nikolaj Roth Payam Javadian Priscilla Huen Seyed Hossein Payandeh Simone M. Søndergaard-Pedersen Steffen R. Jensen Steinar Birgisson</p>	<p>Ahmad Rinno Alexander Sangsong Fogh Anders S. Jakobsen Andreas Paul Anette G. Keilland Bjarke Svane-Boysen Camilla Hjort Kronbo Emil Andreasen Klahn Frederik Gjørup Frederik Munkholm Søndergaard-Pedersen Hjalte Reuss Schmidt Ida Gjerlevsen Nielsen Jacob Ginnerup Andreasen Jakob Bæk Grinderslev Jakob Mikkelsen Jakob Sigvardt Jinlong Yu Jonas Beyer Jonas Palle Kirstine Dalgaard Krista Nielsen Lasse Rabøl Jørgensen Line Bilgrav Nielsen Louise Møller Malene Laugesen Mathilde Holm Nygaard Matthew Craven Mette Borup Niels Frederik-Juhl Niklas Durhuus Vichairat Rolf Kjeldsen Simon Fruergaard Simon Helming Nielsen</p>	<p>Anna Zink Aref Mamakhel Bo Richter Britta Lundtoft Jacob Becker Marianne Sommer Peter Hald</p>
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Bilag 1: DANSCATT personoversigt 2016

			Vicki Nue	Solveig Kjeldgaard Steffan Schmidt Steffen Pedersen Sven Lemming Overgaard Søren Haugaard Madsen Troels Christiansen	
<b>Henning Friis Poulsen,</b> DTU Physics, DTU Wind, DTU Cen, DANCHIP, and DTU Energy, Technical University of Denmark	Anders Dahl Bente Lebech Cathrine Frandsen Didier Blanchard Dorte Juul Jensen Henning Friis Poulsen Innokenty Kantor Jacob Ross Bowen Jean-Claude Grivel Jens Wenzel Andreasen Kristoffer Haldrup Luise Theil Kuhn Martin Meedom Nielsen Matti Knaapila Niels Bech Christensen Peter Stanley Jørgensen Rune E. Johnsen Søren Fæster Søren Schmidt Tianbo Yu Yubin Zhang	Anders Clemen Jakobsen Anders Filsøe Pedersen Christian Rein Hugh Simons Kasper Skov Kjær Malgorzata Makowska Mika Torkkeli Morten Sales Nicolai Fog Gade-Nielsen Rasmus Toft-Petersen Rosa Barabash Tobias Harlang	Alberto Cereser Chaoling Xu Diana Zederkof Elisa Biasin Ellen Fogh Frederik Beyer Hansen Giovanni Fevola Jessica Lefevre Jin Zhang José Xavier Sierra Trujillo Jun Sun Lea Hildebrandt Rossander Mads Laursen Marta Majkut Mathias Kure Peter Mahler Larsen Peter Vester Salvatore De Angelis Sonja Rosenlund Ahl Tiago Ramos Yuri Aparecido Opata	Andreas Lauritzen Julia Dyrnum Kimmie K. Moerner Mariana Mar Lucas Mathias Huss-Hansen Michael Korning Sørensen	Carsten Gundlach Erik Knudsen Finn Saxild Hanne Sørensen Jette Oddershede John Johnson Marianne Sundby Peter Kjær Willendrup
<b>Wolfgang Pantleon</b> DTU Mechanical Engineering, Technical University of Denmark	Grethe Winther Jesper Hattel Karen Pantleon Marcel Somers Thomas Christiansen Wolfgang Pantleon	Matteo Villa Chitta Ranjan Das	Annika Martina Diederichs Federico Bottoli Frank Nissen Nikolai Ytterdal Juul Sunday Chukwudi Okoro Toto Andriollo		Flemming Bjerg Grumsen

Bilag 1: DANSCATT personoversigt 2016

<p><b>Kenny Ståhl</b> DTU Chemistry, Technical University of Denmark</p>	<p>Hans Mølager Christensen Kenny Ståhl Klaus B. Møller Pernille Harris René Wugt Larsen</p>	<p>Asmus O. Dohn Christian Engelbrekt Jonas Andersen Mátyás Imre Pápai Sanaullah Kahn</p>	<p>Alina Kulakova Gianluca Levi Kasper Tidemand Line Ryberg Mats Simmermacher Mostafa Abedi Nicklas Skjoldager Pernille Sønderby Sowmya Indrakumar Sujata Mahapatra Ulf Molich</p>	<p>Christian Sørensen Kathrine Øgendahl Laura Aaboe Andersen</p>	<p>Maria Blanner</p>
<p><b>Anker Degn Jensen</b> DTU Chemical Engineering, Technical University of Denmark</p>	<p>Anker Degn Jensen Jakob Munkholt Christensen</p>	<p>Martin Høj</p>	<p>Kristian Viegaard Raun Trine Arndal</p>		
<p><b>Finn Christensen</b> DTU Space, Technical University of Denmark</p>	<p>Finn Christensen Desiree Ferreira</p>		<p>Sonny Massahi Chantal Silvestre</p>		
<p><b>Kell Mortensen</b> Niels Bohr Institute, University of Copenhagen</p>	<p>Brian M Andersen Heloisa N. Bordallo Jacob Kirkensgaard Jens Als-Nielsen Kell Mortensen Kim Lefmann Linda Udby Lise Arleth Robert Feidenhansl</p>	<p>Alexander Karl Ingemar Björling Astrid Tranum Rømer Erik Brok Murillo Longo Martins Nicholas Skar-Gislinge Sergey Kaphisnikov Søren Roi Midtgaard</p>	<p>Anton Kovyakh Aghiad Ghazal Andreas Nørgård Larsen Anine Borger Anna Fedrigo Everton Carvalho dos Santos Dainius Jakubauskas Erik Dreier Christensen</p>	<p>Camilla Buhl Larsen Erik Dreier Christensen Johannes Martiny Morten Sales Rosanna Ignazzi</p>	<p>Keld Theodor Marianne Jensen</p>

Bilag 1: DANSCATT personoversigt 2016

	Steen Hansen Prof Poul Erik Lindelof		Frederik Grønbæk Tidemand Henrik Jacobsen Johannes Beil Jose Enedilton Medeiros Pereira Julie Hougaard Overgaard Kristian Romlund Rix Mads Bertelsen Marcella Berg Morten Holm Christensen Nicolai Tidemand Johansen Pia Jensen Ray Sonja Lindahl Holm Torsten Lauridsen Ursula Bengård Hansen		
<b>Michael Gajhede</b> Dept. of Drug Design and Pharmacology, University of Copenhagen	Bente Vestergaard Jette S. Kastrup Karla Frydenvang Michael Gajhede Ole Kristensen Osman Mirza	Carlotta Marasini Jerzy Dorosz Saara Laulumaa Saskia Bucciarelli Thor Seneca Thorsen	Ersoy Cholak Anja P. Larsen Kirstine Bendtsen Nils Skovgaard Sarah Jones Stine Møllerud Thomas S. Petersen	Abdallah Abdulrahman Adriana Lauroba Arpan Sharma Aura Leahu Kristoffer Brasen Daniel Rønnow Schacht Mathias Poulsen Sebastian Winther	

Bilag 1: DANSCATT personoversigt 2016

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## Danscatt ph.d.-projekter 2016

### DTU Mechanical Engineering, Technical University of Denmark

Sunday Chukwudi Okoro, High-temperature corrosion on biodust firing

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Chaoling XU, Nucleation of recrystallization at selected sites in deformed fcc metals. DTU Wind Energy

### DTU Energy, Technical University of Denmark

Mie Møller Storm, *Preparation and Characterization of Cathode Materials for Lithium-Oxygen Batteries.*  
Malgorzata Grazyna Makowska, *In situ Neutron Imaging of Solid Oxide Fuel Cells.*

### DTU Chemistry, Technical University of Denmark

Pernille Sønderby, Solution behaviour of Human Serum Albumin and GLP-1 variants, DTU Chemistry

### DTU Physics, CEN and DANCHIP, Technical University of Denmark

Pedersen, Anders Filsøe; **Elucidating oxygen electrocatalysis with synchrotron X-rays: PEM fuel cells and electrolyzers : An experimental study.** Department of Physics, Technical University of Denmark, 2016. 291 p.

Majkut, Marta; **Mapping of strain mechanisms in barium titanate by three-dimensional X-ray diffraction.** Department of Physics, Technical University of Denmark, 2016. 159 p.

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### Dept. of Pharmacy, University of Copenhagen

Intan Diana Mat Azmi, Soft Cubosome and Hexosome Nanocarrier Design for Drug Delivery  
Aghiad Ghazal, Combination of SAXS with microfluidics for investigation pharmaceutical formulations  
Shen Yu Helvig, NANO-engineered LYMPHOTROPIC Cubosomes and Hexosomes

Mark Gontsarik, Tailoring Antimicrobial Peptides for Bacteria Membrane Destruction.

**Affiliation:** Laboratory for Biointerfaces, Empa, Swiss Federal Laboratories for Materials Science and Technology, Lerchenfeldstrasse 5, 9014 St. Gallen, Switzerland

### **Dept. of Chemistry, University of Copenhagen**

Diwaker Jha, *Improved flow property determination from nanotomography of porous media* Reza Gooya, *Improved Insight into Transport Phenomena in Porous Materials at Submicrometer Resolution*

Kristian E. H. Frandsen, *Structural characterization of Lytic Polysaccharide MonoOxygenases - Enzymatic interactions with lignocellulosic- and starch substrates*

Andreas Konstantatos, *Lanthanide Single-Molecule Magnets Framed by Alkali Metals & Magnetic and Spectroscopic Studies of 3d Transition Metal Complexes*

### **Niels Bohr Institute, University of Copenhagen**

Morten Sales (KL)

Development of Instrumentation for Spin-Echo Induced Spatial Beam Modulations for Small Angle Scattering Investigations

Thomas Stankevic (RF)

Nano-focused X-ray beam for mapping strain in core-shell nano-wires.

Mikkel Skov Nielsen (RF)

Applications of novel X-ray imaging modalities in food science

Sonja L Holm (KL)

Neutron scattering investigations of correlated electron systems and neutron instrumentation

Anna Fedrigo (KL)

Neutron Instrumentation and Neutron Investigation of Archaeometallurgical Arms and Armour

Henrik Jacobsen (KL)

Complex magnetic systems studied with neutron scattering

### **Dept. of Chemistry, Aarhus University**

Bjarne Hansen *"Synthesis and characterisation of metal boranes for energy storage"*, 2016, Aarhus Universitet.

Espen Eikeland *"Intermolecular interactions at high pressure – a crystallographic study"*, 2016, Aarhus Universitet.

Fiona Bach-Gansmo *"Bone ultrastructure with focus on osteocyte lacunae"*, 2016, Aarhus Universitet.

Mette Filsø *"Crystallographic studies of inter-atomic interactions and ion migration"*, 2016, Aarhus Universitet.



Mie Birkbak "*Multimodal X-ray imaging of hierarchical materials*", 2016, Aarhus Universitet.  
Morten Bormann Nielsen "*High pressure. A different approach to materials science*", 2016, Aarhus Universitet.

Simon Frølich "*Multiscale biological materials*", 2016, Aarhus Universitet.  
Vicki Nue "*Harnessing Catechol Chemistry for Material Design*", 2016, Aarhus Universitet.  
Nanna Wahlberg "Core electron density deformation from PXRD"

Henrik Hellstern "A dual stage hydrothermal flow reactor for green and sustainable synthesis of hybrid nanomaterials"

### **Dept. of Physics, Chemistry and Pharmacy, University of Southern Denmark**

Chen Shen, "Active compounds in biomimetic membranes - translating external trigger signals into mechanical responses of a lipid matrix" PhD thesis 2016 (SDU).  
Suraj S.C. Pushparaj, "Structural investigations of layered double hydroxides" PhD thesis 2016 (SDU).

### **Dept. of Molecular Biology, Aarhus University**

Dorota Focht: Et strukturelt studie af substrat promiskuiteten i den bakterielle SLC6 homolog

Dennis Vestergaard Pedersen: Strukturelle og funktionelle studier af komplement faktor P og dets funktion som positiv regulator i det humane komplement system

Janus Asbjørn Schatz-Jakobsen: Strukturel beskrivelse af inhibering af den terminale del af komplement systemet

Maja Holch Nielsen: Strukturel analyse af antioxidant proteinet TSA2

Claus Tofting-Olesen: Studier af ikke-ribosomale peptid syntetaser

Mateusz Dyla: Pumpning af ioner på enkelt-molekyle niveau

Nicholas Egholm Sofos: Strukturel analyse af protein komplekset NEXT

Kehan Xu: Strukturelle studier af bakterielle toksin-antitoxin systemer – undersøgelse af VapC toksinets katalytiske mekanisme, samt auto-regulering af VapBC TA systemet

## Bilag 4: Danscatt Outreach, kurser, studenterafhandling, publikationer m.v. 2016

Dept. of Chemistry, Aarhus University

Bidrag til konferencer, kongresser m.m. 2016:

Title of event	Name(s) of speaker(s)	Venue	Date
A multitude of metal borohydrides; facile synthesis from the elements	Bo Richter	15th International Symposium on Metal-Hydrogen Systems, Interlaken, Schweiz	07/08/2016
The chemistry of nucleation	Bo Brummerstedt Iversen	Gilleleje, CINF summerschool	8/8/2016
Accurate crystallography Coppins style: densities, excited states and beyond crystals	Bo Brummerstedt Iversen	Buffalo, New York	22/10/2016
Disruptive Materials technologies	Bo Brummerstedt Iversen	DanicaPension, København	17/5/16
The chemistry of nucleation	Bo Brummerstedt Iversen	DESY, Hamborg	15/11/2016
Orbital engineering of thermoelectric materials	Bo Brummerstedt Iversen	Kirkenes, Norge	13/9/2016
The chemistry of nucleation	Bo Brummerstedt Iversen	Oxford University, UK	29/11/2016
The chemistry of nucleation	Bo Brummerstedt Iversen	Telluride, USA	3/8/2016
Accurate crystallography Coppins style: densities, excited states and beyond crystals	Bo Brummerstedt Iversen	Tsukuba, Japan	18/11/2016
The chemistry of nucleation	Bo Brummerstedt Iversen	University of Zurich, Schweiz	16/11/2016
Application of powder X-ray diffraction in materials science	Mads Ry Vogel Jørgensen	Sustain DTU - ATV conference - 2016	30/11/2016
Bimetallic Strontium/Samarium – Alkali Metal Borohydrides Adopting Perovskite Structures	Kasper Trans Møller	E-MRS 2016, Warszaw, Polen	19/09/2016
Multi-functional energy storage materials	Torben René Jensen	E-MRS 2016, Warszaw, Polen	19/09/2016

Bilag 4: Danscatt Outreach, kurser, studenterafhandling, publikationer m.v. 2016

Exchange-coupled magnets	Mogens Christensen	Danish Magnetic Association, Aarhus	01/05/2016
Experimental Electron Density of Low Barrier Hydrogen Bonds in $H_3Co(CN)_6$	Kasper Tolborg	30th European Crystallographic Meeting, Basel, Schweiz	28/08/2016
Intermolecular interactions at high pressure	Espen Zink Eikeland	30th European Crystallographic Meeting, Basel, Schweiz	28/08/2016
On the magnetic behaviour of unique linear Fe-complexes using the electron density	Jacob Overgaard	30th European Crystallographic Meeting, Basel, Schweiz	28/08/2016
HEIMDAL - In kind potential	Mogens Christensen	Danish Instrument Builders, København	25/01/2016
HEIMDAL – Neutron powder diffraction with extended length scale for ESS	Mogens Christensen	15th European Powder Diffraction Conference, Bari, Italien	12/06/2016
In situ crystal growth studies and the potential at ESS	Mogens Christensen	Mat2Cell, Uppsala, Sverige	6/10/2016
Exchange-spring Magnets for Increased Energy Product	Mogens Christensen	Danish Magnetic Association Meeting, Odense	24/11/2016
Insights into single molecule magnetism from charge and spin density studies	Jacob Overgaard	7th European Charge Density Meeting, Polen	26/06/2016
<i>Heat conduction in thermoelectric materials</i>	Mogens Christensen	Neutrons for Energy, Bad Reichenhall, Tyskland	18/07/2016
<i><math>M_2B_{10}H_{10} + MH</math> (<math>M = Li</math> and <math>Na</math>) composite under hydrogen pressure</i>	Steffen Jensen	15th International Symposium on Metal-Hydrogen Systems, Interlaken, Schweiz	07/08/2016
<i>New boron and nitrogen based metal hydrides</i>	Torben René Jensen	15th International Symposium on Metal-Hydrogen Systems, Interlaken, Schweiz	07/08/2016
<i>New directions for higher boranes</i>	Bjarne Rosenlund Søndertoft Hansen	15th International Symposium on Metal-Hydrogen Systems, Interlaken, Schweiz	07/08/2016
<i>Pressure Influence on Metal Borohydride Formation from Aluminium Boride and Metal Hydrides</i>	Kasper Trans Møller	15th International Symposium on Metal-Hydrogen Systems, Interlaken, Schweiz	07/08/2016
<i>Multi-functional energy storage materials</i>	Torben René Jensen	10th Int. Symposium Hydrogen & Energy, Zao, Japan	21/02/2016
<i>Nano-scale imaging of bone</i>	Nina Wittig	Novo Scholarship Symposium 2016, KBH	14/11/2016

Bilag 4: Danscatt Outreach, kurser, studenterafhandling, publikationer m.v. 2016

<i>New types of hydrides with high H<sub>2</sub> densities</i>	Torben René Jensen	Task 32 IEA HIA Expert Meeting, Sendai, Japan	26/02/2016
<i>When Electron Microscopy is not Enough - Unravelling the Chemistry of Nanoparticle Formation by In Situ Total X-ray Scattering</i>	Espen Drath Bøjesen	SCANDEM, Trondheim, Norge	06/06/2016
<i>Structure-property relations of perovskites - Polymorphism and High Pressure Studies of Iridates</i>	Martin Bremholm	15th European Powder Diffraction International Conference, Bari, Italy	12/06/2016
<i>Bone hierarchical structure investigated in 3D by nanotomography, diffraction/scattering computed tomography and X-ray fluorescence</i>	Henrik Birkedal	EMRS 2016, Fall Meeting, Warsaw, Poland	19/09/2016
<i>3D Structures of Biomineral Architectures by New X-ray Imaging Techniques</i>	Henrik Birkedal	Goldschmidt 2016, Yokohama, Japan	26/06/2016
<i>Attachment on the Rocks: The Adhesion System of Anomia</i>	Henrik Birkedal	Goldschmidt 2016, Yokohama, Japan	26/06/2016
<i>Diffraction Scattering Computed Tomography: Peering into Complex Materials</i>	Henrik Birkedal	EPDIC 15, Bari, Italy	12/06/2016
<i>Self-healing hydrogel materials inspired by blue mussel byssus chemistry</i>	Henrik Birkedal	Euro Bio-inspired Materials 2016, Potsdam, Germany	22/02/2016

**Other contributions:**

<b>Title of Contribution</b>	<b>Author (external authors in Italics)</b>	<b>Event and place</b>	<b>Date</b>
Diffraction scattering computed tomography	Henrik Birkedal	1st DANMAX User Meeting, University of Southern Denmark	03/02/2016
HEIMDAL – complementarities with X-rays	Mogens Christensen	1st DanMAX Users Meeting, Odense	03/02/2016
Material Chemistry in Batteries	Steinar Birgisson	Danish Chemical Society: Annual Meeting 2016, Odense	9/06/2016
Update on battery activities at CMC at AU	Steinar Birgisson	Danish Battery Symposium 2016, Lyngby, Danmark	07/04/2016
Pressure Influence on Metal Borohydride Formation from Aluminium Boride and Metal Hydrides	Kasper Trans Møller	Institute of Materials Research, Helmholtz-Zentrum Geesthacht, D-21502 Geesthacht	02/11/2016

Bilag 4: Danscatt Outreach, kurser, studenterafhandlinger, publikationer m.v. 2016

Pressure Influence on Metal Borohydride Formation from Aluminium Boride and Metal Hydrides	Kasper Trans Møller	iNANO Autumn School 2016, Farsø	07/10/2016
Multi-functional metal hydrides	Torben René Jensen	Curtin University of Technology, Australien	14/10/2016
Foredrag	Jacob Overgaard	Bremen University	05/12/2016
Foredrag	Jacob Overgaard	Physical Chemistry Colloquium Stuttgart University, Tyskland	19/01/2016
Study of higher boranes with metal hydrides under hydrogen pressure	Steffen Jensen	Diamond Seminar	16/06/2016
Exchange coupled magnets	Mogens Christensen	Aalborg University Department Meeting	27/04/2016
HEIMDAL – Neutron powder diffraction with extended length scale	Mogens Christensen	Danscatt Annual meeting 2016, Copenhagen , Danmark	26/05/2016
In operando studies of battery materials	Steinar Birgisson	CMC Annual Meeting 2016, Aarhus, Denmark	26/04/2016
Breaking the Wall of the Earth	Morten Bormann Nielsen	Falling Walls Lab Aarhus, Stakladen, Aarhus University	28/09/2016
Breaking the Wall of the Earth	Morten Bormann Nielsen	Falling Walls Lab Finals, Akademie der Künste, Berlin	08/11/2016

**Undervisning og kurser:**

<b>Description</b>	<b>Author (external authors in Italics)</b>	<b>Event and place</b>	<b>Date</b>
Foredragsholder	Jacob Overgaard	1st Robert Stewart School on Charge Densities, Nancy, Frankrig	23/08/2016

**Poster contributions:**

<b>Title of poster</b>	<b>Authors (external authors in Italics)</b>	<b>Event and place</b>	<b>Date</b>
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Bilag 4: Danscatt Outreach, kurser, studenterafhandlinger, publikationer m.v. 2016

<i>Novel Ammonium Metal Borohydrides</i>	Grinderslev, J. (Intern), Jepsen, L. H. (Intern), <i>Cerny, R. (Ekstern), Lee, Y. (Ekstern)</i> , Møller, K. T. (Intern), Jensen, T. R. (Intern)	Danscatt Annual meeting 2016, Copenhagen , Danmark	26/05/2016
<i>Novel Ammonium Metal Borohydrides</i>	Grinderslev, J. (Intern), Jepsen, L. H. (Intern), <i>Cerny, R. (Ekstern), Lee, Y. (Ekstern)</i> , Møller, K. T. (Intern), Jensen, T. R. (Intern).	Hydrides as Energy Materials	01/06/2016
In situ reduction of as-prepared $\gamma$ -Iron Oxide Nanoparticles	Garbus, P. G. (Intern), Ahlburg, J. (Intern), Christensen, M. (Intern), Andersen, H. L. (Intern), <i>Keller, L. (Ekstern)</i>	30th European Crystallographic Meeting, Basel, Schweiz.	28/08/2016
Heat management in high-pressure hydrogen tanks	Borg, E. (Intern), Jensen, T. R. (Intern)	Hydrides as Energy Materials	01/06/2016
Tuning the size and properties of magnetic CoFe <sub>2</sub> O <sub>4</sub> nanocrystallites	Andersen, H. L. (Intern)	iNANO Autumn School 2016, Farsø, Danmark.	07/10/2016
RuAs <sub>2</sub> - A thermoelectric disappointment	Færch Fischer, K. F. (Intern), Iversen, B. B. (Intern)	1st International Summer School On Thermoelectrics, Golden, USA	25/07/2016
Metal-Organic Framework Nanosheets for Fast-Response and Highly Sensitive Luminescent Sensing of Fe <sup>3+</sup>	Xu, H. (Intern), Iversen, B. B. (Intern)	Danscatt Annual meeting 2016, Copenhagen , Danmark	26/05/2016
High pressure structural studies of two SrIrO <sub>3</sub> perovskite polymorphs	Kronbo, C. H. (Intern), Nielsen, M. B. (Intern), Munkholm Kevy, S. (Intern), <i>Parisiades, P. (Ekstern)</i> , Bremholm, M. (Intern)	Danscatt Annual meeting 2016, Copenhagen , Danmark	26/05/2016
Magnetic anisotropy in a dysprosium single molecule magnet	Klahn, E. A. (Intern)	DanScatt annual meeting, København, Danmark.	26/05/2016
High-pressure X-ray diffraction study of GaF <sub>3</sub>	Jørgensen, J. (Intern), <i>Filinchuk, Y. (Ekstern), Dmitriev, V. (Ekstern)</i>	15 <sup>TH</sup> European Powder Diffraction Conference, Italien	12/06/2016
Experimental Electron Density of Low Barrier Hydrogen Bonds in H <sub>3</sub> Co(CN) <sub>6</sub>	Tolborg, K. (Intern), Jørgensen, M. R. V. (Intern), Overgaard, J. (Intern), Iversen, B. B. (Intern)	7th European Charge Density Meeting, Polen.	26/06/2016

Synthesis and structure of Sr(BH <sub>4</sub> ) <sub>2</sub> -2NH <sub>3</sub> BH <sub>3</sub>	Jørgensen, M. (Intern), Jensen, T. R. (Intern)	15th International Symposium on Metal-Hydrogen Systems, Interlaken, Schweiz.	07/08/2016
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**Out-reach:**

Type of Communication/Subject/Topic	Contributor	Event and place	Date
Magneter	Mogens Chrisensen	High school visit, Deutches Gymnasium Aabenraa, AU	29/04/2016
Materialeforskning ved verdens kraftigste neutronkilde	Mogens Christensen	Forskningens Døgn 2016	19/01/2016
Eksplсивstoffer: Om eksplсивstofferne kemi, virkemåde og kulturhistorie	Peter Hald	Gymnasieforedrag, Institut for Kemi, AU	18/01/2016
Eksplсивstoffer: Om eksplсивstoffers kemi, virkemåde og kulturhistorie	Peter Hald	UNF Odense: Eksplсивstoffer	19/01/2016
Eksplсивstoffer: Om eksplсивstoffers virkemåde, kemi og kulturhistorie	Peter Hald	Gymnasieforedrag, Silkeborg Gymnasium	11/01/2016
Et nyt energisystem	Torben René Jensen	Gymnasieforedrag, Teknisk Gymnasium Viby J	10/05/2016

**BSc grader 2016:**

Ahmad Rinno "High pressure studies of Na<sub>2</sub>IrO<sub>3</sub> and NaIrO<sub>3</sub>", 2016, Aarhus Universitet. Andreas Paul "Single crystal crystallography", 2016, Aarhus Universitet.

Emil Andreasen Klahn "Determination of the anisotropic magnetic susceptibility in Dy(tBu-acac)<sub>3</sub>bpy as seen by polarized neutrons", 2016, Aarhus Universitet.

Frederik Gjørup "In-situ PXRD studie af udglødningen af magnetisk ordnet strontium hexaferrit nanopartikler", 2016, Aarhus Universitet.

Frederik Munkholm Søndergaard-Pedersen, "Preliminary PDF Study and Solvothermal Synthesis of Gamma Alumina", 2016, Aarhus Universitet.

Hjalte Reuss Schmidt "Investigation of Magnetic Properties through Topological Analysis", 2016, Aarhus Universitet.

Jacob Ginnerup Andreasen "Potassium Alanate as a Hydrogen Storage Material", 2016, Aarhus Universitet.

Jakob Mikkelsen "Negative thermal expansion of the protonated and Cu<sup>2+</sup>-exchanged chabazite zeolite", 2016, Aarhus Universitet.

Jonas Palle "Imaging of bone composition and nanocrystal properties", 2016, Aarhus Universitet.

Krista Nielsen "*Synthesis and Characterization of MOF MIL-125(Ti)*", 2016, Aarhus Universitet.

Jonas Beyer "*Advanced Rietveld Study of the Thermoelectric  $Ba_8Ga_{16+x}Ge_{30-x}$  Clathrate Structure*", 2016, Aarhus Universitet.

Lasse Rabøl Jørgensen "*Purification, Te-doping and High Temperature Stability Analysis of  $SrZn_2Sb_2$  Thermoelectric*", 2016, Aarhus Universitet.

Jonas Palle "*Imaging of bone composition and nanocrystal properties - A study of bone structure and composition by synchrotron X-ray diffraction and fluorescence tomography*", 2016, Aarhus Universitet.

Line Bilgrav Nielsen, Iversen "*Synthesis and characterization of  $MoS_2$  Nanoparticles*", 2016, Aarhus Universitet.

Mathilde Nygaard "*Electron density and Magnetic Properties of the  $[Co(SPh)_4]^{2-}$  Complex*", 2016, Aarhus Universitet.

Niels Frederik-Juhl "*Supercritical Synthesis of Nickel Nanoparticles*", 2016, Aarhus Universitet.

Rolf Kjeldsen "*Magnetic Self-Healing Hydrogels*", 2016, Aarhus Universitet.

### **MSc grader 2016, inkl. "Del A" rapporter (ph.d. stud.):**

Alexander Sangsong Fogh "*Syntese af metal samariumborhydrid og hydrogenering af natriumhydrid og aluminium borid*", 2016, Aarhus Universitet.

Anna Zink Eikeland "*Optimizing the magnetic properties of  $SrFe_{12}O_{19}$* ", 2016, Aarhus Universitet.

Henrik Lyder Andersen, "*Hydrothermal Synthesis of Magnetic Spinel Ferrite Nanocrystallites*", 2016, Aarhus Universitet.

Jakob Grinderslev "*Synthesis and characterization of novel ammonium metal borohydrides*", 2016, Aarhus Universitet.

Jiawei Zhang "*Designing high-performance layered thermoelectric materials*", 2016, Aarhus Universitet.

Lirong Song "*Synthesis and Characterization of Bulk and Thin Film Thermoelectric Materials: A study on Zn-Sb and Mg-Sb systems*", 2016, Aarhus Universitet.

Louise Hjørning Møller "*Investigation of Cobalt-dioxolene Complexes – A Study of Synthesis, Structural and Magnetic Properties, Photo and High-Pressure Crystallography*" 2016, Aarhus Universitet.

Martin Roelsgaard "*Studies of Nanoparticle Formation and Battery Materials by In Situ X-ray Diffraction Methods*", 2016, Aarhus Universitet.

Mette Borup "*High-pressure single crystal diffraction study: clathrates of Dianin's compound*", 2016, Aarhus Universitet.

Nina Kølln Wittig "*Nano-scale imaging of bone*", 2016, Aarhus Universitet.

Steffen Riis Jensen "*A Study on Hydrogen Storage Materials*", 2016, Aarhus Universitet.

Jakob Bach Sigvardt "*Design and development of a levitation setup and high pressure melt study of Martian mantle*", 2016, Aarhus Universitet



## **DTU Physics, DTU CEN, DANCHIP, Technical University of Denmark**

### **Conference articles:**

Dake, Jules M.; Oddershede, Jette; Sørensen, Henning O.; Werz, Thomas; Shatto, J. Cole; Uesugi, Kentaro; Schmidt, Søren; Krill III, Carl E. / **Direct observation of grain rotations during coarsening of a semisolid Al-Cu alloy**. In: National Academy of Sciences. Proceedings, Vol. 113, No. 41, 2016, p. E5998 – E6006. (with KU Chemistry)

Schönfeldt, Troels; Batkov, K.; Klinkby, Esben Bryndt; Lauritzen, Bent; Mezei, Ferenc; Takibayev, A.; Willendrup, Peter Kjær; Zanini, L. / **A model for non-thermalized neutron spectra emitted from para-hydrogen**. Proceedings of the 21st Meeting of the International Collaboration on Advanced Neutron Sources (ICANS XXI): Dawn of High Power Neutron Sources and Science Applications. ed. / T. Oku; M. Nakamura; K. Sakai; M. Teshigawara; H. Tatsumoto; M. Yonemura; J. Suzuki; M. Arai. Japan Atomic Energy Agency, 2016. p. 134-140 3.2.12 (K E K Proceedings; No. 2015-7). (J A E A - Conf; No. 2015-002).

### **Oral presentations:**

Jette Oddershede, Intragranular Orientation Spread Induced by Grain Interaction, 3rd International Congress on 3D Materials Science (3DMS), St. Charles, USA. July 10-13, 2016 (with DTU Mechanical Engineering).

Henning Friis Poulsen, Lorentz Workshop: "Quantitative 3D X-Ray Imaging: From Tomographic Images to Metrics", X-ray methodologies for airport security. Seminar at TSA Headquarter, Arlington, Washington DC (USA) , 24/2 2016

Henning Friis Poulsen, X-ray microscopy: a tool for multiscale characterization. Seminar at HERO-M center, KTH, Stockholm 10/5 2016

Henning Friis Poulsen, 3D Multiscale Characterization and Visualization of Crystalline Materials. DTU Vision Day 2016, DTU, Kgs. Lyngby 24/5 2016

Henning Friis Poulsen, Dark-Field X-Ray Microscopy: Multiscale Structure and Stress Mapping. At: 3rd international congress on 3D Materials Science, St. Charles (USA). 10/7-13/7 2016

Henning Friis Poulsen, Multiscale mapping using hard x-ray diffraction imaging. At: Opportunities for In-Situ Characterization During Advanced Manufacture, Argonne Nat. Lab, Chicago (USA) Aug 29-30, 2016

Henning Friis Poulsen, Multiscale movies of microstructure evolution. At: Conference for Materials Science and Technology, MS&T 2016, Salt Lake City (USA) 23-27/10 2016.

Henning Friis Poulsen, Multigrain Indexing of Unknown Multiphase Materials. AT: High Pressure multigrain Crystallography workshop, Argonne Nat. Lab, Chicago (USA) 28-29/10, 2016

Henning Friis Poulsen, MAX IV: World's best x-ray microscope. At: Danish Optical Society Annual Conference 2016, 24-25/11, 2016.

Jin Zhang, Optimize material parameters with 4D experiments and phase-field simulations, 8th International Conference on Multiscale Material Modeling 2016, Dijon, France. October 9-14, 2016

Innokenty Kantor, DanMAX users meeting: "Full field imaging and dark field microscopy at DanMAX" (talk), Odense, 03 Feb 2016

Sonja Rosenlund Ahl, "In-Situ Multiscale 3D-Mapping of Embedded Recrystallizing Grains in Aluminium", 12/7-16, 3DMS 2016, St. Charles, Illinois, USA

Sonja Rosenlund Ahl, "Quantifying the onset of recrystallization in deformed metals using x-rays", 7/2-16, Dansk fysik selskabs årsmøde 2016, Middelfart, DK

Sonja Rosenlund Ahl, "Dark Field X-Ray Microscopy for Studies of Very Low Angle Boundaries", 15/2-16, TMS2016, Nashville, Tennessee, USA

Sonja Rosenlund Ahl, "Quantifying the onset of recrystallization in deformed metals using x-rays", 30/11-16, Sustain DTU 2016, Kgs. Lyngby, DK

Anders Clemen Jakobsen, "Mapping of Embedded Dislocations in Diamond with Sub 200 nm Resolution", 3DMS 2016, St. Charles, IL, USA.

Anders Clemen Jakobsen, "Mapping Dislocations In Diamond Crystals Using Dark-Field X-ray Microscopy With 200 nm Resolution", Dislocations 2016. Purdue University, Lafayette, Indiana, USA.

Hugh Simons, Talk at Danfysik Selskab.

Hugh Simons, Talk at 2016 international workshop of topological structures in ferroic materials.

Hugh Simons, Invited talk at 2016 International Symposium for the Applications of Ferroelectrics .

Hugh Simons, Talk at International Congress on 3D Materials Science (3DMS) 2016.

Søren Schmidt, NEUWAVE-8, Abingdon, UK, – tale om diffraktionsbaseret neutron imaging.

Søren Schmidt, ITNMR-8 2016, Beijing, Kina – tale om diffraktionsbaseret neutron imaging.

Carsten Gundlach, 1/2-2016: 'Imaging at DTU - examples of micro CT x-ray tomography', ATV-SEPMAPP workshop om overfladeteknikker.

Carsten Gundlach, 12/12-2016: 'The 3D imaging center at DTU', NEXIM afslutningskonference

Carsten Gundlach, 16/12-2016: '3D imaging center at DTU', Zeiss XEN workshop in Wien.

Kristoffer Haldrup, Direct, Sub-Picosecond Tracking of Structural and Electronic Degrees of Freedom Using X-Ray Free Electron Lasers, Nordic Femtochemistry XII, Örenäs, Sverige.

Peter Kjær Willendrup, "Integrating software: SASview, McStas and Mantid for powerful virtual SANS experiments", NOBUGS 2016 conference, København, November 2016

### Abstracts and posters:

Diederichs, Annika Martina; Lienert, Ulrich; Poulsen, Henning Friis; Pantleon, Wolfgang / **Advanced microstructural analysis of cyclically deforming metallic materials towards lifetime improvement.** 2016. Abstract from Sustain-ATV Conference 2016, Kgs. Lyngby, Denmark. (with DTU Mechanical Engineering)

Jørgensen, Mads Ry Vogel; Kantor, Innokenty; Bergbäck Knudsen, Erik; Poulsen, Henning Friis; Iversen, Bo Brummerstedt / **DanMAX - The Danish beamline for in situ materials studies at MAX IV.** 2016. Poster session presented at European Powder Diffraction Conference 2016, Bari, Italy. (with AU Chemistry)

Jin Zhang, Measure material parameters by bridging 3D experiments and simulations, 3rd International Congress on 3D Materials Science (3DMS), St. Charles, USA. July 10-13, 2016

Peter Kjær Willendrup, DFS 2016: "New developments in the McStas neutron Monte Carlo ray-tracing package"(poster)

Peter Kjær Willendrup, DANSCATT 2016: "New developments in the McStas neutron Monte Carlo ray-tracing package"(poster)

Peter Kjær Willendrup, NOBUGS 2016: "New developments in the McStas neutron Monte Carlo ray-tracing package" (poster)

Innokenty Kantor, Danscatt annual meeting 2016: "DanMAX - The Danish beamline for in situ materials studies at MAX IV" (poster), Copenhagen, 26 May 2016

Innokenty Kantor, XTOP-2016: "DanMAX - The Danish beamline for in situ materials studies at MAX IV" (poster), Brno, 4-8 Sept 2016

### Anden formidling/outreach, m.v.:

Martin Meedom Nielsen, 6. oktober 2016, interview med Die Zeit:

<http://www.zeit.de/2016/42/photovoltaik-roentgen-laser-european-xfel-probebetrieb>

Kristoffer Haldrup, 15. oktober 2016, interview med Kristeligt Dagblad: <https://www.kristeligt-dagblad.dk/viden-forskning/et-skridt-mod-endoloese-maengder-af-gratis-energi>

Kristoffer Haldrup, Interview på DR2 21. juni 2016, om åbningen af MaxIV.

Henning Friis Poulsen, ESS og MAX IV som vækstmotorer for hovedstadsregionen. At: ATV rundbordsmøde: Industriens behov for materialeforskning og –teknologi og innovation. Esbjerg, 12/2 2016

Niels Bech Christensen, præsentation om BIFROST-instrument ved DIBS'16: Danish Instruments for Big Science

Hugh Simons, 17/11 2016, "Multiferroics: emergent supermaterials combining elastic, electrical and magnetic functionality", Fysikaften, DTU Fysik.

Carsten Gundlach, 20/3-2016: ' X-ray micro computed tomography basics and examples of use at DTU Imaging Industry Portal', DTU alumni

Carsten Gundlach, 26/8-2016: 'Røntgen mikrotomografi', Foredrag hos Odense By museer

Carsten Gundlach, 7/10-2016: '3D imaging center at DTU – Examples of tomography', Foredrag hos Grundforskningscenter IDUN, DTU Nanotech

**Carsten Gundlach, møder med virksomheder:**

- 9/2-2016 Møde om LINX hos VELUX A/S, Østbirk
- 10/2-2016 Møde hos Rockwool International A/S, Hedehusene
- 12/2-2016 Møde hos Tetra Pak AB, Lund, Sverige
- 18/2-2016 Møde hos Frichs A/S, Åbyhøj
- 19/2-2016 Møde hos Grundfos A/S, Bjerringbro
- 1/3-2016 Møde hos Xnovotech, Køge
- 3/3-2016 Møde hos DI, København
- 7/4-2016 Møde hos LM Wind Power A/S, Lunderskov
- 2/6-2016 Møde hos Tetra Pak, Lund
- 12/6-2016 Møde hos Tetra Pak, Lund
- 30/8-2016 Møde og foredrag hos Fiberline A/S, Middelfart
- 27/9-2016 Møde hos Tetra Pak, Lund
- 6/12-2016 Møde hos Rockwool International A/S, Vamdrup

**Undervisning og kurser:**

Niels Bech Christensen, Søren Schmidt, "X-ray and Neutron Experiments at International Research Facilities", B.Sc. course

Niels Bech Christensen, Søren Schmidt, kursus 10200 "The structure and dynamics of materials studied with X-rays and neutrons", M.Sc. course (Med DTU Energi m.fl.)

Cathrine Frandsen, undervisning i neutronspreddning som del af kursus "Magnetisme og magnetiske materialer" (med Niels Bohr Institute).

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

Kristoffer Haldrup, kursus 10031, "Introduktion til Fysik og Nanoteknologi". Fire ugers forløb om røntgenfysik.

Kristoffer Haldrup, Erhvervspraktikanter fra folkeskolen 2\* om året, titel på foredrag: "Super-intens røntgenstråling - Hvad er det, og hvad kan man bruge det til?"

Carsten Gundlach, 25/1-2016: 'Mapping the contours: Micro-CT scanning and polynomial texture mapping'. På kurset 'Analytical Tools for Organic Material Studies (ATOMS) An introduction to new investigative science for the humanities' på CTR – KU.

Carsten Gundlach, 17/8-2016: 'Imaging at DTU - examples of micro CT x-ray tomography'. Ph.D. sommerskole på DTU Byg.

Carsten Gundlach, 19/8-2016: 'X-ray micro computed tomography basics and examples', Foredrag på 3 ugers kursus I spredningsteknikker, DTU Fysik.

Carsten Gundlach, 26/10-2016: 'X-ray microtomography at 3D imaging center', Foredrag på DTU Fysik kursus 10200.

Peter Kjær Willendrup, SINE2020 Workshop, "Neutrons: Cradle to Grave workshop", Coimbra, Portugal, September 2016 (<http://coimbra2016.essworkshop.org>)

Peter Kjær Willendrup, McStas skoler:

- Bariloche, Argentina Februar 2016
- ESS, Lund, Sverige Maj 2016
- I forbindelse med NOBUGS, København November 2016

#### **MSc kandidater og BSc:**

Niels Bech Christensen, "Crystal and Magnetic Structures of Lithium Orthophosphates", Michael Korning Sørensen og Andreas Bott Kristensen (BSc)

Søren Schmidt, Carsten Gundlach, "Karakterisering af revnespidser med røntgentomografi", Ida Møller Haubech Hansen (BSc)

Søren Schmidt, "Indeksering af ukendte strukturer ved brug af røntgenstråling", Jes Ærsøe Hyllested (MSc)

Carsten Gundlach (medvejleder), "In situ TEM and X-ray Nano Tomography of Anode Materials in Batteries", Jeppe Ormstrup (MSc)

## **DTU Mechanical Engineering, Technical University of Denmark**

### **Contributions to conferences and congresses in 2016:**

T.L. Christiansen, K.V. Dahl, M.S. Jellesen, M.A.J. Somers, Thermochemical surface engineering; playground for science and innovation, Metal 2016, Brno, Czech Republic, 25/5-27/5 2016, invited

T.L. Christiansen, K.V. Dahl, M.S. Jellesen, M.A.J. Somers, Thermochemical surface engineering; playground for science and innovation, 5th Asian Conference on Heat Treatment and Surface Engineering, Hangzhou, China, 12/11-14/11 2016, invited

A.M. Diederichs, D. Orlov, W. Pantleon, Monitoring microstructural evolution during reversed deformation by high-resolution reciprocal space mapping, MAX4ESSFUN Annual Meeting 2016, Lund, Sweden, 6/10-7/10 2016.

A.M. Diederichs, U. Lienert, H.F. Poulsen, W. Pantleon, Advanced microstructural analysis of cyclically deforming metallic materials towards lifetime improvement, Sustain-ATV Conference 2016, Kgs. Lyngby, Denmark, 30/11 2016.

N.Y. Juul, J. Oddershede, G. Winther, Measured Resolved Shear Stresses on Slip Systems in Austenitic Steel Grains, 3rd International Congress on Materials Science, St. Charles, USA, 10/7-13/7 2016

F. Nießen, M. Villa, D. Apel, O. Keßler, M. Reich, M. Somers, J. Hald, In-situ investigation of the kinetics of reverse austenite formation in supermartensitic stainless steel, Thermec'2016, Graz, Austria, 29/5-3/6 2016

W. Pantleon, Disorientations, dislocations and slip systems, Dislocations 2016, West-Lafayette, USA, 19/9-23/9 2016, invited

W. Pantleon, Auf der Jagd nach Versetzungen: vom Röntgenkeller zur Strahlenhütte, Wiss. Kolloquium 100 Jahre Institut für Werkstoffwissenschaft, Freiberg, Germany, 6/10-7/10 2016, invited

M.A.J. Somers, Expanded austenite: from fundamental parameters to prediction of composition- and stress-depth profiles, 4th Symposium on Surface Hardening and Corrosion Resistant Materials, Valetta, Malta, 22/6-24/6 2016, invited

C. Wejdemann, H.F. Poulsen, U. Lienert, W. Pantleon, Tracking subgrains during strain path changes by high resolution reciprocal space mapping, TMS 2016 145th Annual Meeting & Exhibition, Nashville, USA; 14/2-18/2 2016

G. Winther, Intragranular orientation spread induced by grain interaction, TMS 2016 145th Annual Meeting & Exhibition, Nashville, USA; 14/2-18/2 2016, invited

G. Winther, Analysis of grain-scale experimental data in a crystal plasticity framework, 8th International Conference on Multiscale Materials Modeling, Dijon, France, 9/10-14/10 2016, invited

### **Education and courses:**

41691 Ph.D. course on application of X-ray diffraction in materials science F17

## DTU Energy, Technical University of Denmark

### Contributions to conferences and congresses in 2016:

Blanchard, D., *Quasi-Elastic Neutron Scattering Studies on Solid Electrolytes for all-solid-state Lithium Batteries*, European Crystallographic Meeting 2016, Aug 30, 2016, Basel, Switzerland, Invited talk.

Blanchard, D., *Quasi-Elastic Neutron Scattering studies for Material Research*, Sep 2, 2016, 50 Years of Neutron Backscattering, Munich, Germany, Invited Talk.

Andreasen, J.W., *Imaging Structure Formation in Energy Materials by in situ X-ray Scattering and Ultra-high Resolution Tomography*, Yearly Meeting, Danish Physical Society, Jun 6, 2016, Middelfart, Denmark, Invited talk.

Johnsen, R.E. *In situ X-ray diffraction studies of electrode materials in working metal-ion batteries and other layered materials*. Functional Materials seminar, Sep 20, 2016, Physics Department, Technical University of Munich, Germany, Invited talk.

Johnsen, R.E. & Norby, P. *Micro-battery cells for detailed in situ X-ray diffraction studies of electrode materials in working metal-ion batteries*. E-MRS 2016 Spring Meeting, CC, - In situ studies of functional nano materials at large scale facilities, May 2-6, 2016, Lille, France, Contributed talk.

De Angelis, S., Bowen, J. R. and Jørgensen, P. S., *Ex Situ 3D Nano-Ptychography of Ni-YSZ SOFC Anode during Redox Cycling*, Pacific Rim Meeting (ECS), Oct 2-7 2016, Honolulu, Hawaii, Contributed talk.

Ramos, T., Jørgensen, J.S., Andreasen, J.W., *Automated tomographic alignment of translation and rotation uncertainties and application to phase-contrast tomography*, CINEMAXII summer school, Aug 29, 2016, Fuglsang, Denmark, Poster

Ramos, T., Scipioni, R., Christiansen, A. S., Norby, P., Jensen, S. H., Giakoumidis, S., Andreasen, J. W., *In situ Ptychographic tomography of a microscale LiFePO<sub>4</sub> battery*, DESY Photon Science Users' Meeting 2016, Jan 27, 2016, Hamburg, Germany, Poster

Ramos, T., Jørgensen, J.S., Andreasen, J.W., *Alignment Algorithms for Enhanced High-Resolution Tomography*, DESY Photon Science Users' Meeting 2016, Jan 27, 2016, Hamburg, Germany, Poster

Ramos, T., Jørgensen, J.S., Andreasen, J.W., *Alignment Algorithms for Enhanced High-Resolution Tomography*, Yearly Meeting, Danish Physical Society, Jun 6, 2016, Middelfart, Denmark, Poster

Mathiesen, J.K., Johnsen, R.E., & Norby, P. *Understanding the Domain Structure of Graphite upon Lithium Intercalation and De-intercalation*, 45th Danish Crystallography Meeting & 8th DANSCATT Meeting, May 26 - 27, 2016, University of Copenhagen, Denmark, Poster.

Mathiesen, J.K., Johnsen, R.E. & Norby, P. *Understanding the Domain Structure of Graphite upon Lithium Intercalation and De-intercalation*, School and Conference on Analysis of Diffraction Data in Real Space, Mar 7 - 11, 2016, Grenoble, France, Poster.

Sierra Trujillo, J. X., Bowen, J. R., Jørgensen, P. S., Simon, H., Detlefs, C., Cook, P., Poulsen, H. F., *Characterization of YSZ membranes using Dark Field X-Ray Diffraction Microscopy*, HERCULES course, ESRF, Grenoble, France, April 2016, Poster

Rossander, L. H., Larsen-Olsen, T. T., Dam, H. F., Norrman, K., Schmidt, T. M., Corazza, M., Rajkovic, I., Andreasen, J. W. and Krebs, F. C. *In situ roll-to-roll X-ray crystallization studies of slot-die coated perovskite solar cell active layers*, HERCULES – Higher European Research Course for Users of Large Experimental Systems, Mar 29 – April 29, 2016, Grenoble, France, Poster.

**Other communication / outreach, etc.:**

*Lattice-Boltzmann method: the link between X-ray tomography and fluid modeling*, 47511 CINEMAX II: 3D Modelling and Imaging of Material Microstructure - Ph.D. Summer School, Aug 2016, lecture.

**Education and courses:**

10200 *The structure and dynamics of materials studied with X-rays and neutrons*, Fall 2016.

10209 *X-ray and Neutron Experiments at International Research Facilities*, Jun 2016.

47511 *CINEMAX II: 3D Modelling and Imaging of Material Microstructure* - Ph.D. Summer School, Aug 2016.



## **DTU Chemistry, Technical University of Denmark**

### **Bidrag til konferencer og kongresser 2016:**

Pernille Harris, Invited presentation

GLP-1 conjugated to rHSA variants with modified FcRn binding properties. Impact on molecular structure and half-life. 7th Annual Protein Formulation Development & Drug Delivery Forum" on 7th - 8th June 2016 at the Avenida Palace Hotel, Barcelona, Spain

Klaus B. Møller: Inviteret foredrag "Molecules in motion observed with X-rays", MOLIM General Meeting 2, Okt. 10-12, 2016, Dubrovnik, Kroatien

### **Anden formidling/outreach, m.v:**

Interview on TV2 News, 8 minutes on scientific breakthrough,

<http://livsstil.tv2.dk/sundhed/2016-04-08-danske-og-engelske-forskere-finder-enzym-kan-behandle-depressioner-og-adhd>.

Featured research in ACS Chemical & Engineering News,

<http://cen.acs.org/articles/94/i15/Structure-enzyme-converts-neurotransmitter-dopamine.html?type=paidArticleContent>.

Featured research in Scientific American,

<http://www.scientificamerican.com/article/hacking-an-enzyme-s-structure-could-lead-to-drugs-for-alzheimer-s-and-schizophrenia/>.

Videnskabens Verden DR P1, Danish radio broadcast, half hour interview and feature,

<http://www.dr.dk/radio/ondemand/p1/videnskabens-verden-2016-05-10#!/>.

News radio broadcast, DR P1 and P4, in Danish.

ScienceNordic.com, featured research,

<http://sciencenordic.com/breakthrough-depression-schizophrenia-and-high-blood-pressure>.

Videnskab.dk, featured research, in Danish,

<http://videnskab.dk/krop-sundhed/gennembrud-adhd-skizofreni-og-forhojet-blodtryk>.

### **Undervisning og kurser:**

Applications of X-ray and neutron scattering in biology, chemistry and physics. (KU & DTU)

Klaus B. Møller: 4 lectures at 'Molecular Dynamics and Chemical Kinetics: Exploitation of Solar Energy' Summer School on Photo physics, photo chemistry, capture of solar energy and molecular design of devices, August 15 to August 23, 2016, University of Copenhagen.

### **Patenter 2016:**

The crystal structure of dopamine  $\beta$ -hydroxylase; European patent application No. 16164227.7 filed on 7<sup>th</sup> April 2016.

**Navne på MSc kandidater og BSc:**

Kathrine Kirk Øgendahl

Line Abildgaard Ryberg

## Dept. of Health and Medical Sciences, University of Copenhagen

### Contributions to conferences and congresses in 2016:

Yaghmur, A. (2016) Soft drug nanocarriers based on cubosomes and hexosomes, Copenhagen Nanomedicine Day 2016, Faculty of Health and Medical Sciences, University of Copenhagen (Invited Talk).

Azmi, I. D. M., Wu, L., Wibroe, P. P., Nilsson, C., Østergaard, J., Stürup, S., Gammelgaard, B., Urtti, A., Moghimi, S. M., Yaghmur, A. (2016) Modulatory effect of human plasma on liquid crystalline dispersions, Copenhagen Nanomedicine Day 2016, Faculty of Health and Medical Sciences, University of Copenhagen (Poster).

Ghazal, A., Gontsarik, M., Kutter, J., Lafleur, J., Labrador, A., Mortensen, K., and Yaghmur, A. (2016) Direct monitoring of calcium-triggered phase transitions in cubosomes using SAXS combined with microfluidics, Copenhagen Nanomedicine Day 2016, Faculty of Health and Medical Sciences, University of Copenhagen (Poster).

Indruszewski, T., Moghimi, S. M., Yaghmur, A. (2016) Self assembled lyotropic liquid crystalline nanoparticles as potential theranostic nanopharmaceuticals. CLINAM, Basel, Switzerland (Poster).

Yaghmur, A. (2016) Cubosome and Hexosome Nanocarriers as Versatile Platforms for Drug Delivery, International Workshop: Synchrotron and Neutron Scattering in Biomaterials and Soft Matter, Malmö, Sweden (Poster).

Azmi, I. D. M., Wibroe, P. P., Lu, L-P., Kazem, A. I., Amentisch, H., Moghimi, S. M., and Yaghmur, A. (2016) A Structurally Diverse Library of Safe-by-Design Citrem-Phospholipid Lamellar and Non-lamellar Liquid Crystalline Nano-Assemblies, International Workshop: Synchrotron and Neutron Scattering in Biomaterials and Soft Matter, Malmö, Sweden. (Oral).

### Other communication / outreach, etc.:

The article of the PhD student Mark Gontsarik under supervision of Dr. Stefan Salentinig (Empa's) and published in the *Journal of Physical Chemistry Letters* was covered by different journalists and different websites including the following:

<https://www.empa.ch/web/s604/peptide>

<https://www.sciencedaily.com/releases/2016/10/161018093821.htm>

<https://www.medinside.ch/de/post/schweizer-forscher-entwickeln-waffe-gegen-superkeime>

<http://derstandard.at/2000046070413/Biochemiker-entwickeln-neue-Waffe-gegen-Superkeime>

[http://diepresse.com/home/science/5103842/Multiresistente-Keime\\_Hilft-Tasmanischer-Teufel](http://diepresse.com/home/science/5103842/Multiresistente-Keime_Hilft-Tasmanischer-Teufel)

<http://scienmag.com/peptides-vs-superbugs/>

<http://phys.org/news/2016-10-peptides-superbugs.html>

<http://www.gdp.ch/scienza-e-tecnologia/resistenza-agli-antibiotici-unarma-piu-id141988.html>

Bilag 4: Danscatt Outreach, kurser, studenterafhandlinger, publikationer m.v. 2016

<http://www.bernerzeitung.ch/wissen/medizin-und-psychologie/forscher-entwickeln-neue-waffe-gegen-superkeime/story/25570526>

**Front page from journals in 2016: Front page and cover story in the Journal of Controlled Release**

**Front page:** See the cover of Journal of Controlled Release, vol. 221, 10 January 2016

**Cover story:** The cover story: *Hemocompatible and immune-safe library of citrem-phospholipid liquid crystalline nanoplatforms.*

**Names of MSc candidates and BSc:**

Master Students completed their studies: Kirstin Khaliqi, Mohammed Jawad, Erdal Avici, Simon Pham, Ömer Faruk Özdemir, Ali Kazem

## Dept. of Chemistry, University of Copenhagen

### Bidrag til konferencer og kongresser 2016:

#### Oral presentations:

Leila Lo Leggio 14th Workshop in Protein.DTU "Applied Protein Science", Kgs. Lyngby, Denmark. 9. May 2016. *Polysaccharide Breaking News. Lytic polysaccharide monooxygenases: potential, structures and substrate binding* (invited)

Leila Lo Leggio, European Crystallography Meeting, Basel, Switzerland. 28. Aug - 1. September 2016. *Lytic polysaccharide monooxygenases and their interaction with polysaccharide substrates* (invited)

Leila Lo Leggio, ALAMY 6, 11-15 September 2016, Smolenice Castle, Slovakia. *Structural studies on the AA13 family of lytic polysaccharide monooxygenases*

Kim Krighaar Rasmussen, Synchrotron and Neutron Scattering in Biomaterials and Soft Matter Malmö, Sweden, 26-28 October 2016 *Structural and dynamics studies of a truncated variant of CI repressor from bacteriophage TP901-1*

Kristian E.H. Frandsen, DANSCATT meeting, 26-27 May 2016, Copenhagen *The molecular basis of polysaccharide cleavage by lytic polysaccharide monooxygenases*

S. H. J. Eiby, S. Nedel, D. J. Tobler, A. Bischoff, B. C. Christiansen, A. S. Hansen, H. G. Kjaergaard, S. L. S. Stipp, Goldschmidt 2016, Yokohama, Japan, 27 June-1 July 2016 *The role of anion (Cl-, SO42- and CO32-) ratio and concentration on reformation of calcined hydrotalcite* (Presented by H. O. Sørensen)

H. O. Sørensen, Y .Yang, S. Bruns, S. L. S. Stipp, Goldschmidt 2016, Yokohama, Japan, 27 June-1 July 2016 *Why pH buffering may lead to a more homogeneous rock dissolution*

D. Müter, K. N. Dalby, H. O. Sørensen, M. Guizer-Sicairos, M. Holler, S. L. S. Stipp, Goldschmidt 2016, Yokohama, Japan, 27 June-1 July 2016 *Nano-Mechanical Properties of Chalk from Ptychographic Imaging*

Y .Yang, S. Bruns, S. L. S. Stipp, H. O. Sørensen, Goldschmidt 2016, Yokohama, Japan, 27 June-1 July 2016 *Infiltration instability amplifies the discrepancy between geometric and reactive surface areas in rocks*

H. O. Sørensen, D. Müter, K. N. Dalby, R. Gooya, S. Bruns, A. Moaddel, S. L. S. Stipp, 45th Danish Crystallographers Meeting & 8th DanScatt Meeting, Copenhagen, May 26-27 *From dust to parameters – X-ray tomography on natural samples*

Y .Yang, S. Bruns, S. L. S. Stipp, H. O. Sørensen, 45th Danish Crystallographers Meeting & 8th DanScatt Meeting, Copenhagen, May 26-27 *Effect of dissolved CO2 on the morphological evolution of natural porous materials: simulated water-rock interactions based real microstructures of North Sea chalk*

H. O. Sørensen, invited talk at DTU Chemistry, DTU, Kgs. Lyngby, Denmark, 18 May 2016 *Macroscale properties of porous media for energy applications studied at the microscale*

Kirsten M. Ø. Jensen, DESY User Meeting 2016, February 28-29, Hamburg, Germany, *The Nanostructure Problem in Materials Chemistry* (Invited)

Kirsten M. Ø. Jensen, EPDIC15 (European Powder Diffraction Conference), June 11<sup>th</sup>-16<sup>th</sup> 2016, *Total Scattering and PDF analysis for nanostructure analysis in Materials Chemistry Bari, Italy* (Invited, Plenary)

Y. Yang, S. Bruns, S. L. S. Stipp, H. O. Sørensen, AGU Fall Meeting, San Francisco, USA, Dec. 12-16 December 2016 *Dissolved CO<sub>2</sub> stabilizes dissolution front migration and increases breakthrough porosity for natural porous materials*

Jesper Bendix, Coordination Chemistry Symposium, Okayama University, Sept. 2, 2016, Okayama, Japan *Metalloligands providing high-symmetry lanthanide SMM's and actinide chains assembled via metal-metal interactions*

Jesper Bendix, 2<sup>nd</sup> Bordeaux Olivier Kahn Discussions BOOK-D, Bordeaux, CRPP, May 26-28, 2016 *Metalloligands providing high-symmetry lanthanide SMM's and actinide chains assembled via metal-metal interactions*

Mikkel Agerbæk Sørensen, Coordination Chemistry Symposium, Okayama University, Sept. 2, 2016, Okayama, Japan *Tetragonal Lanthanide Complexes as Test Subjects for SMM Design Criteria*

Mikkel Agerbæk Sørensen, 2<sup>nd</sup> Bordeaux Olivier Kahn Discussions BOOK-D, Bordeaux, CRPP, May 26-28, 2016 *Symmetry-Tunable Lanthanide Complexes: Test Subjects for SMM Design Criteria* (Flash presentation)

Morten Gotthold Vinum, Coordination Chemistry Symposium, Okayama University, Sept. 2, 2016, Okayama, Japan *Magnetostructural correlations in a family of tetragonal single-chain magnets*

Anders Ø. Madsen, 45th Danish Crystallographers Meeting & 8th DanScatt Meeting, Copenhagen, May 26-27. *Can we get better understanding of phase stability and transformations in polymorphic drug crystals from inelastic scattering studies?*

Anders Ø. Madsen, 7<sup>th</sup> European Charge Density Meeting. June 26<sup>th</sup> - July 1<sup>st</sup> 2016. *Combining multipole modeling and lattice dynamics.*

#### **Poster presentations:**

Anders K. Varming, DANSCATT meeting, 26-27 May 2016, Copenhagen *Structural Characterization of the TP901-1 CI Repressor Protein*

Annette E. Langkilde, DANSCATT meeting, 26-27 May 2016, Copenhagen *Preparations for a macromolecular neutron diffraction experiment –aiming at multiple temperature high resolution data*

Folmer Fredslund, DANSCATT meeting, 26-27 May 2016, Copenhagen *Structural characterization of the thermostable *Bradyrhizobium japonicum* D-sorbitol dehydrogenase*

Tobias Tandrup, DANSCATT meeting, 26-27 May 2016, Copenhagen. *Structure determination of engineered GH51  $\alpha$ -L-arabinofuranosidase of *Thermobacillus xylanilyticus**

R. Gooya, S. Bruns, D. Müter, A. Moaddel, R. P. Harti, S. L. S. Stipp, H. O. Sørensen, 45th Danish Crystallographers Meeting & 8th DanScatt Meeting, Copenhagen *Effect of Tomography Resolution on the Calculated Microscopic Properties of Porous Material*

S. Bruns, S. L. S. Stipp, H. O. Sørensen, 45th Danish Crystallographers Meeting & 8th DanScatt Meeting, Copenhagen *Iterative Non-Local Means for Tomography Reconstructions of Geological Samples: Benchmarking with Experimental Noise Footprints*

D. Müter, H. O. Sørensen, K. N. Dalby, S. L. S. Stipp, 45th Danish Crystallographers Meeting & 8th DanScatt Meeting, Copenhagen *Nanoscale mechanical properties of chalk from X-ray tomography*

Kim K. Rasmussen Current Topics in Protein Science, 5. December 2016, DTU, Kgs. Lyngby *Combining complementary techniques to unravel the presumably stochastic life cycle of TP901-1*

Troels Lindahl Christensen, DANSCATT meeting, 26-27 May 2016, Copenhagen, *Size Dependent Structure in Molybdenum Oxide Nanoparticles and Ultra Small Particles*

Mikkel Juelsholt, 26-27 May 2016, Copenhagen, Synthesis and structural characterization of WO<sub>3</sub> nanoparticles

Jesper Bendix, 15<sup>th</sup> ICMM, Sept. 4-8, 2016, Sendai Japan, *High-Symmetry Lanthanide SMMs and Actinide Chains Assembled via Metal-Metal Interactions*

Mikkel Agerbæk Sørensen, 15<sup>th</sup> ICMM, Sept. 4-8, 2016, Sendai Japan, *Tetragonal Lanthanide Complexes as Test Subjects for SMM Design Criteria*

Mikkel Agerbæk Sørensen, 2<sup>nd</sup> Bordeaux Olivier Kahn Discussions BOOK-D, Bordeaux, CRPP, May 26-28, 2016 *Symmetry-Tunable Lanthanide Complexes: Test Subjects for SMM Design Criteria* (Flash presentation)

Morten Gotthold Vinum, 15<sup>th</sup> ICMM, Sept. 4-8, 2016, Sendai Japan, *Magnetostructural correlations in a tetragonal Fe<sup>II</sup>-Re<sup>IV</sup> single-chain magnet*

Morten Gotthold Vinum, 2<sup>nd</sup> Bordeaux Olivier Kahn Discussions BOOK-D, Bordeaux, CRPP, May 26-28, 2016, *Magnetostructural correlations in a tetragonal Fe<sup>II</sup>-Re<sup>IV</sup> single-chain magnet.*

Anders Ø. Madsen, European Crystallography Meeting, Basel, Switzerland. 28. Aug - 1. September 2016. Thermal diffuse scattering from molecular crystals - A case study of pyrazinamide.

#### **Anden formidling/outreach, m.v.:**

Kirsten M. Ø. Jensen: Udtalelse til artikel i Weekendavisen: *Til Lysfest i Lund*, 24. juni 2016.

Kirsten M. Ø. Jensen: Foredrag ved 'Senioruniversitetet Værløse', 21 og 24 November, 2016. 2 foredrag af 90 minutter.

#### **Undervisning og kurser:**

Undergraduate courses (Crystallography-BSc and Crystallography-MSc), course responsible Leila Lo Leggio.

Materials Chemistry, course responsables Anders Ø. Madsen and Henning O. Sørensen.

Structural tools in nano-science (MS course) course responsible Nicolas Bovet.

Advanced Physical Chemistry, Master course, Course responsible Henrik Grum Kjærgaard.

**Forside fra tidsskrifter 2016:**

Nature Chemical Biology, April 2016, Vol 12 nr 4 i forbindelse med Frandsen et al (2016) *Nature Chemical Biology*, **12**, 298-303. doi:10.1038/nchembio.2029

**Popular articles:**

Lo Leggio, L., Tovborg, M., Johansen, K.S. (2016) Enzymatisk nedbrydning af polysaccharider, *Dansk Kemi* 97, 23-25 (in danish).

**Navne på MSc kandidater og BSc:**

BSc. Mikkel Juelsholt, Synthesis and Characterization of Tungsten Oxide Nanoparticles.

BSc. Cecilia Dam Weihe, Lytic polysaccharide monooxygenases: Determination of a Structure. And Description of Crystallization Experiments.

BSc. Christina Basse Riel, Synthesis and Characterization of Copper Nanoparticles.

BSc. Mark Alexander Olsen. Structure determination of the metastable theophylline form III – by X-ray powder diffraction.

MSc. Laura Voigt, The effect of aluminium on green rust composition, structure and reactivity.

MSc. Simon Holm Jacobsen Eiby, Green rust formation and reactivity.

MSc. Phillip Miguel Kofoed. The colour and thermostability of a morphochrome and its quinone.



## **Dept. of Health and Medical Sciences, University of Copenhagen**

### **Bidrag til konferencer og kongresser 2016:**

Kastrup, J. S. (invited speaker). Insight from structures of ligand-binding domains of ionotropic glutamate receptors. 26th Neuropharmacology Conference - Ionotropic Glutamate Receptors, San Diego, California, USA, November 10-11, 2016.

Møllerud, S., Thorsen, T. S., Kristensen, L. B., Pickering, D. S., and Kastrup, J. S. Structural and pharmacological characterization of the kainate receptor subunit GluK5. Poster at the DANSCATT Annual Meeting, University of Copenhagen, May 26-27 2016.

Kristensen, L.B., Kristensen, O., Møllerud, S., Frydenvang, K., Pickering, D. S. and Kastrup, J. S. Structure of the ligand-binding domain of the kainate receptor subunit GluK4. Poster at the DANSCATT Annual Meeting, University of Copenhagen, May 26-27 2016.

Leahu, A., Larsen, A.P., Frydenvang, K., Valembois, S., Francotte, P., Pirotte, B., and Kastrup, J.S. Structural characterization of the ligand-binding domain of the ionotropic glutamate receptor GluA2 in complex with new positive allosteric modulators. Poster at the DANSCATT Annual Meeting, University of Copenhagen, May 26-27 2016.

Møllerud, S. Structural and pharmacological characterization of the kainate receptor subunit GluK5. Poster at Drug Research Academy Summer School, August 24-25 2016.

Vestergaard, B. (invited speaker). SAXS on protein fibrillation. March 2016. Dobson-Knowles-Vendrusculo biophysics seminar series, University of Cambridge.

Marasini, C. (invited speaker) Sucrose effect on protein fibrillation. Italian Biophysics Society meeting, August 2016.

Skamris, T. (invited speaker) Aggregation and stability of antibodies in response to acidic treatment during production. American Association of Pharmaceutical Sciences Symposium, November 16, Denver, Colorado.

Vestergaard B. (invited speaker) Structural analysis of transthyretin fibrillation. EMBO conference 'Molecular Machines – Integrative Structural and Molecular Biology', Heidelberg, Nov 20-23 2016.

Vestergaard B. Neutron analysis of protein fibrillation. CoNEXT general meeting. Magleås kursuscenter, October 24<sup>th</sup>. 2016.

### **Undervisning og kurser:**

Kastrup, J. S. "Lægemidler mod hjernens sygdomme". Lectures offered to Gymnasia.

Kastrup, J. S. (course director). PhD course Receptor Structure and Function, Faculty of Health and Medical Sciences, University of Copenhagen, May 9 –13 2016.

Vestergaard B. 2 lectures at the EMBO global exchange lecture series: Structural and Biophysical methods for biological macromolecules in solution. 19-26 June 2016, Suwon, Korea

**Navne på MSc kandidater og BSc:**

Aura Leahu  
Mathias Poulsen  
Sebastian Winther  
Silvia Barbateskovic  
Arpan Sharma  
Lea Jessen  
Ved Mehta  
Christoffer Brasen  
Selene Baiget

## Niels Bohr Institute, University of Copenhagen

### Navne på MSc kandidater og BSc:

#### MSc

Andreas N Larsen (LA)

Camilla Buhl Larsen (KL)

Exact diagonalization studies of 2D quantum spin systems

Daniel T Martin (KM)

Degradation of metals and coatings at high temperatures

Erik Dreier Christensen (KL)

Boleite – A quantum spin droplet.

Johannes Martiny (BMA)

Rozanna Ignazzi (HNB)

Mobility of functional groups.

#### BSc

Alexander K Lauritsen (HNB)

Martin Olsen (KL) Optimizing neutron guides for ESS

Martin W Willumsen (RF)

Sara Blemmer (LA)

Thomas S Halberg (RF)

Tue Holm-Jensen (JK)

Magnus F Bøe (BMA)

*Suppression of the critical temperature in s-wave superconductors by magnetic and non-magnetic impurities*

## **Dept. of Science, Systems and Models, Roskilde University**

### **Bidrag til konferencer og kongresser 2016:**

#### **Dorthe Posselt:**

Presentation of DanMAX and DanMAX organization, Name of the conference: 1<sup>st</sup> DanMAX user meeting, Type of participation: Oral, Date and place: February 3, 2016, SDU (Denmark)

Restructuring of diblock copolymer thin films during solvent vapor treatment investigated by GISAXS Name of the conference: Materials Physics Seminar, Type of participation: Oral seminar, Date and place: August 25, Helsinki University, Helsinki (Finland).

Influence of straight medium chain alcohols on the dynamics of phospholipid model membranes, Name of the conference: Biomembrane Days, Type of participation: Poster, Date and place: 5-7 September 2016, Berlin (Germany).

#### **Henriette Wase Hansen:**

$G_{\infty}$ , mean-squared displacement and the alpha relaxation – what are the connections?, Name of the conference: Viscous liquids and the glass transition. XIV. International workshop, Type of participation: Oral contribution, Date and place: June 16 - June 18, 2016, Sømmerin, Holbæk (Denmark)

$G_{\infty}$ , mean-squared displacement and the alpha relaxation – what are the connections?, Name of the conference: 'Future of Chemical Physics', JCP, Type of participation: Poster, Date and place: August 31 - 2 September, Oxford (UK)

A test of the “isomorph theory”, Name of the conference: QENS 2016, Type of participation: Poster Date and place: September 5-8 2016, Postdam (Germany)

#### **Alejandro Sanz:**

High pressure cell for simultaneous neutron scattering and dielectric spectroscopy. Name of the conference: 50 years of neutron backscattering. International workshop. Type of participation: Oral contribution. Date and place: 2-3 September 2016, Garching (Germany).

### **Undervisning og kurser:**

#### **Dorthe Posselt:**

Cross-institutional Mastercourse: Applications of X-ray and neutron scattering in biology, chemistry and physics, August 2016.

Cross-institutional PhD course: Molecular Biophysics, October 2016.

PhD opponent, University of Gothenburg (Monika Vitala), June 2016.

PhD opponent, University of Helsinki (Inkeri Kontro), August 2016.

#### **Navne på MSc kandidater og BSc:**

Anders Samsøe-Petersen, Influence of impurities on the micellar crystal structure of Pluronic P85.

## **Dept. of Physics, Chemistry and Pharmacy, University of Southern Denmark**

### **Bidrag til konferencer og kongresser 2016:**

Dorthe B. Ravnsbæk, "Aging in high power Li-ion battery electrodes – when boring is best!", DESY Photon Science User Meeting, Hamburg, Germany, 28. January 2016.

Christine McKenzie, "Selectively Harnessing the Potential Reactivity of O<sub>2</sub>", Fusion conference on Small Molecule Activation, Cancun, Mexico, May 21 2016

Christine McKenzie, "An Iron Catalyst for O-Transfer Reactions: Coordination and Halogen-Bonding Assisted Iodosylbenzene Activation" Girona Seminar on Predictive Catalysis, Girona Spain, April 19 2016

Christine McKenzie, "Harnessing the Oxidizing Power of Air", Annual meeting of COSTCM1205 action, Ljubljana, Slovenia, March 22, 2016

S. Tougaard (Keynote speaker), "Novel applications of inelastic background analysis: 3D imaging and HAXPES", 7th International Symposium on Practical Surface Analysis (PSA-16), 16/10- 21/10, 2016, Daejeon, Sydkorea

C. Zborowski, O. Renault, E. Martinez, A. Torres, Y. Yamashita, G. Grenet, S. Tougaard

"Inelastic Background Analysis in HAXPES: Application to deeply buried Ta/Al interfaces in advanced power devices" European Conference on Surface Science (ECOSS-32), 28/8 – 2/9- 2016, Grenoble, Frankrig

S. Tougaard, "Non-destructive imaging of nanostructures by analysis of the photoelectron peak shape" European Conference on Surface Science (ECOSS-32), 28/8 – 2/9- 2016, Grenoble, Frankrig

Ulla Gro Nielsen, "How the method of synthesis governs the local and global structure of LDHs" SMARTER-5 Bayreuth, Germany, September, 2016

Ulla Gro Nielsen, "Solid state NMR studies of layered inorganic materials with application in environmental remediation", Developments and Applications of Solid State NMR to Materials Science, Chemistry and Engineering Conference, 13/05/2016 → 17/05/2016, Varna, Bulgarien

### **Anden formidling/outreach, m.v.:**

Dorthe B. Ravnsbæk, "Bedre og billigere batteries", Folkeuniversitet, Aarhus 12. October 2016 and Emdrup 17. November 2016

### **Undervisning og kurser:**

Christine McKenzie, KE810 Bioinorganic Chemistry (PhD course at SDU where synchrotron methods are covered)

Christine McKenzie, Training School EPR and Mössbauer Spectroscopy, Max Planck Institute, Mülheim, Germany, 14-16 December, 2016S. Tougaard, "Quantitative Analysis of Surfaces by Electron Spectroscopy, XPS and AES"

Bilag 4: Danscatt Outreach, kurser, studenterafhandlinger, publikationer m.v. 2016

(two days of lectures and hands on practical application of software held at the full week workshop), Ecole  
Thematique: "Workshop on XPS analysis", 26/9-30/9, 2016 i Roscoff, Frankrig

## **Haldor Topsoe**

### **Anden formidling/outreach, m.v.:**

Interview til Weekendavisen vedr. MAX-IV (*Til lysfest i Lund* af Annette K. Nielsen) 29-06-2016.

### **Undervisning og kurser:**

Lecture at "Summer school on synchrotron and neutron radiation" at DTU (Kenny Ståhl) entitled "Industrial use of X-ray absorption spectroscopy" 17-08-2016.