

# 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 venligst bilag 1 for en fuldstændig liste over personer der har deltaget i aktiviteter med relation til DANSCATT.

DANSCATTs bestyrelse har følgende medlemmer:

Formand Henning Friis Poulsen, DTU Fysik  
Næstformand Kell Mortensen, KU Niels Bohr Institutet  
Niels Bech Christensen, DTU Fysik  
Robert Feidenhans'l, KU Niels Bohr Institutet  
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

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

### 4. Økonomi

Oprindeligt bevilget beløb (kr.)	Ekskl. overhead:	4.000.000	Inkl. overhead:	4.000.000
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Eventuel tillægsbevilling (kr.)	Ekskl. overhead:		Inkl. overhead:	
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Forklar væsentlige afvigelser mellem budget og regnskab og i givet fald årsagerne hertil

Ingen væsentlige afvigelser.

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 users community of X-ray and Neutron large scale installations are organized within the instrumentcentre DANSCATT. The user community span from Biology, Chemistry, Physics, materials science to industrial applications, including several companies. The main activity of DANSCATT is to facilitate access to the international large scale facilities by supporting travel where necessary. 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. In total approximately 225 publications were published in 2014 with support from DANSCATT. The access is essential for the Danish user groups to be at the forefront of science as also indicated by the large amount of important publications 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 Danish user community and is enabling interdisciplinary projects by its network activities. Denmark is participating in international facilities like ESRF in Grenoble, European XFEL in Hamburg and the neutron facility ILL in Grenoble. 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.

### 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- og samfundsmæssige resultater
- Forskeruddannelse
- Samarbejde, herunder tværinstitutionelt, tværdisciplinært og internationalt samarbejde

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

### 6. Stipendier

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

Postdoc Amy Poole (K, England, fødselsdato 01.10.1978), Paul Scherrer Institutet, 3 måneder  
Postdoc Markos Skoulatos (M, Grækenland, fødselsdato 04.07.1983), Paul Scherrer Institutet, 2 måneder  
Ph.d.-studerende Sonja Lindahl Holm (K, Danmark, cpr.nr. 110186-1542), Paul Scherrer Institutet, 7 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 venligst bilag 2 for en samlet oversigt, i alt 225 publikationer (fejlmargen +/- 3% på grund af sampublicationer). DANSCATT har støttet med gennemsnitligt 18.000 kr. per publikation.

Artikler, ikke peer reviewed

Doktordisputatser

Torben R. Jensen, Inorganic Nanomaterials for Hydrogen Storage, 2014, Dept. of Chemistry, Aarhus University

Ph.d.-afhandlinger

Jonas Okkels Birk: New Techniques in Neutron Scattering, Niels Bohr Institute, University of Copenhagen  
Kaare Bjerregaard-Andersen: The sodium-coupled bicarbonate-chloride exchanger – structural insights into the role of the N-terminal cytoplasmic domain. Dept. of Molecular Biology and Genetics, Aarhus University  
Emil Dedic: Structural basis for maturation of stable RNA in yeast nucleus. Dept. of Molecular Biology and Genetics, Aarhus University  
Kasper Andersen Borup: High temperature resistivity, Hall effect, and Seebeck coefficient measurements, Dept. of Chemistry, Aarhus University  
Per Sigaard Christensen: Hydrothermal liquefaction of waste biomass - optimizing reaction parameters, Dept. of Chemistry, Aarhus University  
Asmus O. Dohn: Transient Changes in Molecular Geometries and How to Model Them, DTU Chemistry  
Christian Engelbrekt: Green synthesis and structural control of metal and mineral nanostructures, DTU Chemistry  
Nicholas Skar Gislinge: Developing Nanodiscs as a Tool for Low Resolution Studies of Membrane Proteins. Niels Bohr Institute, University of Copenhagen  
Casper Jon Steenberg Ibsen: Crystallization of Apatites: Kinetics, pH, Additives and Formation of Hierarchical Structures, Dept. of Chemistry, Aarhus University  
Mikkel Søes Ibsen: Novel roles for OAS proteins in the defense against viral infections. Dept. of Molecular Biology and Genetics, Aarhus University  
Johanne M. Jensen: Struktur og funktionsstudier af bakterielle peptidtransportører, Dept. of Drug Design and Pharmacology, University of Copenhagen  
Kaspar Klenø: Exploration of the challenges of neutron optics and instrumentation at long pulsed spallation sources. Niels Bohr Institute, University of Copenhagen  
Dmytro Korablov: Mg-based hydrides and alkali metal borohydrides for solid state hydrogen storage: mechano-chemical activation and doping, Dept. of Chemistry, Aarhus University  
Anna D. Lande: Structural Studies of Neuroligand Interaction with the Sorting Receptors Sortilin and SorLA & Novel Role of the Dynein Complex in Germline Apoptosis in C. Elegans. Dept. of Molecular Biology and Genetics, Aarhus University  
Hanna Leemreize: Biological and bioinspired mineralization – probing heterogeneous materials, Dept. of Chemistry, Aarhus University  
Morten Brix Ley: Complex Metal Hydrides - Synthesis and Multifunctionality, Dept. of Chemistry, Aarhus University  
Phillip Malcho: Catalytic Deoxygenation of Renewable Chemicals - Structure-Performance Studies, DTU Chemistry  
Selma Maric: Development of a stealth carrier system for structural studies of membrane proteins in solution, Niels Bohr

Institute and Plant Biology, University of Copenhagen

Murillo Longo Martins: Synthesis and characterization of a bio-nanocomposite for cancer treatment, Niels Bohr Institute, University of Copenhagen

Jeppe Olsen: Studies of positive modulation of  $\alpha 4\beta 2$  nicotinic acetylcholine receptors, Dept. of Drug Design and Pharmacology, University of Copenhagen

Kasper S. Pedersen: Approaches to Fluoride-Bridged Molecular Magnetic Materials, Trigonal Lanthanide Single-Ion Magnets, Dept. of Chemistry, University of Copenhagen

Martin Cramer Pedersen: Mathematical, computational, and statistical aspects of model refinement from small-angle scattering data, Niels Bohr Institute, University of Copenhagen.

Kirsten Schuh, Hydrothermal synthesis of molybdenum based oxides for the application in catalysis, Karlsruhe Institute of Technology (KIT), (defended, published 2015)

Paulina Seweryn: Structural characterization of the carbon-phosphorus lyase & biochemical and structural studies of nuclear exosome co-factors: Rrp6, Rrp47 and Mpp6, Dept. of Molecular Biology and Genetics, Aarhus University

Azadeh Shahsavar: Structural Studies of Pentameric Ligand-Gated Ion Channels: Acetylcholine Binding Protein Model System and Full-Length bacterial homologue, GLIC, Dept. of Drug Design and Pharmacology, University of Copenhagen

Yanbin Shen, Electrode Materials for Lithium/Sodium-Ion Batteries: From Formation Mechanism to Intercalation Mechanism, Dept. of Chemistry, Aarhus University

Marc Sigrist. Magneto-structural correlations in  $[Mn_3O]^{7+}$  core SMMs and selected 4d, 5d and 4f SMMs, Dept. of Chemistry, University of Copenhagen

Piotr Siupka: The cytokine system in vertebrate immunology - from evolution to function, Dept. of Molecular Biology and Genetics, Aarhus University

Dadi Þorsteinn Sveinbjörnsson: Design and Characterisation of Solid Electrolytes for All-Solid-State Lithium Batteries, DTU Energy

Hanne Sørensen: Analysis and Application of Whey Proteins depleted Skim Milk Systems – Microstructure. Food Science and Niels Bohr Institute, University of Copenhagen. 2014

Xinshen Tian: Structural and biophysical characterization of humanized monoclonal antibodies by small angle X-ray scattering, Dept. of Drug Design and Pharmacology, University of Copenhagen

Tim Brandt van Driel: Time Resolved X-Ray Scattering of Molecules in Solution: Approaching the Molecular Movie, DTU Physics

Ole West, Failure analysis and thermomechanical surface engineering of bearings in the wind turbine drive train, DTU Mek

Videnskabelige bøger/antologier

Videnskabelige rapporter

Bidrag til bøger/antologier/rapporter

Ghodke, S. D., G.V. Jensen, A.S.P. Svane, K. Weise, A. Søndergaard, M.A. Behrens, J.Skov Pedersen, N.C. Nielsen, J. Søndergaard Pedersen, R. Winter, and D.E. Otzen. Polymorphism, Metastable Species and Interconversion: The Many States of Glucagon Fibrils. Chapter 34 in: Bio-nanoimaging – Protein Misfolding and Aggregation, Elsevier Science, 373-386, 2014

Haldrup, Kristoffer; Nielsen, Martin Meedom. Measuring and understanding ultrafast phenomena using X-rays. The Future of Dynamic Structural Science. ed. Judith A.K. Howard; Hazel A. Sparkes; Paul R. Raithby; Andrei V. Churakov. Springer Science+Business Media B.V., 2014. p. 91-113 (NATO Science for Peace and Security Series A: Chemistry and Biology).

Hansson and P. Norby “In-situ Powder X-ray Diffraction in Heterogeneous Catalysis” Chapter 4 in “In-situ Characterization of Heterogeneous Catalysts” by José Rodriguez. Jonathan Hanson and Peter J. Chupas (Eds.) 2013, John Wiley & Sons Inc. (9781118000168).

Mortensen, Kell. Characterization of Polymer Blends and Block Copolymers by Neutron Scattering: Miscibility and Nano Scale Morphology. In “Characterization of Polymer Blends: Miscibility, Morphology and Interfaces” (Eds: S. Thomas, Y. Grohens, J. P. Pillai; Publ: John Wiley & Sons Ltd.) 2014.

Nilsson, C., J. Østergaard, S.W. Larsen, C. Larsen, A. Urtti, A. Yaghmur; PEGylation of Phytantriol-Based Lyotropic Liquid Crystalline Particles - The Effect of Lipid Composition, PEG Chain Length, and Temperature on the Internal Nanostructure, Activity Annual Report 2013 Max-Lab (Lund University, Sweden)

Oddershede, Jette ; Schmidt, Søren; Lyckegaard, Allan; Lauridsen, Erik Mejdal; Wright, Jonathan Paul; Winther, Grethe. Grain centre mapping - 3DXRD measurements of average grain characteristics. In: Strain and dislocation gradients from

diffraction, Rozaliya Barabash, Gene Ice (Editors), Imperial College Press, London, 2014, p. 254-279

Pantleon, Wolfgang; Wejdemann, Christian; Jakobsen, Bo; Poulsen, Henning Friis; Lienert, Ulrich. High-Resolution Reciprocal Space Mapping for Characterizing Deformation Structures. In: Strain and dislocation gradients from diffraction, Rozaliya Barabash, Gene Ice (Editors), Imperial College Press, London, 2014, p. 322-357.

Poulsen, Henning Friis; Schmidt, Søren; Juul Jensen, Dorte; Sørensen, Henning Osholm; Lauridsen, Erik Mejdal; Olsen, Ulrik Lund; Ludwig, Wolfgang; King, Andrew ; Wright, Jonathan Paul; Vaughan, Gavin B. M. 3D -Ray Diffraction Microscopy. In: Strain and Dislocation Gradients from Diffraction: Spatially-Resolved Local Structure and Defects . ed. Rozaliya Barabash; Gene Ice. World Scientific Publishing Co Pte Ltd, 2014. p. 205-253.

Working papers/arbejdspapirer/preprints

Konferenceartikler, peer reviewed

Se venligst bilag 3

Konferenceartikler, ikke peer reviewed

Se venligst bilag 3

Patenter, patentansøgninger

Datasæt (x hvis afleveret til Dansk Data Arkiv)

Planlagte publikationer (angiv type)

#### Anden formidling

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

Se også bilag 3 for flere formidlingsaktiviteter.

EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark June 15-18, 2014

ESOF Conference. Copenhagen Jun 22-26, 2014

Niels Bech Christensen, Danmarks Tekniske Universitet om ESS, TV2 Lorry 9/9 2014,

Lefmann, K. MAX-IV og ESS i Lund, en kæmpe chance for nordisk forskning indenfor materialer og bio-videnskaber, Folkemødet, Allinge, juni 2014

Lefmann, K., A. Bakke, Nordic Neutron Scattering Communities 2008-2013 - a bibliometric study, February 2014

Karen Pantleon, Danmarks Tekniske Universitet, Member of the Helmholtz Zentrum Berlin HZB Scientific Selection Panel, College C6 Material Sciences and Hard Condensed Matter, 2014

## Rådgivning

Fx artikler, videnskabelige rapporter, mm.

## Undervisning

Fx lærebøger, kompendier, kurser, kandidatuddannelser

DANSCATT bidrager til at en lang række studerende (se venligst bilag1) på både bachelor-, master- og ph.d.-niveau kan deltage i måletidsrejser og foretage eksperimenter, både i forbindelse med kurser og som en del af arbejdet med deres specialer og afhandlinger. Der er blevet vejledt mere end 32 MSc og 30 BSc i 2014.

DANSCATT har endvidere bidraget til følgende ph.d.-kurser og -skoler (flere findes i bilag 3):

Summerschool: Applications of X-ray and neutron scattering in biology, chemistry and physics. Collaboration between University of Copenhagen, Technical University of Denmark, Lund University and Roskilde University.

Ecostore Summerschool, Hvide Sande, Denmark, October 8, 2014.

iNANO Autumn School 2014, Grenå, Denmark October 10-12, 2014

International PhD-School "Geometry and Topology of Liquid Crystals" at RMIT, Melbourne

## 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. Formidlingsegnet 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?

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

Fremtidens avancerede materialer og lægemidler vil kræve større kendskab og 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 målerejser til disse faciliteter. Danmark er medlem af faciliteter som ESRF og ILL i Grenoble og European XFEL i Hamborg. Desuden er Danmark 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 development goes in the direction of smaller source sizes, better x-ray optics, new detectors with higher efficiency and better resolution combined with advanced software analysis tools. Several laboratories do no longer have in-house structural x-ray facilities, but only rely on the access to international facilities. DANSCATT ensures access and supports beamtime travels to these facilities. Denmark is a member of facilities like ESRF and ILL in Grenoble and the European XFEL in Hamburg. Furthermore, Denmark is co-hosting the European Spallation Source (ESS) in Lund. DANSCATT

ensures the Danish qualifications in this area on a long term basis that will give Danish research groups and companies the biggest impact at these facilities.

Maks. 5 vigtigste publikationer

D. Müter, H.O.Sørensen, D. Jha, R. Harti, K.N. Dalby, H. Suhonen, F. Engstrøm, R. Feidenhans'l, S. L. Stipp. Resolution dependence of petrophysical parameters derived from X-ray tomography of chalk. Appl. Phys. Lett. 105, 043108; doi: 10.1063/1.489196

Tyrsted, C.; Lock, N.; Jensen, K. M. Ø.; Christensen, M.; Bøjesen, E. D.; Emerich, H.; Vaughan, G.; Billinge, S. J. L.; Iversen, B. B., Evolving atomic structure during nanoparticle formation, IUCr-J 2014, 1, 165-171.

Wang, K., Sitsel, O., Meloni, G., Autzen, H. E., Andersson, M., Klymchuk, T., Nielsen, A. M., Rees, D. C., Nissen, P., and Gourdon, P. (2014) Structure and mechanism of Zn<sup>2+</sup>-transporting P-type ATPases, Nature 514, 518-522.

Wenkai Zhang, Roberto Alonso-Mori, Uwe Bergmann, Christian Bressler, Matthieu Chollet, Andreas Galler, Wojciech Gawelda, Ryan G. Hadt, Robert W. Hartsock, Thomas Kroll, Kasper S. Kjær, Katharina Kubiček, Henrik T. Lemke, Huiyang W. Liang, Drew A. Meyer, Martin M. Nielsen, Carola Purser, Joseph S. Robinson, Edward I. Solomon, Zheng Sun, Dimosthenis Sokaras, Tim B. van Driel, György Vankó, Tsu-Chien Weng, Diling Zhu, Kelly J. Gaffney, Tracking Excited State Charge and Spin Dynamics in Iron Coordination Complexes, Nature, 509, 345-349 (2014), doi:10.1038/nature13252

Søren Roi Midtgaard, Martin Cramer Pedersen, Jacob J.K. Kirkensgaard, Kasper K. Sørensen, Kell Mortensen, Knud J. Jensen, Lise Arleth. Self-Assembling Peptides form Nanodiscs that stabilize Membrane Proteins. Soft Matter 10, 738-752, 2014. DOI: <http://dx.doi.org/10.1039/c3sm51727f>

E. Brok, M. Sales, K. Lefmann, L.T. Kuhn, W.F. Schmidt, B. Roessli, P. Robinson, S.A. Mcenroe, R.J. Harrison, Experimental evidence for lamellar magnetism in hemo-ilmenite by polarized neutron scattering, Phys. Rev. B 89, 054430 (2014)

Andre væsentlige resultater

Gem som

Reset Form

<b>Groupleader</b>	<b>VIP's (Professors, Senior scientists etc.)</b>	<b>Postdocs</b>	<b>PhD students</b>	<b>Students</b>	<b>TAP's (Technicians, Administrative staff etc.) and Scientific assistants</b>
<b>David Field</b> Electron-Molecule Scattering, Dept. of Physics and Astronomy, Aarhus University	David Field	Andrew Cassidy	Jakob Jørgensen		
<b>Søren S. Thirup</b> Dept. of Molecular Biology, Aarhus University	Bjørn P. Pedersen Ditlev E. Brodersen Gregers R. Andersen Jan K. Jensen Lasse B. Jenner Poul Nissen Rune Hartmann Søren S. Thirup Thomas Boesen	Alessia Arduin Andreas Bøggild Anne-Marie L. Winther Antoni Kowalski Azadeh Shahsavari Claus Olesen Esben Quistgaard Florian Hilbers Frederik T. Hansen Hans Henrik Gad Ingrid Dach Jacob L. Andersen Johannes Bauer Joseph Lyons Kasper R. Andersen Kristian Stødkilde Laure Yatime Magnus Kjærgaard Maike Bublitz Mick Blaise Miriam Rose Ash Nick S. Laursen Peter Paulsen Rune Kidmose	Anna D. Lande Casper Larsen Claus Olesen Dennis V. Pedersen Dorota Focht Dovile Januliene Emil Dedic Ewa Terczynska-Dyla Goran Bajic Haili Lin Henriette Autzen Jacob Ulstrup Janus A. Schatz-Jacobsen Jaslyn M.M.E. Wong Jeryl X.J. Cheng Jonas L. Gregersen Kehan Xu Kira Gysel Maja Holch Nielsen Manuela Gorgel Mateusz Dyla Meilee Ling Mikkel S. Ibsen Morten Torvund-Jensen	Christian Thrysøe Diana Kowalik Jakob Ulstrup Janus Dam Adler Jeppe A. Nielsen Joachim P. Vilstrup Julie Bolding Kirstine Louise Bendtsen Line Eriksen Luna Tjerrild Marlene Sørensen Martin Hansen Metta A. Berentsen Milena Laban Rasmus Pihl Sanne Ea Jørgensen Trine Gadeberg	Anne Marie Nielsen Anne N. Holdensen Christine J.F. Nielsen Dorthe J. Strandbygaard Gitte Ratz Jesper L. Karlsen Karen Bech Karen Margrete Nielsen Karen Marx Karthiga Thavachelvam Khaled Taj Lan B. Van Lotte T. Pedersen Sofia Mortensen Susanne Vends Tetyana Klymchuk

			Nicholas E. Sofos Nikolsj D. Drachmann Oleg Sitsel Patricia R. Fuertes Paulina Seweryn Peter Paulsen Piotr Siupka Rasmus K. Jensen Rasmus Kock Flygaard Sigrid T. Larsen Tobias Kromann-Hansen		
<b>Bo Brummerstedt Iversen,</b> Dept. of Chemistry, Aarhus University	Bo Brummerstedt Iversen Dorthe B. Ravnsbæk Henrik Birkedal Jacob Overgaard Jens-Erik Jørgensen Mads Ry Jørgensen Martin Bremholm Mogens Christensen Torben R. Jensen	Ann-Christin Dippel Dipankar Saha Gilles Philippot Hazel Reardon Lai Chin Wu Marian Stingaciu Mark Paskevicius Martin Søndergaard Nikolay Tumanov Niels Bindzus Per R. Christensen Simon Johnsen Venkatesha Hathwar	Anders B. Blichfeld Anders J. Mørup Bjarne R. S. Hansen Casper W. Andersen Casper Ibsen Cecilia Granados Miralles Elisabeth Grube Ellen Jensen Elsa Roedern Espen D. Bøjesen Espen Eikeland Fiona Bach-Gansmo Gharib Doost Hanna Leemreize Henrik Hellstern Jean-Fabien Petit Jiawei Zhang Kasper Borup Kasper Møller Kristian Andreasen Lars H. Jepsen Lirong Song Maja Krüger Thomsen Marco Calizzi	Alexander Sangsong Fogh Amanda Andersen Anders C. S. Jensen Anders S. Jakobsen Anna Pistilli Anna Zink Aske Jørgensen Bjørn S. Bruun Camilla Hjort Kronbo Daniel Huertas Sánchez Dorrit B. Nielsen Elpinikki Lappa Erika Dematteis Giuditta Perversi Henriette Ravn Jakob Bæk Grinderslev Jakob Sigvardt Karl F. Fischer Kasper Houlberg Kirstine Dalgaard Kristian Kläning Louise Møller Maika Klemmer Martin Bondesgaard	Aref Mamakhel Bo Richter Britta Lundtoft Henrik L. Andersen Jacob Becker Marianne Sommer Payam Javadian Peter Hald

			Marie Krogsgaard Matilde Saura Mattia Sist Mette S. Filsø Mie Birkbak Morten B. Ley Morten Bormann Nielsen Nanna Wahlberg Paulina Kuziora Peter Nørby Priscilla Huen Sebastian Christensen Seyed Hossein Payandeh Simon Frølich Simone M. Søndergaard-Pedersen Solveig R. Madsen Steinar Birgisson Vicki Nue Yanbin Shen	Martin Roelsgaard Martin Schmidt Mathias Jørgensen Mathilde Gestin Mette Borup Morten Christiansen Nina Kølln-Wittig Niklas Durhuus Vichairat Nikolai Moestrup Pernille Mikkelsen Peter Søgaard Rasmussen Peter Thygesen Ram Sarusie Sanna Sommer Steffan Schmidt Steffen Pedersen Steffen R. Jensen Svend Lemming Jacobsen Thomas Gillain Torben G. Jensen Troels Christiansen Ubonrat Mueanchat	
<b>Henning Friis Poulsen,</b> DTU Physics, Technical University of Denmark (including DTU Wind, DTU Cen, DANCHIP, and DTU Energy Conversion)	Bente Lebech Christian Danvad Damsgaard Didier Blanchard Henning Friis Poulsen Jens Wenzel Andreasen Kristoffer Haldrup Luise Theil Kuhn Martin Meedom Nielsen Morten Christensen Morten Vesterager Madsen	Anders Clemen Jakobsen Anette Vickery Britt Rosendahl Christian Wejdemann Hugh Simons Jacob Larsen Kasper Skov Kjær Mahrez Amri Marie Lund Traulsen Tim Brandt van Driel	Alberto Cereser Ane Sælland Christensen Dadi Þorsteinn Sveinbjörnsson Chaoling Xu Emil Bøje Lind Pedersen Ellen Fogh Elisa Biasin Jacob Madsen Lea Hildebrandt Rossander Mads Laursen Malgorzata Makowska	Anton Bay Andersen Jacob Peter Thorsbro Jonas Lundholm Bertelsen Katrine Elsøe Marcus Schultz	Carsten Gundlach Erik Brok Erik Knudsen Finn Saxild Hanne Sørensen Jan Kehres Jette Oddershede Ove Rasmussen Peter Kjær Willendrup

	Niels Bech Christensen Niels Hessel Andersen Philip Zielke Poul Norby Rune Esben Johnsen Simone Sanna Sørensen Schmidt Tejs Vegge Yubin Zhang		Marta Majkut Michael Corazza Mie Møller Storm Peter Mahler Larsen Peter Vester Salvatore De Angelis Sonja Rosenlund Ahl		
<b>Wolfgang Pantleon</b> DTU Mechanical Engineering, Technical University of Denmark	Grethe Winther Karen Pantleon Marcel Somers Thomas Christiansen Wolfgang Pantleon	Matteo Villa	Bastian Brink Federico Bottoli Nikolai Ytterdal Juul Ole West Sunday Chukwudi Okoro		Flemming Bjerg Grumsen
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<b>Anker Degn Jensen</b> DTU Chemical Engineering, Technical University of Denmark	Anker Degn Jensen Jan-Dierk Grunwaldt Jakob Munkholt Christensen	Hudson Carvalho Martin Høj	Trine Arndal		
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	Lars Fahl Lundegaard Lone Bech Peter Nicolai Ravnborg Vennestrøm Ton V. W. Janssens				
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Institut					
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## List of Publications 2014 (bilag 2)

### Dept. of Physics and Astronomy, Aarhus University

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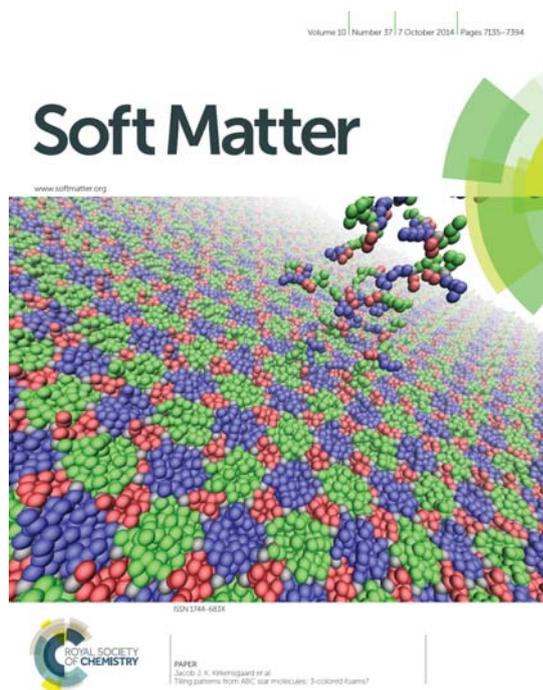
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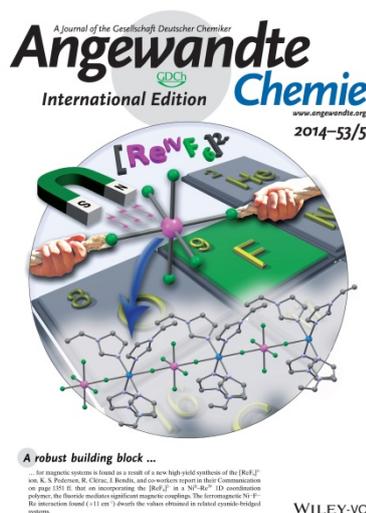
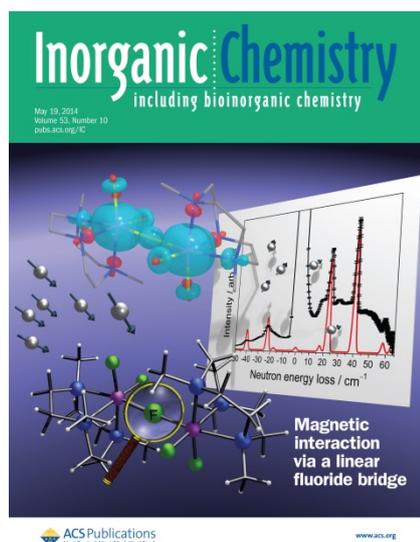
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## **List of Conferences, talks, posters and outreach activities 2014 (bilag 3)**

**Dept. of Physics and Astronomy, Aarhus University**

### **Contributions to conferences etc. 2014:**

LYDAN Leiden, The Netherlands, January 2014: Persistent Surface Voltages in Diluted Molecular Films: The implications for CO ice layers

ECOSS Antalya, Turkey, Sept 2014: Spontaneous organisation in molecular films to produce polarised solids

**Dept. of Molecular Biology and Genetics, Aarhus University**

”Krystallografi: atomer og molekyler i 3D”, 22. March 2014, Aarhus Universitet  
Organized by Lasse Bohl Jenner og Charlotte Rohde Knudsen

”40 years of Biostructural Chemistry”, 21. March 2014, Aarhus Universitet.  
Organized by Charlotte Rohde Knudsen & Lasse Bohl Jenner

”Membrane Transport Proteins Gordon Research Conference”, 13-18 July 2014, Mount Snow  
Resort, Vermont. Organized by Poul Nissen

”Diffraction methods in Structural Biology”, 26-27 July 2014, Bates College, Maine. Organized by  
Maike Bublitz

## INVITED TALKS

Title of event	Venue	Name(s) of speaker(s)
Invited seminar	Institute of Physics, CAS, Beijing	Bo Brummerstedt Iversen
Invited talk	Technical University of Dresden German Solid State Chemistry Meeting	Bo Brummerstedt Iversen
Invited talk	European Powder Diffraction Conference, Aarhus	Bo Brummerstedt Iversen
Invited seminar	University of Oregon, Eugene	Bo Brummerstedt Iversen
Prize lecture	Grundfos	Bo Brummerstedt Iversen
Invited seminar	Harbin Institute of Technology	Bo Brummerstedt Iversen
Invited seminar	Department of Physics, Aarhus	Bo Brummerstedt Iversen
Invited talk	Inanscon conference, Middelfart	Bo Brummerstedt Iversen
Invited talk	ISHA conference, Bordeaux	Bo Brummerstedt Iversen
Invited talk	IUCr conference, Montreal	Bo Brummerstedt Iversen
Invited talk	Kavli Symposium, Trondheim	Bo Brummerstedt Iversen
Invited talk	MRS Fall Meeting, Boston	Bo Brummerstedt Iversen
Invited talk	Selskabet for Naturlærens Udbredelse, København	Bo Brummerstedt Iversen
Invited talk	Technical University of Porto	Bo Brummerstedt Iversen
International Year of Crystallography in Copenhagen, "Diffraction Reveals, Size, Shape and Orientation of Nanomagnets"	H.C. Ørsted Institute, Copenhagen, Denmark, January 22-23, 2014	Mogens Christensen
SPIE Optical Engineering + Applications : Developments in X-Ray Tomography IX "Diffraction computed tomography reveals the inner structure of complex biominerals"	San Diego, California, USA August 19, 2014	Henrik Birkedal
Department of Physics, BOKU, "Permanent underwater attachment in the mermaid's toenail"	Universität für Bodenkultur Wien Vienna, Austria, October 8, 2014	Henrik Birkedal
MCARE 2014: Materials Challenges in Alternative & Renewable Energy Novel multi-purpose hydrides Invited tutorial talk	Clearwater, USA February 17-20, 2014	Torben René Jensen
MRS Spring Meeting & Exhibit "Investigation of New Hydrides Using In-Situ Powder Diffraction"	San Francisco, California, USA April 21-25, 2014	Torben René Jensen
IDHEA International Discussion on Hydrogen Energy and Applications "New ideas for hydrogen storage"	Nantes, France May 12-14, 2014	Torben René Jensen
The HyFillFast project: Fast, efficient and high capacity hydrogen refueling and onboard storage	ENERGY AND ENVIRONMENT FOR THE FUTURE, The Programme Commission on Sustainable Energy and Environment, Innovation Fund Denmark, 24 – 25 November, København	Torben René Jensen
MRS Spring Meeting, "Diffraction Tomography: A Window on Complex Hierarchical Materials" Abstract AAA6.04	San Francisco, USA April 23, 2014	Henrik Birkedal
E-MRS, "Formation of apatite nanocrystals from amorphous calcium phosphate – insight from in situ X-ray diffraction"	Lille, France May 26, 2014	Henrik Birkedal
Euro Bio-Inspired Materials "Mussel Power – Mimicking Nature"	Potsdam, Germany March 18-21, 2014	Marie Krosgaard
23rd Congress and General Assembly of the IUCr, "Synchrotron charge density studies of chemical bonding in the polymorphs of FeS <sub>2</sub> "	Montreal, Canada August 05-12, 2014	Jacob Overgaard
23rd Congress and General Assembly of the IUCr, "In situ growth of SrFe <sub>12</sub> O <sub>19</sub> "	Montreal, Quebec, Canada August 04-13, 2014	Mogens Christensen
23rd Congress and General Assembly of the IUCr, "Accurate Charge Densities from Synchrotron Powder Diffraction"	Montreal, Quebec, Canada August 04-13, 2014	Niels Bindzus

23rd Congress and General Assembly of the IUCr, <i>“Material Design Inputs from Charge Density Analysis in Organic Semiconductors”</i>	Montreal, Quebec, Canada August 04-13, 2014	Venkatesha Rama Hathwar
23rd Congress and General Assembly of the IUCr, <i>“Nuclear Enhanced MEM Used to Analyze Local Distortion in Lead Chalcogenides”</i>	Montreal, Quebec, Canada August 04-13, 2014	Sebastian Christensen
23rd Congress and General Assembly of the IUCr, <i>“Effect of Pressure on Mixed Valence FeII/FeIII Complex”</i>	Montreal, Quebec, Canada August 04-13, 2014	Solveig Røgild Madsen
23rd Congress and General Assembly of the IUCr, <i>“In- and ex situ PXRD studies of ZnO nanoparticle growth in sub-critical water”</i>	Montreal, Quebec, Canada August 04-13, 2014	Espen Draht Bøjesen
EPDIC14 – The European Powder Diffraction Conference, <i>“HEIMDAL”</i>	Aarhus University, Department of Chemistry, Denmark, June 15-18, 2014	Mogens Christensen

## OTHER CONTRIBUTIONS:

Title of Contribution	Author (external authors in <i>Italics</i> )	Event and place	Date
Conference organization	Bo Brummerstedt Iversen, Henrik Birkedal, Jens-Erik Jørgensen, Martin Bremholm	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
Conference organization	Bo Brummerstedt Iversen,	Danish Chemical Society, 10 <sup>th</sup> Aarhus Winter Meeting 2014, Department of Chemistry, Aarhus University, Denmark	January 24, 2014
<i>“DANMAX for diffraction”</i>	Mogens Christensen	Nordic X-Ray Science Days Lund, Sweden	Sept. 29 – Oct. 1, 2014
<i>“Materialers fødsel – og deres indre struktur”</i>	Mogens Christensen	UNF Chemistry CAMP Aarhus, Denmark	18/07/2014
<i>“ESS - Neutrons for nanocharacterisation”</i>	Mogens Christensen	Technet_nano - Stakeholder Day, Alsion, Syddansk Universitet, Sønderborg, Denmark	March 20, 2014
<i>“Hydrogen Containing Solids - New Perspectives”</i>	Torben René Jensen	Seminar on Hydrogen and Proton Conducting Materials Technical University of Denmark, Department of Energy Conversion and Storage, Lyngby, Denmark	August 7, 2014
<i>“Nanomagnetism – for permanent magnets”</i>	Mogens Christensen	Magnetic Materials symposia Uppsala, Sweden	December 11, 2014
<i>“Nanomagnets”</i>	Mogens Christensen	Aarhus-Harbin Workshop on Nanomaterials Harbin, China	January 3-9, 2014
<i>“In situ diffraction studies of the maghemite formation under control by mussel-inspired additives”</i>	Vicki Nue, Henrik Birkedal	MRS Spring Meeting, San Francisco, USA	April 23, 2014
<i>“Synthesis of Hydrogen storage materials, solvent based, mechanochemistry and Schlenk techniques”</i>	Torben R. Jensen	Ecostore Summerschool Hvide Sande, Denmark	October 8, 2014
<i>“Synthesis of Battery materials, solid state and hydrothermal synthesis, oxides and nitrides”</i>	Torben R. Jensen	Ecostore Summerschool Hvide Sande, Denmark	October 8, 2014
<i>“New Materials for Energy Storage” (Invited lecture)</i>	Torben R. Jensen	Hydrogen Storage Workshop, Department of Advanced Materials and Technologies, Military University of Technology, Warsaw, Poland.	December 3-4, 2014
<i>“Effect of pressure on mixed valence FeII/FeIII complex”</i>	Solveig Røgild Madsen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting	May 23, 2014

		Lyngby, Denmark	
"Mussel Power – Mimicking Nature"	Marie Krogsgaard	Scandinavian Society for Biomaterials 7 <sup>th</sup> Annual Meeting iNANO, Aarhus, Denmark	March 26-28, 2014
<i>Influence of osteopontin on apatite formation</i>	Casper J. S. Ibsen	COST Action TD0903 - BIOMINERALIX - Final conference, Granada, Spain	April 14-16, 2014
<i>Carbonate Modifies Apatite Nanocrystal Formation</i>	Casper J. S. Ibsen	MRS Spring Meeting, San Francisco, USA	April 21-25, 2014
<i>Compact Bone Studied by Diffraction Tomography</i>	Mie Birkbak	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014

## POSTER CONTRIBUTIONS:

Title of poster	Authors (external authors in <b>Italics</b> )	Event and place	Date
<i>A biomineralized underwater attachment system operating under tension – Nano-mechanical properties of Anomia simplex</i>	Simon Frølich, Henrik Birkedal	Bio-inspired Materials Conference, Berlin Germany	March 2014
<i>A biomineralized underwater attachment system operating under tension – Nano-mechanical properties of Anomia simplex</i>	Simon Frølich, Henrik Birkedal	Gordon Research Seminar: Biomineralization New London, NH, USA	August 2014
<i>A biomineralized underwater attachment system operating under tension – Nano-mechanical properties of Anomia simplex</i>	Simon Frølich, Henrik Birkedal	12th iNANO Annual Meeting, Aarhus, Denmark	January 2014
<i>A series of new manganese borohydride ammoniates</i>	Lars H. Jepsen, Morten B. Ley, <b>Y. Filinchuk</b> , Torben R. Jensen	12th iNANO Annual Meeting, Aarhus, Denmark	January 16, 2014
<i>Accurate Charge Densities from Powder Diffraction</i>	Niels Bindzus, Nanna Wahlberg, Jacob Becker, <b>A-C. Dippel</b> , Bo B. Iversen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Alkali Metal Strontium Borohydrides</i>	Kasper T. Møller, Morten B. Ley, <b>R. Schouwink</b> , <b>R. Cerny</b> , Torben R. Jensen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Alkali and alkali earth metal borohydride ammoniates for energy storage</i>	J. Grinderslev, Lars H. Jepsen, Torben R. Jensen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Denmark.	May 22, 2014
<i>Alkali earth metal borohydride ammoniates</i>	Ram Sarusie, Lars H. Jepsen, <b>M.H. Sørby</b> , <b>R. Cerný</b> , Torben R. Jensen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Alkali earth metal borohydride ammoniates as future NH<sub>3</sub> and/or H<sub>2</sub> storage materials</i>	Ram Sarusie, Lars H. Jepsen, Torben R. Jensen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Denmark	May 22, 2014
<i>Amine Templated Two Dimensional Tin Sulfides</i>	Nina Lock, Mette Ø. Filsø, Mogens Christensen, Bo B. Iversen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Between diamonds and a hard place: A SrMnO<sub>3</sub> study</i>	Morten B. Nielsen, Martin Bremholm, <b>D. Ceresoli</b> , <b>P. Parisiades</b> , Bo B. Iversen	Danish Chemical Society, 10 <sup>th</sup> Aarhus Winter Meeting 2014, Department of Chemistry, Aarhus University, Denmark	January 25, 2014
<i>Between diamonds and a hard place: A SrMnO<sub>3</sub> study</i>	Morten B. Nielsen, Martin Bremholm, <b>D. Ceresoli</b> , <b>P. Parisiades</b> , Bo B. Iversen	12th iNANO Annual Meeting, Aarhus, Denmark.	January 16, 2014
<i>Bi- and trimetallic borohydrides in the Li-K-Mg system</i>	Ubonrat Mueanchat, Elsa Roedern, Torben R. Jensen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Denmark.	May 22, 2014
<i>Bimetallic Borohydrides Synthesized from Sr(BH<sub>4</sub>)<sub>2</sub> and Alkali Metal</i>	Kasper T. Møller, Morten B. Ley, <b>P. Schouwink</b> , <b>R.</b>	MH 2014, Manchester, Storbritannien	July 20-25, 2014

<i>Borohydrides</i>	<b>Cerný</b> , Torben R. Jensen		
<i>Cobalt ferrites nanoparticles obtained by hydrothermal continuous flow synthesis method</i>	Marian Stingaciu	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Coccolithophorids, Mussel Shells and Chalk - a comparison of the microstructure of biogenic calcite of different origin</i>	Simon Frølich	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Continuous hydrothermal flow synthesis and characterization of SnO<sub>2</sub> nanoparticles - control of size and morphology</i>	Henriette Ravn Larsen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Core polarization of silicon in <math>\alpha</math>-silicon</i>	Nanna Wahlberg, Bo B. Iversen, Niels Bindzus, Lasse Bjerg, Jacob Becker	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Core polarization of silicon in <math>\alpha</math>-silicon</i>	Nanna Wahlberg, Bo B. Iversen, Niels Bindzus, Lasse Bjerg, Jacob Becker	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>Decomposition of <math>g</math>-Mg(BH<sub>4</sub>)<sub>2</sub>-X composites, X = LiH, NaH, CaH<sub>2</sub>, MgH<sub>2</sub></i>	Elisabeth Grube	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Determination of the transition pressure from <math>\alpha</math>-Mn(BH<sub>4</sub>)<sub>2</sub> to <math>\delta</math>-Mn(BH<sub>4</sub>)<sub>2</sub></i>	<b>D.B. Nielsen</b> , Elsa Roedern, Torben R. Jensen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>Development of a direct synthesis of ZnSb</i>	Anders B. Blichfeld, Bo B. Iversen, Simon Johnsen	International Conference on Thermoelectrics - ICT2014	July 9, 2014
<i>Effect of Pressure on a Mixed Valence Fe<sup>II</sup>Fe<sup>III</sup><sub>2</sub> Complex</i>	Solveig R. Madsen, Jacob Overgaard, Bo B. Iversen	23rd Congress and General Assembly of the IUCr, Montreal, Canada.	August 8, 2014
<i>Electrochemical performance of LiM(BH<sub>4</sub>)<sub>3</sub>Cl, M = La, Ce, Gd</i>	Morten Brix Ley, <b>R. Janot</b> , <b>R. Filinchuk</b> , Torben R. Jensen	International symposium on Metal-Hydrogen Systems 2014, Manchester, Storbritannien	July 24, 2014
<i>Exploring Host-Guest Interactions in Organic Clathrates: A Single Crystal High Pressure X-Ray Diffraction Study</i>	Espen Eikeland, Solveig R. Madsen, Jacob Overgaard, Bo B. Iversen	HERCULES, Grenoble, Frankrig.	March 2014
<i>Extracting the resistivity tensor from van der Pauw measurements</i>	Karl F.F. Fischer, Kasper A. Borup, Bo B. Iversen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>Formation, Growth and Phase Transition of Colloidal Monodisperse Spherical Copper Sulphide Nanocrystals: An In Situ XRD Study</i>	Peter Nørby	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Formation and Growth of Magnetic <math>\gamma</math>-Fe<sub>2</sub>O<sub>3</sub> Nanocrystallites under Hydrothermal Conditions</i>	Henrik L. Andersen, Kirsten M.Ø. Jensen, Christoffer Tyrsted, Espen D. Bøjesen, Steinar Birgisson, Mogens Christensen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>Formation of Size-Controlled SrFe<sub>12</sub>O<sub>19</sub> Nano-Particles by Hydrothermal Synthesis</i>	Anna Z. Mortensen, Cecilia Granados, Mogens Christensen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Functionally Graded Thermoelectrics by Bulk Crystal Growth</i>	Ellen M.J. Hedegaard, Simon Johnsen, Lasse Bjerg, Kasper A. Borup, Bo B. Iversen	6th International Workshop on Crystal Growth Technology, Berlin, Tyskland	June 16, 2014
<i>High-Pressure Equipment for Investigation of Hydrogen Storage Materials</i>	Kasper T. Møller, Bjarne R.S. Hansen, <b>C.J. Webb</b> , Torben R. Jensen	12th iNANO Annual Meeting, Aarhus, Danmark	January 16, 2014
<i>Hydrothermal formation of Sr-ferrite through an intermediate phase</i>	Cecilia Granados	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>Hydrothermal In and Ex Situ PXRD Study of MSb<sub>2</sub>O<sub>4</sub> (M = Mn, Fe, Co) Functional Materials</i>	Martin Roelsgaard	EPDIC 14, Aarhus, Danmark	June 15-18, 2014

<i>Hydrothermal synthesis of rare earth-free magnetic nanoparticles</i>	Matilde Saura, Cecilia Granados, Espen D. Bøjesen J. Song, M. Dong, Mogens Christensen.	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>In- and ex situ PXRD studies of the influence of various synthesis parameters on the growth of ZnO nanoparticles in sub-critical water</i>	Espen D. Bøjesen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>In situ crystallization of SrFe<sub>2</sub>O<sub>19</sub></i>	Cecilia Granados	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>In situ Powder X-ray Diffraction at High Pressure</i>	Kasper T. Møller, Bjarne R.S. Hansen, <b>C.J. Webb, A.-C. Dippel</b> , Torben R. Jensen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>In situ study of hydrothermal MnO<sub>2</sub> formation</i>	Steinar Birgisson, Yanbin Shen, Bo B. Iversen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>In-situ PXRD studies of ZnO nanoparticle growth: How do various salts influence the hydrothermal growth of ZnO?</i>	Espen D. Bøjesen	12th iNANO Annual Meeting, Aarhus, Danmark.	January 16, 2014
<i>In situ SR-PXD studies of eutectic melting borohydrides</i>	Morten Brix Ley	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>In situ Total Scattering Study of WO<sub>3</sub> Nanoparticle under Hydrothermal Condition</i>	Dipankar Saha	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>In situ X-ray diffraction studies of apatite nanocrystal formation from an amorphous precursor in water</i>	Casper J.S. Ibsen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Integration of Neutron Time-of-Flight Single-Crystal Bragg Peaks in Reciprocal Space</i>	<b>A.J. Schultz</b> , Mads Ry Jørgensen, <b>X. Wang, R. Mikkelsen, D. Mikkelsen, V. Lynch, P. Peterson, M. Green, C. Hoffmann</b>	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>Integration of Neutron Time-of-Flight Single-Crystal Bragg Peaks in Reciprocal Space</i>	<b>A.J. Schultz</b> , Mads Ry Jørgensen, <b>X. Wang, R. Mikkelsen, D. Mikkelsen, V. Lynch, P. Peterson, M. Green, C. Hoffmann</b>	American Conference on Neutron Scattering, Knoxville, TN, USA.	June 4, 2014
<i>Investigating disorder and anharmonicity in cadmium and zinc telluride</i>	Mattia Sist	23rd Congress and General Assembly of the IUCr, Montreal, Canada.	August 5, 2014
<i>Investigation of Orbital Disorder in Ca-doped LaMnO<sub>3</sub></i>	Peter Thygesen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Investigation of Novel Tellurium Based Thermoelectric Material: Synthesis and Characterisation of K<sub>2</sub>SnTe<sub>5</sub></i>	Aske Jørgensen	INASCON, Aarhus, Danmark.	August 11, 2014
<i>LiM(BH<sub>4</sub>)<sub>3</sub>Cl (M = La, Ce, Gd) - New lithium ion conductors</i>	Morten B. Ley, <b>R. Janot, Y. Filinchuk</b> , Torben R. Jensen	556 Wilhelm and Else Heraeus Seminar, Bad Honnef, Tyskland.	March 24, 2014
<i>Location of Cu<sup>2+</sup> in CHA Zeolite Using Rietveld/MEM: Racing towards cleaner air via Cu-CHA zeolite</i>	Casper W. Andersen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>Location of Cu<sup>2+</sup> in CHA Zeolite Using Rietveld/MEM: Racing towards cleaner air via Cu-CHA zeolite</i>	Casper W. Andersen	23rd Congress and General Assembly of the IUCr Montreal, Canada	August 8, 2014
<i>Location of Cu<sup>2+</sup> in CHA Zeolite Using Rietveld/MEM: Racing towards cleaner air via Cu-CHA zeolite</i>	Casper W. Andersen	iNANO Autumn School Poster pris ved iNANO Autumn School 2014	October 10-12, 2014
<i>Low temperature synthesis of unstable</i>	Elsa Roedern, Torben R.	12th iNANO Annual Meeting,	January 16,

<i>metal borohydride ammoniates</i>	Jensen	Aarhus, Danmark	2014
<i>Maghemite nanoparticle formation under the influence of mussel-inspired additives</i>	Vicki Nue, Haraldur P. Gunlaugson, Henrik Birkedal	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Magnesium based materials for hydrogen storage</i>	Elisabeth Grube, Torben R. Jensen	Energy and Environment for the Future, Innovationsfonden, Copenhagen, Denmark	November 24, 2014
<i>Mn(BH<sub>4</sub>)<sub>2</sub> - M(BH<sub>4</sub>)<sub>x</sub> &amp; Mn(BH<sub>4</sub>)<sub>2</sub> - MH<sub>x</sub> composites, M = Li, Na, Mg and Ca</i>	Elsa Roedern, Torben R. Jensen	MH 2014, Manchester, Storbritannien.	July 24, 2014
<i>Nanoconfinement of extremely low melting eutectic metal borohydrides: LiBH<sub>4</sub>-KBH<sub>4</sub></i>	Bjarne R.S. Hansen, Morten B. Ley, Torben R. Jensen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Nature's path to improved semiconductors</i>	Anders C.S. Jensen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>New eutectic system xLiBH<sub>4</sub>-1-xKBH<sub>4</sub> (x = 0.70-0.75)</i>	Morten B. Ley, Elsa Roedern, Torben R. Jensen	International symposium on Metal-Hydrogen Systems 2014, Manchester, Storbritannien	July 24, 2014
<i>New phases in thin-films of the Zn-Sb system</i>	Anders B. Blichfeld, Bo B. Iversen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark	May 22, 2014
<i>Novel Sulfur Diimide Ligands</i>	Maika Klemmer, <b>M. Meinholz, D. Stalke</b>	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>Novel metal borohydride ammoniates</i>	Lars H. Jepsen, Morten B. Ley, Dorthe B. Ravnsbæk, <b>S.H. Hwang, Y. Lee, Y. Filinchuk, R. Cerný</b> , Torben R. Jensen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Nuclear Enhanced X-ray Maximum Entropy Method Used to Analyze Local Distortions in Simple Structures</i>	Sebastian Christensen, Niels Bindzus, Mogens Christensen, Bo B. Iversen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Phase stability of the SrMnO<sub>3</sub> hexagonal perovskite system at high pressure and temperature</i>	Morten B. Nielsen, <b>D. Ceresoli, P. Parisiades, V.B. Prapenka, T. Yu, Y. Wang</b> , Martin Bremholm	Gordon Research Conference, USA.	June 2014
<i>Pushing the limits of structure determination using SR-PXRD and Rietveld/MEM</i>	Casper Welzel Andersen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Size and Shape Control of SrFe<sub>12</sub>O<sub>19</sub> Nanoparticles through Supercritical Synthesis</i>	Matilde Saura, Cecilia Granados, Espen D. Bøjesen, J. Song, M. Dong, M, Mogens Christensen	14th European Powder Diffraction Conference, Aarhus, Danmark.	June 15-18, 2014
<i>Size and Size Distribution Control of Magnetic <math>\gamma</math>-Fe<sub>2</sub>O<sub>3</sub> Nanoparticles</i>	Henrik L. Andersen, Kirsten M.Ø. Jensen, Christoffer Tyrsted, Espen D. Bøjesen, Mogens Christensen	12th iNANO Annual Meeting, Aarhus, Danmark	January 16, 2014
<i>Solvothermal flow synthesis and PXRD study of the Pt<sub>1-x</sub>Ru<sub>x</sub> system</i>	Martin Bondesgaard	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Supercritical Carbonization of Magnesium Silicate Clays</i>	Espen Eikeland	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Synthesis and characterization of Sr<sub>x</sub>Ba<sub>1-x</sub>Fe<sub>12</sub>O<sub>19</sub></i>	Mathilde Gestin	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Synthesis, structural characterization and thermoelectric properties of Sr<sub>x</sub>Ba<sub>1-x</sub>Nb<sub>2</sub>O<sub>6</sub> (x = 0, 0.2-0.8, 1)</i>	Giuditta Perversi	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014

<i>The Effect of Pressure on a Molecular Wire Complex</i>	Solveig R. Madsen, Maja K. Thomsen, Jacob Overgaard, Bo B. Iversen	12th iNANO Annual Meeting, Aarhus, Danmark	January 16, 2014
<i>The core electron density of Boron Nitride</i>	Nanna Wahlberg, Niels Bindzus, <b>T. Straasø</b> , Jacob Becker, <b>J. Als-Nielsen</b> , Bo B. Iversen	12th iNANO Annual Meeting, Aarhus, Danmark	January 16, 2014
<i>The structure of tin telluride</i>	Mattia Sist, Niels Bindzus, Bo B. Iversen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark.	May 22, 2014
<i>Understanding Li2B12H12</i>	Bjarne R.S. Hansen, Torben R. Jensen	12th iNANO Annual Meeting, Aarhus, Danmark	January 16, 2014
<i>Rolling the Dice; polymer controlled nucleation</i>	Anders C.S. Jensen	12th iNANO Annual Meeting, Aarhus, Danmark	January 16, 2014
<i>Natures path to improved semiconductors</i>	Anders C.S. Jensen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Natures path to improved semiconductors</i>	Anders C.S. Jensen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark	May 22, 2014
<i>Watching nanocrystals form</i>	Bo Brummerstedt Iversen	EPDIC14 – The European Powder Diffraction Conference; Dept. of Chemistry, Aarhus University, Denmark	June 15-18, 2014
<i>Osteocytic Osteolysis Induced by Immobilization in Rats</i>	Fiona Bach Gansmo	Euro Bio-Inspired Materials, Potsdam, Germany	March 18-21, 2014
<i>Gels &amp; Threads: Mussel-inspired One-pot Route to Responsive Materials</i>	Marie Krogsgaard	Gordon Research Conference: Bioinspired Materials Newry, Maine, USA	June 22-27, 2014
<i>Probing heterogeneous materials using diffraction tomography</i>	Hanna Leemreize	Euro Bio-Inspired Materials, Potsdam, Germany	March 18-21, 2014
<i>Maghemite nanoparticle formation under the influence of mussel-inspired additives</i>	Vicki Nue, Haraldur P. Gunlaugson, Henrik Birkedal	7 <sup>th</sup> Annual Meeting of the Scandinavian Society for Biomaterials, iNANO, Aarhus University, Denmark	March 2014
<i>Maghemite nanoparticle formation under the influence of mussel-inspired additives</i>	Vicki Nue, Haraldur P. Gunlaugson, Henrik Birkedal	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark	May, 2014
<i>In situ X-ray diffraction studies of apatite nanocrystal formation from an amorphous precursor in water</i>	Casper J. S. Ibsen	43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Lyngby, Danmark	May, 2014
<i>Microstructure of Narwhal Studied by Synchrotron Radiation X-ray Tomographic Microscopy</i>	Mie Birkbak, <b>Karl Anker Jørgensen</b> & Henrik Birkedal	12th iNANO Annual Meeting, Aarhus, Danmark	January 16, 2014
<i>Microstructure of Narwhal Studied by Synchrotron Radiation X-ray Tomographic Microscopy</i>	Mie Birkbak, <b>Karl Anker Jørgensen</b> & Henrik Birkedal	Danish Chemical Society, 10 <sup>th</sup> Aarhus Winter Meeting 2014, Department of Chemistry, Aarhus University, Denmark	January 14, 2014
<i>Compact Bone Studied by Diffraction Tomography</i>	Mie Birkbak, Simon Frølich, Hanna Leemreize, <b>Stuart R Stockb</b> & Henrik Birkedal	Gordon Research Seminar: Biomineralization New London, NH, USA	August 16-17, 2014
<i>Compact Bone Studied by Diffraction Tomography</i>	Mie Birkbak, Simon Frølich, Hanna Leemreize, <b>Stuart R Stockb</b> & Henrik Birkedal	Gordon Research Conference, New London, USA	August 18-22, 2014
<i>Compact Bone Studied by Diffraction Tomography</i>	Mie Birkbak, Simon Frølich, Hanna Leemreize, <b>Stuart R Stockb</b> & Henrik Birkedal	Nordic X-Ray Science Days Lund, Sweden	Sept. 29 – Oct. 1, 2014
<i>Compact Bone Studied by Diffraction Tomography</i>	Mie Birkbak, Simon Frølich, Hanna Leemreize, <b>Stuart R Stockb</b> & Henrik Birkedal	iNANO Autumn School 2014, Grenå, Denmark	October 10-12, 2014

## OUT-REACH

Type of Communication/Subject/Topic	Contributor	Event and place	Date
Invited public talk – “Nanomagneter”	Mogens Christensen	Kemilærerdag, Dept. of Chemistry, Aarhus University	January 17, 2014

SDC teaching	Mogens Christensen	Beijing, China	November 22-29, 2014
Telephone interview: Science Magasin	Mogens Christensen	Max-lab, Lund, Sweden	June 27, 2014
<i>Public Talk: "Hydrogen-samfundet - et nyt energisystem"</i>	Torben R. Jensen	Nanorama Fredagsforedrag Aarhus, Denmark	January 31, 2014
<i>Presentation: "Battery activities at AU"</i> <a href="http://batteriselskab.dk/danish-battery-symposium-2014/agenda">http://batteriselskab.dk/danish-battery-symposium-2014/agenda</a>	Martin Søndergaard	Danish Battery Symposium 2014, Haldor Topsøe, Kgs. Lyngby, Denmark	February 28, 2014
Talk: "In situ study of hydrothermal formation of spinel type LiMn <sub>2</sub> O <sub>4</sub> nanocrystals"	Steinar Birgisson	Danish Battery Symposium 2014, Haldor Topsøe, Kgs. Lyngby, Denmark	February 28, 2014
Talk: "Bulk thermoelectric materials optimization"	Simon Johnsen	Ph.d. school on applied thermoelectrics Aalborg, Denmark	March 11-14, 2014
Presentation: <i>"Under pressure: The phase behaviour of SrMnO<sub>3</sub>"</i>	Morten Bormann Nielsen	iNANO Autumn School 2014, Grenå, Denmark	October 10-12, 2014
Talk: <i>"Glue on the Rocks: Probing the consequences of interaction between organic and inorganic phases in biological materials"</i>	Simon Frølich	iNANO Autumn School 2014 Grenå, Denmark	October 10-12, 2014
Web Publication: Science Highlight <i>"Scientists watch nanoparticles grow at PETRA III"</i>	Dipankar Saha, Kirsten M.Ø. Jensen, Espen D. Bøjesen, Christoffer Tyrsted, Aref Mamakhel, Ann-Christin Dippel, Mogens Christensen, Bo B. Iversen	Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany	March 27, 2014
Talk: <i>"Biomimik – inspireret af naturen"</i> <a href="http://energimuseet.dk/Mark-your-calendar.aspx?CalendarEventID=74">http://energimuseet.dk/Mark-your-calendar.aspx?CalendarEventID=74</a>	Marie Krogsgaard	"Leonardo da Vinci" exhibition, Energimuseet, Bjerringbro, Denmark	2014
Interview: <i>"Fremtidens lim"</i>	Henrik Birkedal	Aarhus Stiftstidende, Denmark <a href="http://stiften.dk/aarhus/serie-om-aarhus-universitet-fabelagtig-forskning-paa-kontorerne">http://stiften.dk/aarhus/serie-om-aarhus-universitet-fabelagtig-forskning-paa-kontorerne</a>	October 21, 2014
Presentation on biological materials and innovation	Simon Frølich	Interskolen, Aarhus, Denmark	December 2014

**DTU Physics, DTU Energy, DTU Wind, DTU CEN, DANCHIP, Technical University of Denmark**

**Contributions to conferences etc. 2014:**

J. W. Andreasen, *High resolution ptychographic tomography of soft matter*, Abstract from 4th Workshop on X-Ray Nano-Imaging of Biological and Chemical Systems at PETRA III, Jan 30, 2014, Hamburg, Germany (Invited speaker).

M. G. Makowska, L. Theil Kuhn, M. Strobl, E. M. Lauridsen, H. L. Frandsen, A. Tremsin, Nikolay Kardjilov; *Observation of nickel oxide reduction in anodes for SOFC using energy-selective neutron imaging*, Abstract from “Neuwave meeting 2014” – workshop on neutron imaging, 2014, Garching, Germany

M. G. Makowska, L. Theil Kuhn, M. Strobl, E. M. Lauridsen, H. L. Frandsen, A. Tremsin, Takenao Shinohara; *Interplay between stress and reduction progress in electrodes for Solid Oxide Electrochemical Cells*, Abstract from “WCNR 2014”, 2014, Grindelwald, Switzerland

M. G. Makowska, L. Theil Kuhn, M. Strobl, E. M. Lauridsen, H. L. Frandsen, A. Tremsin, Takenao Shinohara; *Towards in-situ study of stress enhanced reduction*, Abstract from “Challenges and Opportunities in In Situ Studies of Solid Oxide Electrodes”, 2014, Roskilde, Denmark

E. B. L. Pedersen, P. S. Jørgensen, S. Jiang and J. W. Andreasen. Characterization of organic water dispersible nanoparticles useable in photovoltaics, 2014. Abstract from International Conference of Synthetic Metals 2014, Turku, Finland

P. Norby, *In situ Studies of Lithium Batteries; Using Synchrotron X-ray Radiation to Probe Reactions and Interfaces in Operating Batteries* Distinguished iNANO Lecture, iNANO house, University of Aarhus, Denmark, 7/2 2014.

M. Amri, A. Fitch and P. Norby *In situ high resolution synchrotron X-ray powder diffraction studies of lithium batteries*. Poster at EPDIC 14, June 15-18 2014, Århus, Denmark.

M. Amri & Poul Norby *In-situ high resolution X-ray diffraction studies of conversion battery systems* Abstract from UM14- Nordic X-Ray Science Days. 29 September - 1 October 2014 Lund,

P. Norby: *Electrochemistry live; in situ diffraction studies of battery cells*. Seminar on Battery Materials, Oslo University, Nov. 20. 2014

P. Norby: *Electrochemistry at work; in situ diffraction studies of battery cells* Abstract from UM14- Nordic X-Ray Science Days. 29 September - 1 October 2014 Lund.

Karamehmedović, M., 2014. A lower bound on the stably recoverable information for the Helmholtz equation in R<sup>2</sup>. Inverse Problems from Theory to Application (IPTA) 2014, IOP, Bristol, August 26-28 2014.

Karamehmedović, M., Hansen, P.C., and Schmidt, S., 2014. Modelling and computation for Total Crystallography. DTU Vision Day, Kgs. Lyngby, May 14 2014.

Karamehmedovic, Mirza / **Sparse data structures in 3DXRD**. 2014. Abstract from Sparse Tomo Days, Kgs. Lyngby, Denmark.

Karamehmedović, M., 2014. Inverse scattering: from formulation to application. Invited talk, Faculty of Engineering and Natural Sciences, International University of Sarajevo, Sarajevo, Bosnia and Herzegovina, March 10 2014.

Fogh, Ellen; Toft-Petersen, R.; Nojiri, H.; Kihara, T.; E. Granroth, G.; B. Stone, M.; Lee, J.; Fritsch, K.; Andersen, Niels Hessel; Vaknin, David; Christensen, Niels Bech / **High-field re-entrance of the magnetoelectric effect in LiNiPO<sub>4</sub> investigated in pulsed fields.**

2014. Poster session presented at 4th Annual Niels Bohr International Academy Workshop-School on ESS Science, Copenhagen, Denmark.

Klinkby, Esben Bryndt; Bergbäck Knudsen, Erik; Willendrup, Peter Kjær; Lauritzen, Bent; Nonbøl, Erik; Bentley, P.; Filges, U. / **Application of the MCNPX-McStas interface for shielding calculations and guide design at ESS.**

In: Journal of Physics: Conference Series (Online), Vol. 528, 2014, p. 012032.

Stöhr, Frederik; Michael-Lindhard, Jonas; Simons, Hugh; Hübner, Jörg; Jensen, Flemming; Hansen, Ole; Poulsen, Henning Friis; Garnæs, Jørgen / **Full 3D characterization of high aspect ratio microstructures.**

2014. Poster session presented at 40th International Conference on Micro and Nano Engineering, Lausanne, Switzerland.

Stöhr, Frederik; Michael-Lindhard, Jonas; Simons, Hugh; Hübner, Jörg; Jensen, Flemming; Hansen, Ole; Garnæs, Jørgen; Snigirev, A.; Poulsen, Henning Friis / **Three-Dimensional Characterization of X-ray Refractive Optics.**

Proceedings of the 40th International Conference on Micro and Nano Engineering. 2014.  
2014

Willendrup, Peter Kjær; Bergbäck Knudsen, Erik; Klinkby, Esben Bryndt; Nielsen, T.; Farhi, E.; Filges, U.; Lefmann, K. / **New developments in the McStas neutron instrument simulation package.**

In: Journal of Physics: Conference Series (Online), Vol. 528, 2014, p. 012035.

Bergbäck Knudsen, Erik; Nielsen, Martin Meedom; Haldrup, Kristoffer; Topel, Eric; Schmidt, Søren / **Novel applications of the x-ray tracing software package McXtrace.**

Advances in Computational Methods for X-Ray Optics III. Vol. 9209 2014. p. 92090B (Proceedings of the SPIE).

FX Lin, YB Zhang, SO Poulsen, N Schell, W Pantleon and D Juul Jensen, Kinetics of individual grains during recrystallization of cold-rolled copper, 2014, accepted

M. G. Makowska, L. Theil Kuhn, M. Strobl, E. M. Lauridsen, H. L. Frandsen, A. Tremsin; *Interplay between stress and reduction progress in anodes and anode supports for SOFC*, "DTU Energy Conversion's PhD symposium", 2014, Copenhagen, Denmark

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

### **Proceedings**

Failure analysis and thermochemical surface engineering of bearings for wind turbine drivetrains / West, Ole; Dahl, Kristian Vinter; Christiansen, Thomas Lundin; Somers, Marcel A. J. / In: Proceedings of 2nd International Conference on Energy and the Future of Heat Treatment and Surface Engineering, Chinese Heat Treatment Society, Beijing 2014, p. 361-365, 2014., Chinese Heat Treatment Society,

### **Bidrag til konferencer og kongresser 2014:**

Thermal Stability and Decomposition of Carbon and Nitrogen Expanded Austenite / Material Science & Technology Conference (MS&T'14), Pittsburgh, PA, USA / Bastian Brink (Speaker), Kenny Ståhl, Thomas L. Christiansen, Marcel A. J. Somers, 12-16 October 2014.

Thermal Behavior of Expanded Austenite: Determination of Thermal Expansion and Decomposition using in-situ Synchrotron X-ray Diffraction / Danish Crystallographers Meeting & 6<sup>th</sup> DANSCATT Meeting, Kgs. Lyngby, Denmark / Bastian Brink (Poster presenter), Kenny Ståhl, Thomas L. Christiansen & Marcel A. J. Somers, 22-23 May 2014

Synchrotron X-ray Diffraction Study of Thermal Decomposition of Expanded Austenite / European Powder Diffraction Conference (EPDIC14), Aarhus, Denmark / Bastian Brink (Poster presenter), Kenny Ståhl, Thomas L. Christiansen, Marcel A. J. Somers, 15-18 June 2014.

X-ray diffraction analysis proofing surface sensitive metallographic sample preparation, 143rd TMS Annual Meeting & Exhibition, TMS2014, San Diego, USA / Karen Pantleon (Invited speaker); 16-20 February 2014

High resolution reciprocal space mapping revealing reversible changes in deformation structures during unloading and reloading in tension, 143rd TMS Annual Meeting & Exhibition, TMS2014, San Diego, USA / Wolfgang Pantleon (Invited speaker), Felix Thiel, Ulrich Lienert; 16-20 February 2014

Failure analysis and thermochemical surface engineering of bearings for wind turbine drivetrains / 2nd International Conference on Energy and the Future of Heat Treatment and Surface Engineering; Beijing, P.R: China / Ole West (Speaker), Kristian Vinter Dahl, Thomas Lundin Christiansen, Marcel A.J. Somers, 11-13- October 2014.

Analysis of deformation-induced intragranular orientation spread in IF-steel by a combination of 3DXRD and crystal plasticity, 17th International Conference on Textures of Materials, ICOTOM 17, Dresden, Germany / Grethe Winther (Speaker), 24-29 August 2014

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

### **Bidrag til konferencer og kongresser 2014:**

Frankær, C.G., Ståhl, K. and Harris P.

*Structural characterization of the photoreductive Cu(II) centre in Cu-insulin – combining spectroscopy and diffraction.*

**Radiation Damage 8, Hamburg, Germany (2014)**

Frankær, C.G., Thymark, M., Ståhl, K. and Harris, P.

*X-ray powder diffraction: A powerful analysis tool for industrial protein production.*

**23. IUCr Meeting 2014, Montreal, Canada (2014).**

Brink, B., Ståhl, K., Christiansen, T.L., and Somers, M.A.J.

*Thermal Behavior of Expanded Austenite: Determination of thermal expansion and decomposition using in situ synchrotron X-ray diffraction.*

**DANSCATT/43. DKM, Lyngby, Denmark (2014).**

Brink, B., Ståhl, K., Christiansen, T.L. and Somers, M.A.J.

*Synchrotron X-ray diffraction study of thermal decomposition of expanded austenite.*

**EPDIC-14, Århus, Denmark (2014).**

Ståhl, K.

*Zeolitic materials.*

**European Materials Research Society, 2014 Fall Meeting. Warsaw, Poland (2014)**

Driel, T.B. van, Hartsock, R.W., Kjaer, K.S., Haldrup, K., Christensen, M., Dohn, A., Møller, K., Harlang, T., Zhang, W., Sun, Z., Lemke, H.T., Zhu, D., Ganey, K. and Nielsen, M.M.

*Time-resolved X-ray scattering of molecules in solution: Approaching the molecular movie.*

**DANSCATT/43. DKM, Lyngby, Denmark (2014).**

**DTU Chemical Engineering, Technical University of Denmark**

**Bidrag til konferencer og kongresser 2014:**

**Inhibition and Deactivation of Ni-MoS<sub>2</sub> for Hydrodeoxygenation by Bio-oil Impurities**

Peter M. Mortensen, Diego Gardini, Hudson W. P. de Carvalho, Christian D. Damsgaard, Jan-Dierk Grunwaldt, Peter A. Jensen, Jakob B. Wagner, Anker D. Jensen, Nordic Catalysis symposium 2014, June 15-17, Oslo (Norway) (oral)

**X-ray Absorption Spectroscopy during evolution of the Pd<sub>2</sub>Ga-phase used in methanol synthesis**

Carvalho, Hudson W.P.; Sharafutdinov, I.; Chorkendorff, I.; Damsgaard, C. Grunwaldt, J.D.. Soleil User's Meeting 2014, January 23-24, Saint-Aubin (France)

## Niels Bohr Institute, University of Copenhagen

### Contributions to conferences etc. 2014:

- Mortensen, K. Soft Matter Studies using Small-Angle Scattering Methods. *Denmark-Brazil Workshop on Cooperation on Materials and Energy Campinas*, Sao Paulo, Brazil, December **2014**
- Mortensen, K. Hydrogels based on Molecular Self-assembly Combined Studies of Structure and Rheology. *Workshop on Nanostructured interfaces: Formation, Properties and Applications* (Invited), Lund, Sept **2014**.
- Mortensen, K., Annaka, M. (Invited Plenary) Hydrogels based on Molecular Self-assembly Combined Studies of Structure and Rheology. *Polymer Network Group & Research Group of Polymer Gels - Gel-Symposium*, November **2014**
- Mortensen, K., Chapman, H., Yonath, A.E., Argyriou, D., Zoufal, T. New large-scale research infrastructures: how they will revolutionize our understanding of matter. *ESOF Conference*. Copenhagen Jun 22-26, **2014**
- Lefmann, K. Magnetic dynamics and Phase Transitions in Oxide Nanoparticles, 2. *Öresund Magnetism Workshop*, ESS, Lund, March **2014**
- Bordallo, H.N. Inelastic and Quasi-Elastic Neutron Scattering applied to Materials and Energy. *Workshop on Denmark-Brazil Cooperation on Materials and Energy* 9-10 December 2014, Campinas, Sao Paulo, Brazil
- Bordallo, H.N. Looking at hydrogen motions in confinement: The uniqueness of Quasi-Elastic Neutron Scattering. *3rd International Workshop on "Complex Physical Phenomena in Materials"* -PUC -Rio, Brazil, February 17- 22, 2014.
- Bordallo, H.N.. MIRACLES: The backscattering spectrometer at the European Spallation Source. *QENS/WINS*- 11-16 May, 2014 - L'Escandille, Autrans, France
- Bordallo, H.N. Neutron scattering, a powerful tool to study water in confinement, *Workshop of the International Research Network GdRi - M<sup>2</sup>UN* - Donostia International Physics Center - September 28- October 1, 2014- San Sebastian, Basque Country, Spain

### Other communication activities, patent applications etc.:

- Lefmann, K. Magnetic Dynamics and Phase Transition in Oxide Nanoparticles, Canadian Neutron Research Institute, Chalk River, Canada. February **2014**
- Lefmann, K. Application of ray-tracing Monte Carlo simulations in designing instruments for MAX-IV and ESS, RUC. April **2014**
- Lefmann, K. ESS and CAMEA, NIST, Washington. December **2014**

- Lefmann, K. 1D Ising Ferromagnetism in  $\text{CoCl}_2 \cdot 2\text{D}_2\text{O}$ : Quantum Phase Transition and Relaxation, Johns Hopkins University. December **2014**
- Lefmann, K. Field-induced antiferromagnetism in a high-temperature superconductor, University of Connecticut. December **2014**
- Lefmann, K. Field-induced antiferromagnetism in LSCO and LSCO+O, Brookhaven Nat. Lab. December **2014**
- Lefmann, K. Status of ESS and the CAMEA instrument, Brookhaven Nat. Lab. December **2014**.
- Lefmann, K. MAX-IV og ESS i Lund, en kæmpe chance for nordisk forskning indenfor materialer og bio-videnskaber, Folkemødet, Allinge, juni **2014**
- Lefmann, K. MAX-IV og ESS i Lund, en kæmpe chance for nordisk forskning indenfor materialer og bio-videnskaber, Øresund rundbordsmøde, ESS-DMSC, september **2014**.
- Mortensen K. Strukturelle studier af biomolekylære komplekser og syntetiske polymer systemer ved anvendelse af små-vinkel spredning, SANS og SAXS. Selskabet for Naturlærens Udbredelse. København 7. april **2014**.
- Mortensen K. Gels based on Molecular Self-assembly. Combined Studies of Structure and Rheology. Munich Seminar Series. 13. Munich, Germany, Oct. **2014**.
- Mortensen K. SANS. Meeting on EINFRA-9 Virtual Research Environment proposal. Copenhagen. 31. October **2014**
- Bordallo, H.N. Inelastic Neutron Scattering: A different approach to understand drug stability. ESS and Max IV - New Opportunities in Formulation Research. Lund - 9 January 2014.
- Bordallo, H.N. Molecular Dynamics Simulations: Getting the most out of Inelastic Neutron Data. Topical Meeting on Molecular Dynamics - Royal Academy of Science and Letters - 26 Mai 2014.
- Bordallo, H.N. High Resolution Spectroscopy at the ESS on the Science case for Neutron Spin Echo. Copenhagen. 5. August 2014.
- Bordallo, H.N. Neutron Scattering and Industrial partnership, yet an unexploited field. Danfysik, Taastrup. 20. October 2014.
- Kirkensgaard, J.K.K. Lecturer and co-organizer of International PhD-School "Geometry and Topology of Liquid Crystals" at RMIT, Melbourne
- Kirkensgaard, J.K.K. Talk at Symposium on Geometry and crystalline structure, Canberra, Australia, title: "Complex hierarchically ordered structures in block copolymer melts"

## Dept. of Chemistry, University of Copenhagen

### Contributions to conferences etc. 2014:

#### Conference proceedings:

Lo Leggio, L., Frandsen, K.E.H., Poulsen, J.-C. N., Tovborg, M., De Maria, L., Johansen, K.S. Structural diversity of lytic polysaccharide monoxygenases Proceedings of Mie Bioforum 2014 "Lignocellulose Degradation and Biorefinery" Mie Japan, in press.

#### Oral presentations (no particular order)

D. J. Tobler, J. D. Rodriguez Blanco, K. Dideriksen, K. K. Sand, L. G. Benning, S. L. S. Stipp (2014) Effect of Citric Acid on Amorphous Calcium Carbonate (ACC) Structure, Stability and Crystallisation. Goldschmidt Conference 2014, Sacramento, USA. June 8-13. [Mineralogical Magazine, 77(5) 2491.]

J. D. Rodriguez, D. J. Tobler, Blanco, K. Dideriksen, L. G. Benning, K. K. Sand, S. L. S. Stipp (2014) The Effect of Sr<sup>2+</sup> on the Structure, Stability and Crystallisation of Amorphous CaCO<sub>3</sub>. Goldschmidt Conference 2014, Sacramento, USA. June 8-13. [Mineralogical Magazine, 77(5) 2103.]

D. J. Tobler, J. D. Rodriguez Blanco, K. Dideriksen, K. K. Sand, N. Bovet, L. G. Benning, S. L. S. Stipp (2014) The effect of aspartic acid and glycine on amorphous calcium carbonate (ACC) structure, stability and crystallization. Geochemistry of the Earth's surface (GES-10), Institut de Physique du Globe de Paris, Paris 05, France. August 18-22, 2014.

H. O. Sørensen, D. Mütter, K. Dalby, D. Jha, R. Harti, R. Gooya, Y. Yang, J. Da Silva, M. Guizar-Sicairos, M. Holler, H. Suhonen, R. Feidenhans'l, S. Stipp (2014, invited talk) Ptychography and Tomography for Geology and Geophysics, How can KU take advantage of research facilities like ESS and MAX IV? - Half day workshop about possibilities related to neutron and x-ray scattering at UCPH, Bernstorff Slot, Copenhagen. December 3.

H. O. Sørensen, D. Mütter, K. Dalby, D. Jha, R. Harti, R. Gooya, J. Da Silva, M. Guizar-Sicairos, M. Holler, H. Suhonen, R. Feidenhans'l, S. Stipp (2014) Multiscale Imaging of Chalk, a Natural Porous Material: What do We Learn?, International Conference on X-ray Microscopy 2014, Melbourne, Australia. October 26-31.

R. Gooya, H. O. Sørensen, S. L. S. Stipp (2014) Modelling of flow transport in porous media, from pore scale to non-Darcy flow, International Conference on Numerical and Mathematical Modeling of Flow and Transport in Porous Media, Dubrovnik, Croatia. 29 Sep - 3 Oct.

K. N. Dalby, H. O. Sørensen, D. Mütter, D. Jha, J. C. da Silva, S. L. S. Stipp (2014) From oil field to ptychography: Applications of FIB SEM in NanoGeoScience. Microscopy & Microanalysis 2014, Hartford, CT, United States. August 3-7.

H. O. Sørensen, D. Mütter, K. Dalby, D. Jha, R. Harti, R. Gooya, J. Da Silva, M. Guizar-Sicairos, M. Holler, H. Suhonen, R. Feidenhans'l, S. Stipp (2014) Chalk, a Natural Porous Material: Can we Capture the Essential Properties by 3D Imaging?, International Congress on 3D Materials Science 2014, Annecy, France. June 29-July 2.

J. Dake, J. Oddershede, H. O. Sørensen, S. Schmidt, C. Krill (2014) Experimental Investigation of the Applicability of the MacPherson-Srolovitz Relation to Grain Growth in Al, International

Congress on 3D Materials Science 2014, Annecy, France. June 29-July 2.

J. Dake, J. Shatto, T. Werz, J. Oddershede, H. O. Sørensen, S. Schmidt, C. Krill (2014) Simultaneous Spatial and Orientational Tracking of Ostwald Ripening in Semisolid Al-5 wt% Cu at High Volume Fractions of the Coarsening Phase, International Congress on 3D Materials Science 2014, Annecy, France. June 29-July 2.

K. N. Dalby, H.O. Sørensen, D. Mütter, D. Jha, J. C. da Silva, S. L. S. Stipp (2014) Coherent diffraction imaging of rocks at the nanometer scale, 43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Technical University of Denmark, Kgs. Lyngby. May 22-23.

N. Tsapatsaris, H. N. Bordallo, N. C. R. Momsen, H. O. Sørensen, S. L. S. Stipp (2014) Assessing complex water mobility in chalk deposits, 43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Technical University of Denmark, Kgs. Lyngby. May 22-23.

H. O. Sørensen (2014) Can we predict petrophysical parameters from miniature pieces of chalk? Explorer Meeting, Bad Sooden-Allersdorf, Germany, April 24.

H. O. Sørensen (2014) Can we predict petrophysical parameters from miniature pieces of chalk? Mini-symposium, University of Copenhagen. March 17.

H. O. Sørensen (2014) Can we predict petrophysical parameters from miniature pieces of chalk? Nano-Science Center Seminar, Magleås, Høsterkøb, Denmark. March 15.

H. O. Sørensen (2014) X-ray based techniques as tools to study the micro and nanostructure of natural materials, Sao Paulo workshop, University of Sao Paulo, Sao Paulo, Brazil. February 19.

K. Dideriksen (2014) Green rust: Stability, structure, and thoughts on the interlayer's role in redox reactions. Workshop on "Biogeochemistry and Redox Transformations of Iron". Telluride, CO, USA. August 5-8

Kristian Frandsen Structural studies of copper and zinc loaded *Thielavia terrestris* AA9(GH61) isoform E. Oral presentation at CoLuAa, Copenhagen, 6-7 November 2014.

Vladyslav Soroka Structure of the DBL4 $\gamma$  Domain of Malaria Parasite Erythrocyte Membrane Protein 1. Oral presentation at CoLuAa, Copenhagen, 6-7 November 2014.

Vladyslav Soroka Structure of the DBL4 $\gamma$  Domain of Malaria Parasite Erythrocyte Membrane Protein 1. CoNeXT meeting at Magleås Kursuscenter October 29. 2014

Lila Yang, Expression and characterization of FLRT proteins Fn III domains. CoNeXT meeting at Magleås Kursuscenter October 29. 2014

Leila Lo Leggio, Kristian E. H. Frandsen, Jens-Christian N. Poulsen, Morten Tovborg, Leonardo De Maria, Katja Salomon Johansen. Structural diversity of lytic polysaccharide monooxygenases. Invited oral presentation at Mie Bioforum Nov 18-21, 2014, Mie, Japan

*Homoleptic 5d Fluoride Complexes as Modules for Molecular Spin-Architectures*

Kasper S. Pedersen, Rodolphe Clérac, Anne-Laure Barra, Pierre Dechambenoit, Mikkel A. Sørensen, Marc Sigrist, Thomas Weyhermüller, Høgni Weihe, Hannu Mutka, Stergios Piligkos, Jesper Bendix.

Reaxys – Inspiring Chemistry Conference, 21st-24th September 2014, Grindelwald, Switzerland

*Fluoride-Bridged Magnetic Systems*

J. Bendix

Invited talk, 14 International Conference on Molecular Magnetism, July 5-10, 2014, Sct. Petersburg, Russia

*Homoleptic 5d Fluoride Complexes as Modules for Molecular Spin-Architectures*

K. S. Pedersen, R. Clérac, A.-L. Barra, P. Dechambenoit, M. A. Sørensen, M. Sigríst, T. Weyhermüller, H. Weihe, S. Piligkos, H. Mutka, J. Bendix

14 International Conference on Molecular Magnetism, July 5-10, 2014, Sct. Petersburg, Russia

*Molecule-based Approaches to Magnetic Materials Employing Fluoride Complexes*

J. Bendix.

Invited talk, Gordon Conference on Conductivity & Magnetism in Molecular Materials, Lewiston, Maine, USA, Aug. 3-8, 2014.

*Homoleptic 5d Fluoride Complexes as Modules for Molecular Magnetic Materials*

Kasper S. Pedersen, Rodolphe Clérac, Anne-Laure Barra, Pierre Dechambenoit, Mikkel A.

Sørensen, Marc Sigríst, Thomas Weyhermüller, Stergios Piligkos, Høgni Weihe, Hannu Mutka, and Jesper Bendix

41<sup>st</sup> International Conference on Coordination Chemistry, July 21-25, 2014, Singapore.

**Poster presentations**

H. O. Sørensen, D. Müter, K. N. Dalby, D. Jha, R. Harti, R. Gooya, R. Feidenhans'l, S. L. S. Stipp (2014) Chalk, a natural very fine grained porous material: Can we capture the essential properties by 3D imaging? The International Carbon Conference, University of Reykjavik, Iceland. August 25-29, 2014.

S. S. Hakim, K. N. Dalby, H. O. Sørensen, S. L. S. Stipp (2014) Imaging Rocks in 3D: Optimizing Image Segmentation. The International Carbon Conference, University of Reykjavik, Iceland. August 25-29, 2014.

K. N. Dalby, H. O. Sørensen, R. Harti, D. Jha, S. L. S. Stipp (2014) What precipitates where? How scanning electron microscopy is changing the way we "see" natural surfaces. The International Carbon Conference 2014, University of Reykjavik, Iceland. August 25-29, 2014.

D. Müter, H. O. Sørensen, D. Jha, K. N. Dalby, S. L. S. Stipp (2014) X-ray tomography and finite element simulations of rock mechanics. Microscopy & Microanalysis 2014, Hartford, CT, USA. August 3-7, 2014,

D. Jha, H. O. Sørensen, D. Müter, K. N. Dalby, S. L. S. Stipp (2014) Multi-scale 3D mapping of Tomography Data. Microscopy & Microanalysis 2014, Hartford, CT, United States. August 3-7, 2014

D. Müter, H. O. Sørensen, H. Bock, S. L. S. Stipp, (2014) Nanoscale fluid transport properties of natural porous rocks. 8th Liquid Matter Conference, Lisbon, Portugal. July 20-25, 2014.

D. Jha, H. O. Sørensen, S. Dobberschütz, S. Stipp (2014) Adaptive Ring Artefact Suppression Method for Tomography Applications. International Congress on 3D Materials Science 2014, Annecy, France. June 29-July 2, 2014.

D. Mütter, H. O. Sørensen, J. Oddershede, S. Stipp (2014) Microstructure and Mechanical Optimization in Sea Urchin Shells. International Congress on 3D Materials Science 2014, , Annecy, France. June 29-July 2, 2014.

S. Frølich, S. S. Hakim, H. O. Sørensen, S. Stipp, H. Birkedal (2014) Coccolithophorids, Mussel Shells and Chalk  
- a comparison of the microstructure of biogenic calcite of different origin. 14th European Powder Diffraction Conference, Aarhus. June 15-18, 2014.

D. Jha, H. O. Sørensen, S. Dobberschütz, S. Stipp (2014) Adaptive ring artifact suppression for tomography applications. 43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Technical University of Denmark, Kgs. Lyngby. May 22-23, 2014.

D. Mütter, H. O. Sørensen, J. Oddershede, S. Stipp (2014) Microstructure and mechanical optimisation in sea urchin shells. 43rd Danish Crystallographers Meeting & 6th DanScatt Meeting, Technical University of Denmark, Kgs. Lyngby. May 22-23, 2014.

R. Harti, H. O. Sørensen, K. Dalby, S. L. S. Stipp (2014) Imaging liquids in pores – beyond X-ray tomography, Visionday 2014, Technical University of Denmark, Kgs. Lyngby. May 14, 2014.

Stinne Kirketerp Nielsen, Alexander Holm Viborg, Birte Svensson, Maher Abou Hachem, Leila Lo Leggio Structural studies of  $\beta(1,6)$ -galactosidase from *Bifidobacterium animalis* subsp. *lactis* BI-04 from the GH42 family in complex with small ligands. Poster presentation by Stinne Kirketerp Nielsen at 11th Workshop in Protein.DTU for Young Scientists, 12 May 2014 Technical University of Denmark, Lyngby.

Lila Yang, Kim Krighaar Rasmussen, Maria Hansen, Peter Schledermann Walmod, Leila Lo Leggio Structural Studies of Protein-Protein Interactions: FLRT Interactions with the FGF Receptor. Poster presentation by Lila Yang at 11th Workshop in Protein.DTU for Young Scientists, 12 May 2014 Technical University of Denmark, Lyngby.

Ditte Welner, Kristian Frandsen, Lars Anderson, Kirk M. Schnorr, Stinne Kirketerp Nielsen, Morten Tovborg, Jens-Christian N. Poulsen, Leila Lo Leggio. Structural studies of copper and zinc loaded *Thielavia terrestris* AA9(GH61) isoform E. 13th European Training Course on Carbohydrates, April 13 - 17, 2014 Wageningen, The Netherlands. Poster presented by Kristian Frandsen.

Ditte Welner, Kristian Frandsen, Lars Anderson, Kirk M. Schnorr, Stinne Kirketerp Nielsen, Morten Tovborg, Jens-Christian N. Poulsen, Leila Lo Leggio. Structural studies of copper and zinc loaded *Thielavia terrestris* AA9(GH61) isoform E. Poster presented by Kristian Frandsen. EMBO Practical Course on Computational Structural Biology - from data to structure to function, European Bioinformatics Institute, Cambridge, United Kingdom, UK April 7-11 2014.

Poulsen J.C.N., Ørum S., Viborg, A., Fredslund, F., Nakai, H., Svensson, B., Maher, A.H., Lo Leggio, L. Improvement of protein crystals by addition of water on setup of vapour diffusion crystallization. Poster presentation by Jens-Christian N. Poulsen at 15th International Conference on the Crystallization of Biological Macromolecules, September 17 - 20, 2014 - Hamburg, Germany.

Lila Yang, Kim Krighaar Rasmussen, Maria Hansen, Peter Schledermann Walmod, Leila Lo Leggio Structural Studies of Protein-Protein Interactions: FLRT Interactions with the FGF Receptor. Poster presentation by Lila Yang at CoLuAa, Copenhagen, 6-7 November 2014.

Jahan R, Song J, Eddaoudi M, Madsen AØ, Nowotny M, Serquis A, Bisseyou YBM, Haynes D. International Year of Crystallography Unesco opening declaration.

DOI: 10.13140/2.1.4414.3687 Conference: Unesco Opening Ceremony of the International Year of Crystallography, At Unesco Building, Paris.

Anders Ø Madsen. *Dynamic Quantum Crystallography*. Danish opening of the international year of crystallography. 22. – 23 of January 2014, H.C.Ørsted Institute, University of Copenhagen. Oral presentation.

Marité Cárdenas, Invited speaker to Open Seminar ESS and MAX IV - new opportunities in formulation research. January 9, 2014. Lund, Sweden

Tania Lind, Oral presentation, Biophysics Society, USA, Feb 2014.

Marité Cárdenas, ACS National Meeting Chemistry for Energy. March, Dallas, USA. 2014

Vivien Jagalski, ACS National Meeting Chemistry for Energy. March, Dallas, USA. 2014

Marité Cárdenas, invited speaker to 13th Surface X-ray and Neutron Scattering International Conference, Hamburg, Germany. July 7-11 2014.

*Synthesis and Magnetic Properties of One-Dimensional Fluoride-Bridged Manganese(III) Systems*

M. A. Sørensen, K. S. Pedersen, J. Bendix

14 International Conference on Molecular Magnetism, July 5-10, 2014, Sct. Petersburg, Russia

*Cool surprises with fluoride-bridged systems.*

K. S. Pedersen J. Bendix, R. Clérac, S. Piligkos, H. Weihe, J. Dreiser, G. Lorusso, M. Schau-Magnussen, M. Evangelisti, S. Singh, G. Rajaraman

41<sup>st</sup> International Conference on Coordination Chemistry, July 21-25, 2014, Singapore.

*Magnetic properties of linear chain  $S = 2$  Heisenberg antiferromagnets. In Search of the Haldane Gap.*

M. Agerbæk, J. Bendix

Gordon Conference on Conductivity & Magnetism in Molecular Materials, Lewiston, Maine, USA, Aug. 3-8, 2014.

### **Other communication activities, patent applications etc.:**

Anders Ø. Madsen. Presentation for high school students at the Natural Science Museum. November 2014: Seeing the invisible: Crystallographic research and the synchrotron in Lund.

**Dept. of Pharmacy, University of Copenhagen**

**Contributions to conferences etc. 2014:**

Liposome Research Days 2014, Copenhagen, August 2014

13<sup>th</sup> European Symposium on Controlled Drug Delivery, Egmond Ann Zee, April 2014

11<sup>th</sup> International Conference on Nanosciences and Nanotechnologies, July 2014

Surfactants in Solutions (SIS), Coimbra, June 2014

Danscatt Meeting, DTU, Maj 2014

Trends in Drug Research; The 32<sup>nd</sup> Cyprus Noordwijkerhout Camaerino Symposium, Limassol, May 2014 (invited talk)

**Dept. of Biomedical Sciences, University of Copenhagen**

3<sup>rd</sup> Sept 2014 The 14<sup>th</sup> International ATPase Conference, Lunteren, The Netherlands

16<sup>th</sup> July 2014 Gordon Research Conferences on Membrane Transport Proteins, West Dover,  
Vermont, USA

**Contributions to conferences etc. 2014:**

1. de Ghellinck A, Shen C, Stein P, Fragneto G, Sferrazza M, Klösigen BM. The Interaction of Resveratrol with DPPC Bilayers - a Biophysical Contribution on the Mediterranean Diet. Contributed talk, presented at: Biophysical Society Meeting 2014; 1/28/. p. 41a.
2. Shen C, Klösigen BM. Tracking the Modulation of Membrane Structure in SUVs by DSC - A Comment on Lipid Phase Transition. Poster, presented at: Biophysical Society Meeting 2014; 1/28/. p. 286a.
3. de Ghellinck A, Shen C, Fragneto G, Sferrazza M, Klösigen B. Neutron reflectometry reports tilt angle change in model membranes upon insertion of resveratrol. Poster and contributed talk, presented at: Baltic Neutron School; May 4. – 8., 2014, Tartu, Estonia.
4. Menov L, Bloksgaard M, Klösigen B. Acquired Cholesteatoma investigated by X-ray computed tomography. Poster, presented at: Baltic Neutron School; May 4. – 8., 2014, Tartu, Estland.
5. Löffler RJG, Hansen PL, Klösigen B, Monnard P-A. Functionalized fatty-acid vesicles as soft-matter/polymer hybrid nanocontainers. Poster, presented at: Baltic Neutron School; May 4. – 8., 2014, Tartu, Estonia.
6. Klösigen B. Neutron reflectometry. Invited talk, presented at: Baltic Neutron School; May 4. – 8., 2014, Tartu, Estonia.
7. Shen C, de Ghellinck A, Fragneto G, Sferrazza M, Stein P, Klösigen BM. The Interaction of Resveratrol with Model Membranes from Structure to Thermodynamics. contributed talk at DanScatt Annual Meeting 2014, DTU, Denmark, May 22-23, 2014
8. Christensen, ChK, Tananka Sh, Linder P, Klösigen B. Time-resolved SANS study of structure formation in a solution of the globular protein Lysozyme. Poster at DanScatt Annual Meeting 2014, DTU, Denmark, May 22-23, 2014
9. Shen C, Jørgensen L, Zargarani D, Runge B, Murphy B, Magnussen O, et al. Controlled Modulation of Lipid Bilayer State by a Photosensitive Membrane Effector. Poster, presented at: Biophysical Society Meeting 2015; 1/27/. p. 542a-3a.
10. Shen C, de la Serna JB, Struth B, Klösigen B. DPPC Monolayers Exhibit an Additional Phase Transition at High Surface Pressure. Poster, presented at: Biophysical Society Meeting 2015; p. 85a.