

Rapport skema

Styrelsen for Forskning og Innovation
Bredgade 40
1260 København K



**Styrelsen for Forskning
og Innovation**
Ministeriet for Forskning, Innovation
og Videregående Uddannelser

Dato:

31. marts 2014

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

Det Frie Forskningsråd - Natur og Univers

1. Grundoplysninger

Bevillingens titel:

DANSCATT - Danish Center for the use of Synchrotron, X-ray, and Neutron facilities 2013

Sagsnr. (fx 09-012345)

0602-02877B

Bevillingshavers navn og stilling

Instituttleder Robert Feidenhans'l, Professor

Arbejdsplads (adresse, telefon og
email)

Niels Bohr Institutet, Københavns Universitet
Universitetsparken 5, bygning D
2100 København Ø

Tlf.: 2875 0397 E-mail: robert@fys.ku.dk

Bevillingens hjemmeside
hvis relevant

<http://dancatt.ku.dk/>

Virkemiddel

Instrumentcentre

2. Bevillingsperiode

Oprindelig bevillingsperiode

Fra: 1. januar 2013

Til: 31. december 2013

Seneste godkendte
bevillingsperiode

Fra: 1. januar 2013

Til: 31. december 2013

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 Robert Feidenhans'l, Københavns Universitet
Næstformand Kim Lefmann, Københavns Universitet
Niels Bech Christensen, Risø DTU
Michael Gajhede, Københavns Universitet
Pernille Harris, DTU
Bo Brummerstedt Iversen, Aarhus Universitet
Alfons Molenbroek, Haldor Topsøe A/S
Kell Mortensen, Københavns Universitet
Henning Friis Poulsen, Risø DTU
Søren Thirup, Aarhus Universitet

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

4. Økonomi

Oprindeligt bevilget beløb (kr.)

Ekskl. overhead:

4.024.588

Inkl. overhead:

5.795.407

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 projektførelsen. 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 post doc and technical staff at facilities at the PSI in Switzerland and MAX-lab in Lund, in order to assure preferred access for Danish user groups to these facilities. In total 190 publications were published in 2013 with support from DANSCATT, including about 14 publications in high impact journals. 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.

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 ESS.

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
- Erhvervsmæssige-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))

Post doc Mark Laver (M, England, fødselsdato 01.05.1980), Paul Scherrer Institutet, 6 måneder
Post doc Amy Poole (K, England, fødselsdato 01.10.1978), Paul Scherrer Institutet, 6 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. DANCATT har støttet med gennemsnitligt 20.000 kr. per publikation.

Artikler, ikke peer reviewed

Doktordisputater

Ph.d.-afhandlinger

Intan Diana Mat Azmi: Cubosomes and Hexosomes as Novel Nanocarriers for Targeting Platinum Anticancer Drugs. Dept. of Pharmacy, University of Copenhagen

Jana Baltser: Experiments versus simulations: modeling of instrumentation for X-ray scattering experiments. Niels Bohr Institute, University of Copenhagen

Niels Bindzus: Charge densities from synchrotron powder diffraction. Dept. of Chemistry, Aarhus University
Lasse Bjerg: Modelling of thermoelectric properties. Dept. of Chemistry, Aarhus University

Erik Brok: Spin structures of antiferromagnetic nanoparticles. DTU Physics, Technical University of Denmark

Arvid Piehl Lauritsen Böttiger: Morphology of polymer solar cells. DTU Energy Conversion, Technical University of Denmark

Ingrid Dach: Structural studies of the gastric proton pump and the sarcoplasmic reticulum calcium pump. Dept. of Molecular Biology, Aarhus University

Henrik Friis Dam: Coating, Degradation and Testing of Organic Polymer Devices - Reducing the route from Laboratory to Production Scale Devices. DTU Energy Conversion, Technical University of Denmark

Pernille Galberg: Understanding thermostability and pH dependent properties of proteins: Bacillus circulans xylanase as experimental model system. Dept. of Chemistry, University of Copenhagen

Martin Høj: Nanoparticle synthesis using flame spray pyrolysis for catalysis. One step synthesis of heterogeneous catalysts. DTU Chemical Engineering, Technical University of Denmark

Jesper Langholm Jensen: Structure and Function of Bovine and Camel Chymosin A Protein Chemical Study of the Differences in Milk-Clotting Abilities. Dept. of Chemistry, University of Copenhagen

Kirsten Marie Ø. Jensen: Watching materials form: Particle formation and growth in hydrothermal synthesis. Dept. of Chemistry, Aarhus University
Lina Juknaite: Ionotropic glutamate receptors as drug targets. Structural studies of the extracellular domains. Dept. of Drug Design and Pharmacology, University of Copenhagen

Adriana Kantcheva: The leucine transporter from Aquifex aeolicus as a model for the neurotransmitter sodium symporters – Insights into function and ligand binding. Dept. of Molecular Biology, Aarhus University

Sofie Kastbjerg: Crystallographic studies of thermoelectric materials. Dept. of Chemistry, Aarhus University

Helle Kristiansen: Antiviral Mechanisms of the 2'-5' Oligoadenylate Synthetase Family Novel and Classical Antiviral Activities. Dept. of Molecular Biology, Aarhus University

Søren Kynde: Modelling small-angle scattering data from complex protein-lipid systems. Niels Bohr Institute, University of Copenhagen

Jacob Larsen: Quantum Phase Transitions in CoCl₂ salts, and the Nature of the Co-existence of Magnetism and Superconductivity in Y₉Co₇ and La_{2-x}Sr_xCuO_{4+y} DTU Physics, Technical University of Denmark

	Thue Trofod Larsen-Olsen: Roll-to-Roll Fabricated Polymer Solar Cells: Towards Low Environmental Impact and Reporting Consensus. DTU Energy Conversion, Technical University of Denmark Lina Malinauskaitė: Structural and Functional Studies of the Neurotransmitter: Sodium Symporter Family: Insight into the Transport Mechanism. Dept. of Molecular Biology, Aarhus University Daniel Mattle: Structural and functional studies of a Cu⁺ ATPase from <i>Legionella pneumophila</i>. Dept. of Molecular Biology, Aarhus University Søren Roi Midtgaard: Self-assembling peptide and protein nanodiscs for studies of membrane proteins. Niels Bohr Institute, University of Copenhagen Christa Nilsson: Cubosomes and hexosomes as drug nanocarriers. Dept. of Pharmacy, University of Copenhagen Kim Krihaar Rasmussen: Structural Biology of CI from Phage TP901-1. Dept. of Chemistry, University of Copenhagen Mette Stokkebroe Schmökel: Experimental charge density studies of inorganic solids. Dept. of Chemistry, Aarhus University Irek Sharafutdinov: Investigations into low pressure methanol synthesis. DTU Chemical Engineering, Technical University of Denmark Piotr Krzysztof Siupka: The evolution and molecular mechanism of the function of the cytokine system in vertebrates. Dept. of Molecular Biology, Aarhus University Dadi Sveinbjörnsson: Design and Characterization of Solid electrolytes for All-Solid-State Lithium batteries. DTU Energy Conversion, Technical University of Denmark Martin Søndergaard: Synthesis and characterization of inexpensive high-performance thermoelectric materials. Dept. of Chemistry, Aarhus University Christoffer Tyrsted: Formation studies of nanocrystalline materials. Dept. of Chemistry, Aarhus University Christine A. Ussing: Structural Studies of Cys-loop Receptors: Domains, Model Systems and Full Length Receptors. Dept. of Drug Design and Pharmacology, University of Copenhagen Trine Vammen Vendelboe: Expression, purification and characterization of human Dopamine β-monooxygenase. DTU Chemistry, Technical University of Denmark Matteo Villa: Isothermal martensite transformation. DTU Mechanical Engineering, Technical University of Denmark Qiongxiao Wu: Catalytic synthesis of alcoholic fuels for transportation from syngas. DTU Chemical Engineering, Technical University of Denmark
Videnskabelige bøger/antologier	
Videnskabelige rapporter	
Bidrag til bøger/antologier/rapporter	L. Arleth, S. Frøkær, R. Feidenhans'l, U. Gether, S. Larsen, T.B. Nielsen, K. Lefmann, S.S. West; University of Copenhagen and the future use of neutron and X-ray Sources (A White Paper on ESS and MAX IV) C. Nilsson, B. Barrios-Lopez, A. Kallinen, P. Laurinm?ki, S. Butcher, M. Raki, K. Bergstr?m, S. Weng Larsen, J. Østergaard, C. Larsen, A. Urtti, A. Airaksinen, A. Yaghmur; SPECT/CT imaging of radiolabeled cubosomes and hexosomes for potential theranostic applications. Activity Report 2012 Max-Lab.
Working papers/arbejdspapirer/preprints	
Konferenceartikler, peer reviewed	J.M. Christensen, A.D. Jensen, J.-D. Grunwaldt; Mo-based catalysts for CO hydrogenation to higher alcohols - Insights from XAS and activity tests, 2013. Abstract from ANKA/KNMF Users' Meeting 2013, Karlsruhe, Germany M. Høj, A.D. Jensen, J.-D. Grunwaldt; Flame spray synthesis of VOx/Al2O3 catalysts for propane oxidative dehydrogenation, 2013. Abstract from 11th EuropaCat Congress, Lyon, France M. Høj, A.D. Jensen, J.-D. Grunwaldt; Flame Made VOx/Al2O3 Propane Oxidative Dehydrogenation Catalysts, 2013. Abstract from 23rd North American Catalysis Society Meeting, Louisville, Kentucky, USA Q. Wu, G. L. Chiarello, J.M. Christensen, B. Temel, J.-D. Grunwaldt, A.D. Jensen; Supported molybdenum carbide for higher alcohol synthesis from Syngas, 2013. Abstract from 23rd North American Catalysis Society Meeting, Louisville, Kentucky, USA
Konferenceartikler, ikke peer	

Konferenceartikler, ikke peer reviewed	
Patenter, patentansøgninger	A.Riisager, R. Fehrmann, A.J. Kunov-Kruse, P. Malcho, J. Andersen, K. Ståhl; A method for effective conversion of saccharides to furfural compounds. DTU ref. 95497. Patent applied.
Datasæt (x hvis afleveret til Dansk Data Arkiv)	
Planlagte publikationer (angiv type)	
Anden formidling	
Fx forskningsformidlende bøger/antologier, kronikker, tv, mm.	H. Birkedal: Ny lim limer mennesker sammen. Radio interview, P1 morgen. October 1, 2013 A.B. Blichfeld: Besøgsservice. Dept. of Chemistry, Aarhus University. 2013 D.E. Brodersen: Hovedarrangør af Department of Molecular Biology and Genetics, Annual meeting 2013, Aarhus University, Denmark D.E. Brodersen: Lecture for delegation from the Chinese Research Ministry - "Bacterial toxins and bioactive peptides" E.D. Bøjesen: Fra spildvarme til strøm. Forskningens Døgn, Aarhus University. May 3, 2013 M. Christensen: Institute Seminar: A bottom-up approach to high performance magnets. Aalborg University, April 17, 2013 M. Christensen: iNANO Lecture: "High performance magnets - a bottom-up approach". Aarhus University, March 6, 2013 M. Christensen: Lecturing High School teachers. LMFK – Årskursus, Aarhus University. October 24, December 2013 M. Christensen: Public lectures, both demonstrating energy materials. "Supermagnet" & "Materiale kemi og energi". Forskningens døgn, Aarhus University. May 3, 2013 M. Christensen: Student excursion to MAX-lab. MAX-lab, March 2013 M. Christensen: Presentation: "AU" (about Aarhus University). EUDP Kick Off Meeting at TEGnology, Vejle, Denmark. Sept. 18, 2013 M. Christensen: NANOPYME - experiences from a FP7 project. Horizon 2020 meeting, Aarhus University. December 11, 2013 M. Christensen: Nanomaterials for energy applications. Current Nanoscience, guest lecture, Aarhus University. May 12, 2013. M. Christensen: Magnetic materials for the future. iNANO Board Meeting, Aarhus University. January 25, 2013 M.Ø. Filso: Besøgsservice & SRP. Dept. of Chemistry, Aarhus University. 2013 K. Frydenvang, L. Juknaite, J.S. Kastrup; På jagt efter et virkningssted i hjernen. Lægemedelforskning 2013, PharmaSchool, University of Copenhagen S. Hakim; Structure of Organic Compounds on Calcite and Quartz Surfaces. Nano-Chalk Symposium, University of Copenhagen, Denmark. January 31, 2013 K. Haldrup; Super-intens røntgenstråling -Hvad er det, og hvad kan man bruge det til? Vestegnens VUC, December 2013 N.E. Henriksen: Medarrangør af The Copenhagen Conference on Femtochemistry, FEMTO11, 7-12 July, 2013 M. Krogsgaard: Mussels, frites and ... glue? Interview, Jutland Station. December 4, 2013 M. Krogsgaard: Igen, Igen & igen. Interview, Forskerforum. December 3, 2013 K. Lefmann: Superledere, neutroner, og ESS. AOF Svendborg M.B. Ley: Brint (Hydrogen) opbevaring. Forskningens Døgn, Aarhus University. May 3, 2013 A.J. Mørup: Interview/commentary: Nyt energi-eventyr: Kør, flyv og sejl på alt fra madrester til kloakslam. DR Viden (online). February 5, 2013 P. Nissen, D.E. Brodersen, S. Thirup: Arrangør af ESS Neutron Protein Crystallography 2013 21-22 March 2013, Aarhus University, Denmark P. Nørby: Work at PHAUST. The PhD Association at AU, Science and Technology, Aarhus University. 2013 P. Nørby: Om smart energi. Forskningens Døgn, Aarhus University. May 3, 2013 K. Pantleon: Medlem af Helmholtz Zentrum Berlin HZB Scientific Selection Panel, College C6 Material Sciences and

Hard Condensed Matter, 2013

H.F. Poulsen; Industriens udnyttelse af de store internationale Røntgen og neutron faciliteter. Dansk Metallurgisk Selskabs vintermøde 2013, Kolding, Denmark, 16/01/13.

M. Søndergaard: Nye, bedre Li-ion batterier. Forskningens Døgn, Aarhus University. May 3, 2013

H.O. Sørensen; From samples to images, P3 kick-off meeting, University of Copenhagen, Denmark, December 16, 2013

H.O. Sørensen, R. Feidenhans'l; X-ray tomography at the micrometer and nanometer scale. Nano-Chalk Symposium, University of Copenhagen, Copenhagen, Denmark, January 31-February 1, 2013

H.O. Sørensen, Robert Feidenhans'l; X-ray tomography on natural porous materials. Minisymposium on Imaging Porous Media, University of Copenhagen, Copenhagen, Denmark, January 11, 2013.

B. Vestergaard: Medarrangør af Marstrand meeting, discussing our future CoSAXS beamline on MAX-IV, May 2013. ESS and Life Sciences, Lund, May 2013

Rådgivning

Fx artikler, videnskabelige rapporter, mm.

Undervisning

Fx lærebøger, kompendier, kurser, kandidatuddannelser

DANSCATT bidrager til at en lang række studerende (se venligst bilag 1) på både bachelor-, kandidat- 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.

T.B. Van Driel, M.M. Nielsen, K. Haldrup: Erice Summer School, Dynamical Structural Science, Erice, Italy, May 2013

S. Frølich, H. Birkedal: Nano-mechanical Properties of Anomia Simplex. Winterschool arranged by Nanoscience Cambridge, Hintertgamm, Austria. Febr. 2013

M. Krogsgaard: Cell Catch & Release: The Biological Put & Take. iNANO autumn school. Kystvejen hotel, Grenå, Denmark. October 11-14 2013

H. Leemreize: Looking into matter – diffraction tomography studies on the mineralized attachments system of the mermaid's toenail (Anomia simplex). iNANO autumn school. Kystvejen hotel, Grenå, Denmark. October 11-14 2013

H.F. Poulsen: X-ray diffraction microscopy. II International Baltic School "Methods and Instruments of the X-ray investigations"

N. Sofos: EMBO course talk, Harwell Research Complex, Oxford, UK

B. Vestergaard og A.E. Langkilde har undervist i kurset: EMBO course on Small angle X-ray and Neutron scattering, Grenoble, France

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 (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. 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. Apparaturet 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 medlem af faciliteter som ESRF 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. Dancscatt ensures access and supports beamtime travels to these facilities. Denmark is a member of facilities like ESRF in Grenoble and the European XFEL in Hamburg. Furthermore, Denmark is co-hosting the ESS in Lund. Dancscatt 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

Bajic, G., L. Yatime, R.B. Sim, T. Vorup-Jensen, G.R. Andersen; Structural insight on the recognition of surface-bound opsonins by the integrin I domain of complement receptor 3. *Proc Natl Acad Sci U S A*. 2013 Oct 8;110(41):16426-31. doi: 10.1073/pnas.1311261110. Epub 2013 Sep 24. PubMed PMID: 24065820; PubMed Central PMCID: PMC3799375

Kantcheva, A.K., M. Quick, L. Shi, A.M. Winther, S. Stolzenberg, H. Weinstein, J.A. Javitch, P. Nissen; Chloride binding site of neurotransmitter sodium symporters. *Proc Natl Acad Sci U S A*. 2013 May 21;110(21):8489-94. doi: 10.1073/pnas.1221279110. Epub 2013 May 2. PubMed PMID: 23641004; PubMed Central PMCID: PMC3666746

Nyblom, M., H. Poulsen, P. Gourdon, L. Reinhard, M. Andersson, E. Lindahl, N. Fedosova, P. Nissen; Crystal structure of Na⁺, K⁺-ATPase in the Na⁺-bound state. *Science*. 2013 Oct 4;342(6154):123-7. doi: 10.1126/science.1243352. Epub 2013 Sep 19. PubMed PMID: 24051246

Schmøkel, M.S., L. Bjerg, J. Overgaard, F.K. Larsen, G. Madsen, K. Sugimoto, M. Takata, B.B. Iversen; Pushing X-ray charge densities to the limit: Thermoelectric CoSb₃. *Angew. Chem. Intl. Ed*. 2013, 52, 1503-1506

Udby, L., J. Larsen, N.B. Christensen, M. Boehm, C. Niedermayer, H.E. Mohottala, T.B.S. Jensen, R. Toft Petersen, F.C. Chou, N.H. Andersen, K. Lefmann, B.O. Wells; Direct proof of generic magnetic and superconducting phases in a series of superoxygenated high-Tc oxides. *Phys. Rev. Lett* 111, 227001, 2013

Andre væsentlige resultater

Gem som

Reset Form

Participants in Danscatt activities 2013 (Bilag 1)

Groupleader	VIP's (professors, senior scientists etc.)	Postdocs	Ph.D. students	Students	TAP's (technicians, administrative staff etc.) and scientific assistants
Bo Brummerstedt Iversen, Dept. of Chemistry, Aarhus University	Ann-Christin Dippel Bo Brummerstedt Iversen Henrik Birkedal Jacob Overgaard Jens-Erik Jørgensen Martin Bremholm Mogens Christensen Torben Rene Jensen	Dipankar Saha Lai Chin Wu Mads Ry Jørgensen Marian Stingaciu Martin Søndergaard Simon Johnsen Venkatesha Hathwar	Anders Blichfeld Anders Mørup Bjarne R.S. Hansen Casper Ibsen Dmytro Korablov Elisabeth Grube Ellen Jensen Elsa Roedern Espen Bøjesen Espen Eikeland Fiona L.Bach Gansmo Hanna Leemreize Henrik Hellstern Kasper Borup Kasper Møller Kristian Andreasen Lars H. Jepsen Maja Krüger Thomsen Marie Krogsgaard Mattia Sist Mette S. Filsø Mie Birkbak Morten Brix Ley Morten Schulz Nielsen Nanna Wahlberg	Anders C.S. Jensen Andreas K. Bovin Anna Zink Bjørn S. Bruun Casper W. Andersen Cecilia Granados Miralles Giuditta Perversi Henrik L. Andersen Karl F. Fischer Kasper Houlberg Martin Roelsgaard Martin Schmidt Matilde Saura Ram Sarusie Steffen Pedersen Torben G. Jensen Troels Christiansen	Aref Mamakhel Bo Richter Britta Lundtoft Jacob Becker Marianne Sommer Payam Javadian Peter Hald

			Niels Bindzus Per Runge Christensen Peter Nørby Sebastian Christensen Simon Frølich Solveig R. Madsen Steinar Birgisson Vicki Nue Yanbin Shen		
Søren Skou Thirup, Dept. of Molecular Biology, Aarhus University	C.B.F. Andersen Ditlev E. Brodersen Gregers Rom Andersen L.B. Jenner Poul Nissen Rune Hartmann Søren Skou Thirup Thomas Boesen	A.-M. L. Winther A. Bøggild C. Olesen Frederik T. Hansen H.H. Gad J. Jensen Jesper B. Poulsen Johannes Bauer J.L. Andersen J.S. Johansen Kai-Tuo Wang Kristian Stødkilde Jørgensen L. Yatime M. Blaise M. Bublit M.J. Clausen M. Laursen O. Hamming P. Gourdon R. Kidmose	Claus Olesen D. Vaicaityte Ewa Terczynska-Dyla G. Bajic Henriette E. Autzen H. Kristiansen Jeryl Cheng J.A. Schatz-Jakobsen J.L. Gregersen J.M. Wong Kehan Xu Kira Gysel L. Malinauskaite Maja H. Nielsen Manuela Gorgel Mateusz Dyla Mikkel Ibsen Morten Torvund-Jensen N.D. Drachmann N.E. Sofos O. Sitsel	Aljona Kotsubei Caglanur Sahin Casper Larsen Jeppe A. Nielsen Khaled Taj Kirstine Louise Bendtsen L.B. Rasmussen Maibritt Luckmann	

			Patricia R. Fuertes P.A. Paulsen P. Seweryn Piotr Siupka Sigrid T. Larsen S. Sirotkina		
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	Kim Lefmann Lars Øgendal Lise Arleth Robert Feidenhans'l Steen L. Hansen	Julio Tedesco Linda Udby Nikolaos Tsatpatsaris Shantanu Mukherjee Stine Rønholt Søren Kynde Søren Roi Midtgaard	Mads Bertelsen Maria N. Gastiasoro Maria Thomsen Martin Cramer Pedersen Mikkel Schou Nielsen Morten Sales Murillo Longo Martins Pia Jensen Pie Huda Selma Maric Sonja Lindahl Holm Tomas Stankevic Torsten Lauridsen Ursula Bengård Hansen	Kenneth Lønbæk Marcella Berg Mathias Kure Monika Kovacic Niels Christian Rand Momsen Oliver Boda Rosanna Ignazzi Solveig Hedal Turi Schäffer	
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List of Publications 2013 (bilag 2)

Dept. of Chemistry, Aarhus University

- Arakcheeva, A., P. Pattison, A. Bauer-Brandl, H. Birkedal, G. Chapuis; Cimetidine, $C_{10}H_{16}N_6S$, form C: crystal structure and modelling of polytypes using superspace approach. *J. Appl. Cryst.* **2013**, 46, 99-107
- Bach-Gansmo, F.L., S.C. Irvine, A. Brüel, J.S. Thomsen, H. Birkedal; Calcified Cartilage Islands in Rat Cortical Bone. *Calc. Tissue Int.* **2013**, 92, 330-338
- Barreto, L., M. Bianchi, D. Guan, R. Hatch, J.L. Mi, B.B. Iversen, P. Hofmann; Electron-phonon coupling in the two-dimensional electron gas on Bi_2Se_3 . *Phys. Status Solidi* **2013**, 7, 136-138
- Bindzus, N., F. Cargnoni, B.B. Iversen, C. Gatti; A theoretical study on the rotational motion and interactions in the disordered phase of MBH_4 ($M = Na, K \text{ \& } Rb$). *J. Phys Chem.* **2013**, 117, 2308-2316
- Birkedal, H., S. Frølich, H. Leemreize, R. Stallbohm, Y. H. Tseng, (Eds. R. Santos, N. Aldred, S. Gorb, P. Flammang); The mineralized byssus of *Anomia simplex*: A calcified attachment system in Biological and Biomimetic Adhesives, Challenges and Opportunities. RSC Publishing **2013**, 16-25, DOI:10.1039/9781849737135-00016
- Brown, D.R., T. Day, K.A. Borup, H. Lu, X. Shi, L. Chen, B.B. Iversen, G.J. Snyder; Phase Transition Enhanced Thermoelectric Figure-Of-Merit in Cu_2Se . *APL Mater* **2013**, 1, 052107
- Callini, E., L. Pasquini, T.R. Jensen, E. Bonetti; Hydrogen storage properties of Mg-Ni nanoparticles; *Int. J. Hyd. Energy*, **2013**, 38(27), 12207-12212
- Černý, R., P. Schouwink, Y. Sadikin, K. Stare, L. Smrčok, B. Richter, T.R. Jensen; Trimetallic borohydride $Li_3MZn_5(BH_4)_{15}$ ($M = Mg, Mn$), Containing Two Weakly Interconnected Frameworks. *Inorg. Chem.*, **2013**, 52, 9941-9947
- Christensen, S., M. A. Avila, K. Suekuni, R. Piltz, T. Takabatake, M. Christensen; Combined x-ray and neutron diffraction study of vacancies and disorder in the dimorphic clathrate $Ba_8Ga_{16}Sn_{30}$ of type I and VIII. *Dalton transaction* 42, 14766-14775, **2013**, DOI:10.1039/C3DT51328A
- Christensen, S., L. Bjerg, A. Kaltzoglou, F. Juranyi, T. Unruh, T. Fässler, M. Christensen; Guest host interaction and low energy host structure dynamics in tin clathrates. *J. Appl. Phys.* **2013**, 113, 8, 084902
- Dasgupta, T., C. Stiewe, A. Sesselmann, H. Yin, B.B. Iversen, E. Mueller; Thermoelectric studies in β - Zn_4Sb_3 - the complex interdependence between thermal stability, thermoelectric transport and Zinc content. *J. Appl. Phys.* **2013**, 113, 103708
- Dasgupta, T., H. Yin, J. de Boer, C. Stiewe, B.B. Iversen, E. Mueller; Thermal instability of β - Zn_4Sb_3 – insights from transport and structural measurements. *J. Elec. Mater.* **2013**, DOI: 10.1007/s11664-013-2490-6
- Eltzholtz, J.R., C. Tyrsted, M. Bremholm, K.M.Ø. Jensen, M. Christensen, J. Becker-Christensen, B.B. Iversen; Pulsed supercritical synthesis of anatase TiO_2 nanoparticles in a water-isopropanol

mixture studied by in situ powder X-ray diffraction. *Nanoscale* **2013**, 5, 2372–2378

- Filsø, M.Ø., M.J. Turner, J. Gibbs, S. Adams, M.A. Spackman, B.B. Iversen; Visualizing Li-ion migration pathways in battery materials from procrystal electron density void space calculations. *Chem. Eur. J.* **2013**, 19, 15535 – 15544
- Gibbs, G.V., N.L. Ross, D.F. Cox, K.M. Rosso, B.B. Iversen, M.A. Spackman; Bonded radii and the contraction of the electron density of the oxygen atom by bonded interactions. *J. Phys. Chem.* **2013**, dx.doi.org/10.1021/jp310462g
- Gosalawit-Utke, R., C. Milanese, P. Javadian, J. Jepsen, D. Laipple, F. Karmi, J. Puzkiel, T.R. Jensen, A. Marini, T. Klassen, M. Dornheim; Nanoconfined 2LiBH₄-MgH₂-TiCl₃ in carbon aerogel scaffold for reversible hydrogen storage. *Int. J. Hyd. Energy*, **2013**, 38(8), 3275–3282
- Gosalawit-Utke, R., C. Milanese, T.K. Nielsen, F. Karimi, I. Saldan, K. Pranzas, T.R. Jensen, A. Marini, T. Klassen, M. Dornheim; Nanoconfined 2LiBH₄-MgH₂ for Reversible Hydrogen Storages: Reaction Mechanisms, Kinetics and Thermodynamics. *Int. J. Hyd. Energy*, **2013**, 38(4), 1932-1942
- Gradišek, A., D.B. Ravnsbæk, S. Vrtnik, A. Kocjan, J. Lužnik, T. Apih, T.R. Jensen, A.V. Skripov, J. Dolinšek; NMR Study of Molecular Dynamics in Complex Metal Borohydride LiZn₂(BH₄)₅. *J. Phys. Chem. C*, **2013**, 117, 21139–21147
- Hansen, B.R.S., D.B. Ravnsbæk, D. Reed, D. Book, C. Gundlach, J. Skibsted, T.R. Jensen; Hydrogen storage capacity loss in a LiBH₄-Al composite. *J. Phys. Chem. C*, **2013**, 117, 7423-7432
- Hirai, D., M. Bremholm, J.M. Allred, L.M. Schoop, Q. Huang, J. Tao, R.J. Cava; Spontaneous Formation of 1D Chains due to a Charge-Order transition in the □-pyrochlore CsW₂O₆. *Physical Review Letters*, **2013**, 110 (16), 166402
- Holgate, T.C., N. Wu, M. Søndergaard, B.B. Iversen, N.V. Nong, N. Pryds; Kinetics, Stability and Thermal Contact Resistance of Nickel-Ca₃Co₄O₉ Interfaces Formed by Spark Plasma Sintering. *J. Elec. Mater.* **2013**, DOI: 10.1007/s11664-012-2363-4
- Hung, L.T., N.V. Nong, L. Hana, D.L. Minh, K.A. Borup, B.B. Iversen, N. Pryds, S. Linderorth; High-temperature Thermoelectric Properties of Ca_{0.9}Y_{0.1}Mn_{1-x}Fe_xO₃ (0 ≤ x ≤ 0.25). *J. Mater. Sci.* **2012**, 48, 2817-2822
- Huot, J., D.B. Ravnsbæk, J. Zhang, F. Cuevas, M. Latroche, T.R. Jensen; Mechanochemical Synthesis of Hydrogen Storage Materials, *Prog. Mater. Sci.* **2013**, 58, 30–75, <http://dx.doi.org/10.1016/j.pmatsci.2012.07.001>
- Jensen, K.M.Ø., M. Christensen, H.P. Gunnlaugsson, N. Lock, E.D. Bøjensen, T. Proffen, B.B. Iversen; Defects in hydrothermally synthesized LiFePO₄ and LiFe_{1-x}Mn_xPO₄ cathode materials. *Chem. Mater* **2013**, 25, 2282-2290
- Jepsen, K.L.H., J. Skibsted, T.R. Jensen; Investigations of the thermal decomposition of MBH₄-2NH₃BH₃, M = Na, *J. Alloys Comp.*, **2013**, 580, S287–S291
- Johnson, J.A., Q. Lin, L.-C. Wu, N. Obaidi, Z.L. Olson, T.C. Reeson, Y.-S. Chen, J. Zhang; A "pillar-free", highly porous metalloporphyrinic framework exhibiting eclipsed porphyrin arrays. *Chem. Comm.* **2013**, 27, 49, 2828-2830

- Jørgensen, M.R.V., S. Cenedese, H.F. Clausen, J. Overgaard, Y.S. Chen, C. Gatti, B.B. Iversen; Experimental and theoretical charge density of a Zn containing coordination polymer, $\text{Zn}(\text{HCOO})_2(\text{H}_2\text{O})_2$. *Inorg. Chem.* **2013**, 52, 297–305
- Kastbjerg, S., N. Bindzus, M. Søndergaard, S. Johnsen, N. Lock, M. Christensen, M. Takata, M.A. Spackman, B.B. Iversen; Direct Evidence of Cation Disorder in Thermoelectric Lead Chalcogenides, PbTe and PbS. *Adv. Func. Mat.* **2013**, DOI: 10.1002/adfm.201300722
- Korablov, D., D.B. Ravnsbæk, V. Ban, Y. Filinchuk, F. Besenbacher, T.R. Jensen; Investigation of $\text{MBH}_4\text{--VCl}_2$, $\text{M} = \text{Li, Na or K}$. *Int. J. Hyd. Energy*, **2013**, 38, 8376–8383
- Krogsgaard, M., M.A. Behrens, J.S. Pedersen, H. Birkedal; Self-Healing Mussel-Inspired Multi-pH-Responsive Hydrogels. *Biomacromolecules* **2013**, 14, 297–301
- Leardini, F., A. Paolone, O. Palumbo, R. Cantelli, T. K. Nielsen, T. R. Jensen; Anelastic Spectroscopy Investigation of Nano-confined Alanates. *J. Alloys Comp.*, **2013**, 580, S70–S72
- Leemreize, H., J.D. Almer, S.R. Stock, H. Birkedal; Three dimensional distribution of polymorphs and magnesium in a calcified underwater attachment system by diffraction tomography. *J. Roy. Soc. Interface* **2013**, 10, 20130319
- Li, C., L. Yang, J. Xiao, Y. Wu, Y. Luo, D. Li, P. Hald, Q. Meng, B.B. Iversen; ZnO nanoparticle based highly efficient CdS/CdSe quantum dot-sensitized solar cells. *Phys. Chem. Chem. Phys.* **2013**, 15, 8710–8715
- Li, J.L., M. Bremholm, M. Bianchi, K. Borup, S. Johnsen, M. Søndergaard, D. Guan, R.C. Hatch, P. Hofmann, B.B. Iversen; Phase Separation and Bulk p-n Transition in Single Crystals of $\text{Bi}_2\text{Te}_2\text{Se}$ Topological Insulator. *Adv. Mater.* **2013**, 25, 889–893
- Li, J.L., B.B. Iversen; Biomolecule-assisted hydrothermal synthesis of Bi_2Te_3 nanostructures. *AIP Conf. Proc.* **2013**, 1449, 87–90
- Lock, N., M. Christensen, C. Kepert, B.B. Iversen; Effect of Gas Pressure on Negative Thermal Expansion in MOF-5. *Chem. Commun.* **2013**, 49, 789–791
- Lock, N., M. Christensen, Y. Wu, V.K. Peterson, M.K. Thomsen, R. Piltz, A.J. Ramirez-Cuesta, G. McIntyre, K. Norén, C.J. Kepert, G. Kearley, B.B. Iversen; Scrutinizing Negative Thermal Expansion in MOF-5 – a Combined X-ray and Neutron Diffraction, Inelastic Neutron Scattering, *Ab Initio* and X-Ray Absorption Spectroscopy Study. *Dalton Trans.* **2013**, 42, 1996–2007 (Frontcover)
- Lock, N., E.M.L. Jensen, J.L. Mi, A. Mamakhel, K. Norén, Q. Meng, B.B. Iversen; Copper Doped TiO_2 nanoparticles Characterized by X-Ray Absorption Spectroscopy, Total Scattering and Powder Diffraction - A Benchmark Structure-Property Study. *Dalton Trans* **2013**, 42, 9555 – 9564
- Mamakhel, A., C. Tyrsted, P. Hald, B.B. Iversen; Direct formation of crystalline phase pure rutile TiO_2 nanostructures by a facile low temperature hydrothermal method. *Crystal Growth & Design* **2013**, 13, 4730–4734
- Mi, J.L., S. Johnsen, C. Clausen, P. Hald, N. Lock, L. Sø, B.B. Iversen; Highly controlled crystallite size and crystallinity of pure and Fe doped anatase TiO_2 nanocrystals by continuous flow supercritical synthesis. *J. Mater. Res.* **2013**, 28, 333
- Nechaev, I.A., R.C. Hatch, M. Bianchi, D. Guan, C.J. Friedrich, J.L. Mi, B.B. Iversen, S. Blugel, P.

- Hofmann, E.V. Chulkov; Evidence for a direct band gap in the topological insulator Bi₂Se₃ from theory and experiment. *Phys. Rev. B* **2013**, 87, 121111
- Nielsen, T.K., A. Karkamkar, M. Bowden, F. Besenbacher, T.R. Jensen, T. Autrey; Methods to stabilize and destabilize ammonium borohydride. *Dalton Trans*, **2013**, 42, 680–687
- Nørby, P., K.M.Ø. Jensen, N. Lock, M. Christensen, B.B. Iversen; In Situ Synchrotron Powder X-ray Diffraction Study of Formation and Growth of Yttrium and Ytterbium Aluminum Garnet Nanoparticles in Sub- and Supercritical Water. *RSC Adv.* **2013**, 3, 15368–15374
- Olliges-Stadler, I., M.D. Rossell, M. Süess, B. Ludi, O. Bunk, J.S. Pedersen, H. Birkedal, M. Niederberger; A Comprehensive study of the crystallization mechanism involved in the nonaqueous formation of tungstite. *Nanoscale* **2013**, 5, 8517-8525
- Paskevicius, M., M.B. Ley, D.A. Sheppard, T.R. Jensen, C.E. Buckley; Eutectic Melting in Metal Borohydrides. *Phys. Chem. Chem. Phys.*, **2013**, 15, 19774-19789
- Pauw, B.R., J.S. Pedersen, S. Tardif, M. Takata, B.B. Iversen; Improvements and considerations for size distribution retrieval from small-angle scattering data by Monte-Carlo methods. *J. Appl. Cryst.* **2013**, 46, 365-371
- Platts, J.A., M.K. Thomsen, J. Overgaard; Electron Localisation in Ga-Heterocyclic Compounds. *Z. Anorg. Allg. Chem.* **2013**, 639, 11, 1979-1984
- Polanski, M., T. K. Nielsen, I. Kunce, M. Norek, T. Płociński, L.R. Jaroszewicz, C. Gundlach, T.R. Jensen, J. Bystrzycki; Mg₂NiH₄ synthesis and decomposition reactions. *Int. J. Hyd. Energy*, **2013**, 38, 4003-4010. <http://dx.doi.org/10.1016/j.ijhydene.2013.01.119>
- Puszekiel, J., F. Gennari, P.A. Larochette, F. Karimi, C. Pistidda, R. Gosławit-Utke, J. Jepsen, T.R. Jensen, C. Gundlach, J.B. von Colbe, T. Klassen, M. Dornheim; Sorption behavior of the MgH₂–Mg₂FeH₆ hydride storage system synthesized by mechanical milling followed by sintering. *Int. J. Hyd. Energy*, **2013**, 38, 14618-14630
- Ravnsbæk, D.B., E.A. Nickels, R. Černý, C.H. Olesen, W.I.F. David, P.P. Edwards, Y. Filinchuk, T.R. Jensen; Novel alkali earth borohydride Sr(BH₄)₂ and borohydride-chloride Sr(BH₄)Cl. *Inorg. Chem.* **2013**, 52, 10877-10885
- Reis, D.D., L. Barreto, M. Bianchi, G.A.S. Ribeiro, E.A. Soares, W.S. Silva, V.E. Carvalho, J. Rawle, C. Nicklin, W. Principe, J. Mi, B.B. Iversen, P. Hofmann; Surface structure of Bi₂Se₃(111) determined by low-energy electron diffraction and surface X-ray diffraction. *Phys. Rev. B* **2013**, 88, 041404(R)
- Rude, L.H., U. Filsø, V. D’Anna, A. Spyratou, B. Richter, S. Hino, O. Zavorotynska, M. Baricco, M.H. Sørby, B.C. Hauback, H. Hagemann, F. Besenbacher, J. Skibsted, T.R. Jensen; Hydrogen-fluorine exchange in NaBH₄-NaBF₄; *Phys. Chem. Chem. Phys.*, **2013**, 15, 18185-18194
- Saldan, I., M. Schulze, C. Pistidda, R. Gosławit-Utke, O. Zavorotynska, L.H. Rude, J. Skibsted, D. Haase, Y. Cerenius, T.R. Jensen, G. Spoto, M. Baricco, K. Taube, M. Dornheim; Hydrogen sorption in the LiH–LiF–MgB₂ system. *J. Phys. Chem. C*, **2013**, 117, 17360–17366
- Scheins, S., J. Overgaard, G.A. Timco, A. Stash, Y.S. Chen, F.K. Larsen, M.R.V. Jørgensen, S.R. Madsen, M.S. Schmøkel, B.B. Iversen; Pressure versus temperature effects on intramolecular electron transfer in mixed-valence complexes. *Chem. Eur. J.* **2013**, 19, 195 – 205

- Schlenk, T., M. Bianchi, M. Koleini, A. Eich, O. Pietzsch, T.O. Wehling, T. Frauenheim, A. Balatsky, J.-L. Mi, B.B. Iversen, J. Wiebe, A.A. Khajetoorians, Ph. Hofmann, R. Wiesendanger; Controllable magnetic doping of the surface state of a topological insulator. *Phys. Rev. Lett.* **2013**, 110, 126804
- Schmøkel, M.S., L. Bjerg, S. Cenedese, M.R.V. Jørgensen, Y.-S. Chen, J. Overgaard, B.B. Iversen; Atomic properties and chemical bonding in the pyrite and marcasite polymorphs of FeS₂: A combined experimental and theoretical electron density study, *Chem. Sc.* **2013**, 1-3
- Schmøkel, M.S., L. Bjerg, F.K. Larsen, J. Overgaard, S. Cenedese, M. Christensen, G.K.H. Madsen, C. Gatti, E. Nishibori, K. Sugimoto, M. Takata, B.B. Iversen; Comparative study of X-ray charge density data on CoSb₃. *Acta Crystallogr. Sect. A.* **2013**, 69, 570-582
- Schmøkel, M.S., L. Bjerg, J. Overgaard, F.K. Larsen, G. Madsen, K. Sugimoto, M. Takata, B.B. Iversen; Pushing X-ray charge densities to the limit: Thermoelectric CoSb₃. *Angew. Chem. Intl. Ed.* **2013**, 52, 1503-1506
- Schmøkel, M.S., J. Overgaard, B.B. Iversen; Experimental electron density studies of inorganic materials. *Z. Anorg. Allg. Chem.* **2013**, 1922-1932
- Shen, Y., J.R. Eltzholtz, B.B. Iversen; Controlling Size, Crystallinity, and Electrochemical Performance of Li₄Ti₅O₁₂ Nanocrystals. *Chem. Mater.* **2013**, 25, 5023-5030
- Sheppard, D.A., L.H. Jepsen, T.R. Jensen, M. Paskevicius, C.E. Buckley; New directions for hydrogen storage: Sulphur destabilised sodium aluminium hydride. *J. Mater. Chem.* **2013**, 1, 41, 12775-12781
- Skripov, A.V., A.V. Soloninin, M.B. Ley, T.R. Jensen, Y. Filinchuk; Nuclear Magnetic Resonance Studies of BH₄ Reorientations and Li Diffusion in LiLa(BH₄)₃Cl. *J. Phys. Chem. C*, **2013**, 117, 14965–14972
- Straasø, T., J. Becker, B.B. Iversen, J. Als-Nielsen; The Debye-Scherrer Camera at Synchrotron Sources - a Revisit. *J. Sync. Rad.* **2013**, 20, 98-104
- Su, R., M. Christensen, Y. Shen, J. Kibsgaard, B. Elgh, R.T. Vang, R. Bechstein, S. Wendt, A. Palmqvist, B.B. Iversen, F. Besenbacher; Rapid Synthesis of Porous, Mixed Phase Titania Films with Tailored Orientation of Rutile for Enhanced Photocatalytic Performance. *J. Phys. Chem.* **2013**, 117, 27039–27046
- Sun, P., W. Xu, J.M. Tomczak, G. Kotliar, M. Søndergaard, B.B. Iversen, F. Steglich; Highly Dispersive Electron Relaxation and Colossal Thermoelectricity in the Correlated Semiconductor FeSb₂. *Phys. Rev. B* **2013**, 88, 245203
- Søndergaard, M., E.D. Bøjesen, K.A. Borup, M. Christensen, B.B. Iversen; Sintering and annealing effects on ZnO microstructure and thermoelectric properties. *Acta Mater.* **2013**, accepted
- Søndergaard, M., M. Christensen, K.A. Borup, H. Yin, B.B. Iversen; Thermal stability and thermoelectric properties of Mg₂Si_{0.4}Sn_{0.6} and Mg₂Si_{0.6}Sn_{0.4} compounds. *J. Mater. Sci.* **2013**, 48, 2002–2008
- Søndergaard, M., M. Christensen, K.A. Borup, H. Yin, B.B. Iversen; Thermoelectric properties of the entire composition range in Mg₂Si_{0.9925-x}Sn_xSb_{0.0075}. *J. Elec. Mater.* **2013**, DOI: 10.1007/s11664-012-2282-4

- Søndergaard, M., S. Johnsen, P. Sun, Y. Sun, S. Cenedese, C. Gatti, F. Steglich, B.B. Iversen; Strongly correlated intermetallics – FeSb₂, in: *Thermoelectric Nanomaterials* (Ed. K. Koumoto and T. Mori), Springer, Berlin/Heidelberg **2013**
- Tseng, Y.-H., M.E. Birkbak, H. Birkedal; Spatial Organization of Hydroxyapatite Nanorods on a Substrate via a Biomimetic Approach. *Cryst. Growth Des.* **2013**, 13, 4213-4219
- Wu, L.-C., J. Overgaard, S.R. Madsen, M.S. Schmøkel, B.B. Iversen; High-pressure single-crystal X-ray diffraction study of the photomagnetic switching complex – [Y(DMF)₄(H₂O)₃(□-CN)Fe(CN)₅](□H₂O). *J. Chin. Chem. Soc.* **2013**, 60, 929–934
- Yin, H., S. Johnsen, K.A. Borup, K. Kato, M. Takata, B.B. Iversen; Highly Enhanced Thermal Stability of Zn₄Sb₃ Nanocomposites. *Chem. Commun.* **2013**, 49, 6540 – 6542
- Yun, G., L. Chunhui, L. Yanhong, L. Dongmei, Q. Meng, B.B. Iversen; Simple method for manufacturing Pt counter electrodes on conductive plastic substrates for dye-sensitized solar cells. *Appl. Mater. Interfaces* **2013**, 5, 795–800
- Ångström, J., R. Johansson, L.H. Rude, C. Gundlach, R.H. Scheicher, R. Ahuja, O. Eriksson, T.R. Jensen, M. Sahlberg; Hydrogen storage properties of the pseudo binary Laves phase (Sc_{1-x}Zr_x)(Co_{1-y}Ni_y)₂ system. *Int. J. Hyd. Energy*, **2013**, 38(23), 9772 - 9778

Dept. of Molecular Biology, Aarhus University

- Andersen, J.L., T.J. Schröder, S. Christensen, D. Strandbygård, L.T. Pallesen, M.M. García-Alai, S. Lindberg, M. Langgård, J.C. Eskildsen, L. David, L. Tagmose, K.B. Simonsen, P.J. Maltas, L.C. Rønn, I.E. de Jong, I.J. Malik, J. Egebjerg, J.J. Karlsson, S. Uppalanchi, D.R. Sakumudi, P. Eradi, S.P. Watson, S. Thirup; Identification of the first small-molecule ligand of the neuronal receptor sortilin and structure determination of the receptor-ligand complex. *Acta Crystallogr D Biol Crystallogr*. **2014** Feb;70(Pt 2):451-60. doi: 10.1107/ S139900471303 0149. Epub 2014 Jan 29. PubMed PMID: 24531479; PubMed Central PMCID: PMC3940197
- Bajic, G., L. Yatime, A. Klos, G.R. Andersen; Human C3a and C3a desArg anaphylatoxins have conserved structures, in contrast to C5a and C5a desArg. *Protein Sci*. **2013** Feb;22(2):204-12. doi: 10.1002/pro.2200. Epub 2012 Dec 16. PubMed PMID: 23184394; PubMed Central PMCID: PMC3588916
- Bajic, G., L. Yatime, R.B. Sim, T. Vorup-Jensen, G.R. Andersen; Structural insight on the recognition of surface-bound opsonins by the integrin I domain of complement receptor 3. *Proc Natl Acad Sci U S A*. **2013** Oct 8;110(41):16426-31. doi: 10.1073/pnas.1311261110. Epub 2013 Sep 24. PubMed PMID: 24065820; PubMed Central PMCID: PMC3799375
- Brodersen, D.E., G.R. Andersen, C.B. Andersen; Mimer: an automated spreadsheet-based crystallization screening system. *Acta Crystallogr Sect F Struct Biol Cryst Commun*. **2013** Jul;69(Pt 7):815-20. doi: 10.1107/S1744309113014425. Epub 2013 Jun 29. PubMed PMID: 23832216; PubMed Central PMCID: PMC3702333
- Bublitz, M., M. Musgaard, H. Poulsen, L. Thøgersen, C. Olesen, B. Schiøtt, J.P. Morth, J.V. Møller, P. Nissen; Ion pathways in the sarcoplasmic reticulum Ca²⁺-ATPase. *J Biol Chem*. **2013** Apr 12;288(15):10759-65. doi: 10.1074/jbc.R112.436550. Epub 2013 Feb 11. Review. PubMed PMID: 23400778; PubMed Central PMCID: PMC3624456
- Clausen, J.D., M. Bublitz, B. Arnou, C. Montigny, C. Jaxel, J.V. Møller, P. Nissen, J.P. Andersen, M. le Maire; SERCA mutant E309Q binds two Ca(2+) ions but adopts a catalytically incompetent conformation. *EMBO J*. 2013 Dec 11;32(24):3231-43. doi: 10.1038/emboj.2013.250. Epub 2013 Nov 22. PubMed PMID: 24270570
- Kantcheva, A.K., M. Quick, L. Shi, A.M. Winther, S. Stolzenberg, H. Weinstein, J.A. Javitch, P. Nissen; Chloride binding site of neurotransmitter sodium symporters. *Proc Natl Acad Sci U S A*. **2013** May 21;110(21):8489-94. doi: 10.1073/pnas.1221279110. Epub 2013 May 2. PubMed PMID: 23641004; PubMed Central PMCID: PMC3666746
- Kjaer, T.R., S. Thiel, G.R. Andersen; Toward a structure-based comprehension of the lectin pathway of complement. *Mol Immunol*. **2013** Dec;56(4):413-22. doi: 10.1016/j.molimm.2013.05.007. Epub 2013 Aug 1. Review. PubMed PMID: 23911397
- Laursen, M., L. Yatime, P. Nissen, N.U. Fedosova; Crystal structure of the high-affinity Na⁺K⁺-ATPase-ouabain complex with Mg²⁺ bound in the cation binding site. *Proc Natl Acad Sci U S A*. **2013** Jul 2;110(27):10958-63. doi: 10.1073/pnas.1222308110. Epub 2013 Jun 17. PubMed PMID: 23776223; PubMed Central PMCID: PMC3704003
- Mattle, D., O. Sitsel, H.E. Autzen, G. Meloni, P. Gourdon, P. Nissen; On allosteric modulation of P-type Cu(+)-ATPases. *J Mol Biol*. **2013** Jul 10;425(13):2299-308. doi: 10.1016/j.jmb.2013.03.008. Epub 2013 Mar 13. Review. PubMed PMID: 23500486

- Nielsen, M.J., C.B.F. Andersen, S.K. Moestrup; CD163 binding to haptoglobin-hemoglobin complexes involves a dual-point electrostatic ligand-receptor pairing. *Journal of Biological Chemistry* **2013**. doi:10.1074/jbc.M113.471060
- Nyblom, M., H. Poulsen, P. Gourdon, L. Reinhard, M. Andersson, E. Lindahl, N. Fedosova, P. Nissen; Crystal structure of Na⁺, K⁽⁺⁾-ATPase in the Na⁽⁺⁾-bound state. *Science*. **2013** Oct 4;342(6154):123-7. doi: 10.1126/science.1243352. Epub 2013 Sep 19. PubMed PMID: 24051246
- Schröder, T.J., S. Christensen, S. Lindberg, M. Langgård, L. David, P.J. Maltas, J. Eskildsen, J. Jacobsen, L. Tagmose, K.B. Simonsen, L.C. Biilmann Rønn, I.E. de Jong, I.J. Malik, J.J. Karlsson, C. Bundgaard, J. Egebjerg, J.B. Stavenhagen, D. Strandbygård, S. Thirup, J.L. Andersen, S. Uppalanchi, S. Pervaram, S.P. Kasturi, P. Eradi, D.R. Sakumudi, S.P. Watson; The identification of AF38469: an orally bioavailable inhibitor of the VPS10P family sorting receptor Sortilin. *Bioorg Med Chem Lett*. **2014** Jan 1;24(1):177-80. doi: 10.1016/j.bmcl.2013.11.046. Epub 2013 Nov 27. PubMed PMID: 24355129
- Tidow, H., P. Nissen; Special issue--signalling. Introduction--Ca²⁺ signalling and transport in health and disease. *FEBS J*. **2013** Nov;280(21):5384. doi: 10.1111/febs.12507. Epub 2013 Sep 23. PubMed PMID: 23992355
- Tidow, H., P. Nissen; Structural diversity of calmodulin binding to its target sites. *FEBS J*. **2013** Nov; 280(21):5551-65. doi: 10.1111/febs.12296. Epub 2013 May 13. Review. PubMed PMID: 23601118
- Winther, K.S., D.E. Brodersen, A.K. Brown, K. Gerdes; VapC of Mycobacterium tuberculosis Inhibits Translation by Endonucleolytic Cleavage of the Sarcin-Ricin Loop of 23S rRNA. *Nature Communications* **2013**, e-pub ahead of print (PubMed).
- Xu, K., E. Dedic, P. Cob-Cantal, C. Dienemann, A. Bøggild, K.S. Winther, K. Gerdes, D.E. Brodersen; Protein expression, crystallization and preliminary X-ray crystallographic analysis of the isolated Shigella flexneri VapC toxin. *Acta Crystallogr Sect F Struct Biol Cryst Commun*. **2013** Jul;69(Pt 7):762-5. doi: 10.1107/S1744309113014012. Epub 2013 Jun 28. PubMed PMID: 23832203; PubMed Central PMCID: PMC3702320
- Yatime, L., G.R. Andersen; Structural insights into the oligomerization mode of the human receptor for advanced glycation end-products. *FEBS J*. **2013** Dec;280(24):6556-68. doi:10.1111/febs.12556. Epub 2013 Oct 25. PubMed PMID: 24119142

DTU Physics, DTU Energy Conversion, DTU Wind Energy, DTU Cen, and Danchip, Technical University of Denmark

- Blackburn, E., J. Chang, M. Hücker, A.T. Holmes, N.B. Christensen, R. Liang, D.A. Bonn, W.N. Hardy, U. Rütt, O. Gutowski, M. v. Zimmermann, E.M. Forgan, S.M. Hayden; X-ray diffraction observations of charge-density-wave order in superconducting ortho-II YBa₂Cu₃O_{6.54} single crystals in zero magnetic field. *Physical Review Letters* 110, 137004 **2013**
- Canton, S.E., X. Zhang, J. Zhang, T.B. van Driel, K.S. Kjaer, K. Haldrup, P. Chabera, T. Harlang, K. Suarez-Alcantara, Y. Liu, J. Pérez, A. Bordage, M. Pápai, G. Vankó, A.B. Stickrath, G. Jennings, C.A. Kurtz, M. Rovezzi, P. Glatzel, G. Smolentsev, J. Uhlig, A.O. Dohn, M. Christensen, A. Galler, W. Gawelda, C. Bressler, H.T. Lemke, K.B. Møller, M.M. Nielsen, R. Lomoth, K. Wärnmark, V. Sundström; Towards Highlighting the Ultrafast X-Ray Dynamics at the Optically Dark Sites of Photocatalysts. *J. Phys Chem. Lett.*, 4, 1972-1976 **2013**
- Chatzichristodoulou, C., C. Schönbeck, A. Hagen, P.V. Hendriksen; Defect chemistry, thermomechanical and transport properties of (RE₂-xSrx)_{0.98}(Fe_{0.8}Co_{0.2})_{1-y}MgyO₄-δ (RE=La, Pr). *Solid State Ionics*, 232, 68-79 **2013**
- Esmaeili, M., J.B. Floystad, A. Diaz, K. Hoydalsvik, M. Guizar-Sicairos, J.W. Andreasen, D.W. Breiby; Ptychographic X-ray Tomography of Silk Fiber Hydration. *Macromolecules*, 46, 434-439 **2013**
- Farhi, E., Y. Debab, P. Willendrup; iFit: A new data analysis framework. Applications for data reduction and optimization of neutron scattering instrument simulations with McStas. *Journal of Neutron Research*, **2014** pp. 5-18
- Farhi E., C. Monzat, R. Arnerin, T. van Vuure, C. Castán-Guerrero, C. Hennane, P.A. Harraud, G. Campioni, S. Fuard, J. Ollivier, P. Willendrup; Advanced sources and optical components for the McStas neutron scattering instrument simulation package. *Journal of Neutron Research* 17, **2014** pp. 63- 74
- Faure, B., E. Wetterskog, K. Gunnarsson, E. Josten, R.P. Hermann, T. Bruckel, J.W. Andreasen, F. Meneau, M. Meyer, A. Lyubartsev, L. Bergstrom, G. Salazar-Alvarez, P. Svedlindh; 2D to 3D crossover of the magnetic properties in ordered arrays of iron oxide nanocrystals. *Nanoscale*, 5, 953-960 **2013**
- Glaum, J., H. Simons, M. Acosta et al.; Tailoring the Piezoelectric and Relaxor Properties of (Bi_{1/2}Na_{1/2})TiO₃-BaTiO₃ via Zirconium Doping. *J. American Chem Soc.* 96,9, 2881-2886 **2013**
- Hansen, B., D. Ravnsbæk, D. Reed, D. Book, C. Gundlach, J. Skibsted, T.R. Jensen; Hydrogen storage capacity loss in a LiBH₄-Al composite. *The Journal of Physical Chemistry Part C: Nanomaterials, Interfaces and Hard Matter*, Vol. 117, No. 15, **2013**, p. 7423-7432
- Johansen, R.E., P. Norby; Capillary-based micro-battery cell for in situ X-ray powder diffraction studies of working batteries: a study of the initial intercalation and deintercalation of lithium into graphite. *J. Appl. Cryst.* 46 **2013** 1537-1543
- Kjær, K.S., T. Brandt van Driel, J. Kehres, M.K. Haldrup, D. Khakhulin, K. Bechgaard, M. Cammarata, M. Wulff, T.J. Sørensen, M.M. Nielsen; Introducing a standard method for experimental determination of the solvent response in laser pump, x-ray probe time-resolved wide-angle x-

- ray scattering experiments on systems in solution. *Physical Chemistry Chemical Physics*, Vol. 15, No. 36, **2013**, p. 15003-15016
- Knudsen, E.B., A. Prodi, J. Baltser, M. Thomsen, P.K. Willendrup, M. Sanchez Del Rio, C. Ferrero, E. Farhi, M.K. Haldrup, A. Vickery, R. Feidenhans'l, K. Mortensen, M.M. Nielsen, H.F. Poulsen, S. Schmidt, K. Lefmann; McXtrace: A Monte Carlo software package for simulating X-ray optics, beamlines and experiments. *Journal of Applied Crystallography*, Vol. 46, No. 3, **2013**, p. 679-696
- Knudsen, E., A.T. Rømer, P. Christiansen, P. Willendrup, K. Lefmann; Investigation of propagation algorithms for ray-tracing simulation of polarized neutrons. *Journal of Neutron Research* 17, **2014** pp. 27-34
- Knudsen, E.B., H.O. Sørensen, J.P. Wright, G. Goret, J. Kieffer; FabIO: easy access to two-dimensional X-ray detector images in Python. *Journal of Applied Crystallography*, vol. 46, 2013 p 537-539.
- Krizan, J.W., C. de la Cruz, N.H. Andersen, R.J. Cava; Crystal structure and magnetic properties of the $\text{Ba}_3\text{TeCo}_3\text{P}_2\text{O}_{14}$ and $\text{Pb}_3\text{TeCo}_3\text{V}_2\text{O}_{14}$ langasites. *Journal of Solid State Chemistry* 203, 310-320 **2013**
- Krycka, K.L., J.A. Borchers, M. Laver, G. Salazar-Alvarez, A. López-Ortega, M. Estrader, S. Surinach, M.D. Baro, J. Sort, J. Nogués; Correlated material-specific layer and magnetic distributions with onion-like $\text{Fe}_3\text{O}_4/\text{MnO}/\gamma\text{-Mn}_2\text{O}_3$ core/shell nanoparticles. *Journal of Applied Physics* 113, 17B531 **2013**
- Lemke, H.T., C. Bressler, L.X. Chen, D. Fritz, K. Gaffney, A. Galler, W. Gawelda, K. Haldrup, R. Hartsock, H. Ihee, J. Kim, J.H. Lee, M.M. Nielsen, A. Stickrath, W. Zhang, D. Zhu, M. Cammarata; Femtosecond X-ray Absorption Spectroscopy at a Hard X-ray Free Electron Laser: Application to Spin Crossover Dynamics. *J. Phys. Chem A*, 117, 735-740, **2013**
- Liu, H., C.T. Xu, H. Xie, S. Andersson-Engels, D. Lindgren, D. Thomas, C. Gundlach; Balancing power density based quantum yield characterization of upconverting nanoparticles for arbitrary excitation intensities. *Nanoscale*, Vol. 5, No. 11, **2013**, p. 4770-4775
- Lu, X., H. Gretarsson, R. Zhang, X. Lui, H. Luo, W. Tian, M. Laver, Z. Yamani, Y.-J. Kim, A.H. Nevidomskyy, Q. Si, P. Dai; Avoided Quantum Criticality and Magnetoelastic Coupling in $\text{BaFe}_{2-x}\text{Ni}_x\text{As}_2$. *Physical Review Letters*, 110, 257001 **2013**
- Ma, Z.F., W.J. Sun, S. Himmelberger, K. Vandewal, Z. Tang, J. Bergqvist, A. Salleo, J.W. Andreasen, O. Inganäs, M.R. Andersson, C. Müller, F.L. Zhang, E.R. Wang; Structure-property relationships of oligothiophene-isoindigo polymers for efficient bulk-heterojunction solar cells. *Energy & Environmental Science*, 7, 361-369 **2013**
- Myrdal, J., D. Blanchard, D. Sveinbjornsson, T. Vegge; Li-ion Conduction in the $\text{LiBH}_4\text{:LiI}$ System from Density Functional Theory Calculations and Quasi-Elastic Neutron Scattering. *J. Phys. Chem. C* 2013, 117, 9084–9091 **2013**
- Piatek, J.O., B.D. Piazza, N. Nikseresht, N. Tsyrlin, I. Zivkovic, K. Krämer, M. Laver, K. Prokes, S. Matas, N.B. Christensen, H.M. Rønnow; Phase diagram with enhanced spin-glass region of the mixed Ising-XY magnet $\text{LiHo}_x\text{Er}_{1-x}\text{F}_4$. *Physical Review B* 88, 014408 **2013**
- Polanski, M., T.K. Nielsen, I. Kunc, M. Norek, T. Płociński, L.R. Jaroszewicz, C. Gundlach, T.R. Jensen, J. Bystrzycki; Mg_2NiH_4 synthesis and decomposition reactions. *International Journal of Hydrogen Energy*, Vol. 38, No. 10, **2013**, p. 4003-4010

- Poulsen, H.F.; An introduction to three-dimensional X-ray diffraction microscopy. *J. Appl. Cryst.* **2012**, *45*, 1084-1097. (Ikke medtaget i 2012)
- Roudebush, J.H., N.H. Andersen, R. Ramlau, V.O. Garlea, R. Toft-Petersen, P. Norby, R. Schneider, J.N. Hay, R.J. Cava; Structure and Magnetic Properties of $\text{Cu}_3\text{Ni}_2\text{SbO}_6$ and $\text{Cu}_3\text{Co}_2\text{SbO}_6$ Delafossites with Honeycomb Lattices. *Inorg. Chem.* **52** 6083-6095 **2013**
- Rømer, A.T., J. Chang, N.B. Christensen, B.M. Andersen, K. Lefmann, L. Mähler, J. Gavilano, R. Gilardi, C. Niedermayer, H.M. Rønnow, A. Schneidewind, P. Link, M. Oda, M. Ido, N. Momono, J. Mesot; Glassy low-energy spin fluctuations and anisotropy gap in $\text{La}_{1.88}\text{Sr}_{0.12}\text{CuO}_4$. *Physical Review B* **87**, 144513 **2013**
- Simons, H., J.E. Daniels, J. Glaum et al.; Origin of large recoverable strain in $0.94(\text{Bi}_{0.5}\text{Na}_{0.5})\text{TiO}_3\text{-}0.06\text{BaTiO}_3$ near the ferroelectric-relaxor transition. *Appl. Phys. Lett.* **102** Article Number: 062902 **2013**
- Smolentsev, G., A. Guda, X. Zhang, K. Haldrup, E.S. Andreiadis, M. Chavarot-Kerlidou, S.E. Canton, M. Nachtegaal, V. Artero, V. Sundstrom; Pump-Flow-Probe X-ray Absorption Spectroscopy as a Tool for Studying Intermediate States of photocatalytic Systems. *The Journal of Physical Chemistry C*, Vol. 17, No 34, **2013** p. 17367-17375
- Udby, L., J. Larsen, N.B. Christensen, M. Boehm, C. Niedermayer, H.E. Mohottala, T.B.S Jensen, R. Toft-Petersen, F.C. Chou, N.H. Andersen, K. Lefmann, B.O. Wells; Measurements of Unique Magnetic and Superconducting Phases in Oxygen-Doped High-Temperature Superconductors $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4+y}$. *Physical Review Letters*, **111**, 227001 **2013**
- Wejdemann, C., H.F. Poulsen, U. Lienert, W. Pantleon; In Situ Observation of the Dislocation Structure Evolution During a Strain Path Change in Copper. *J O M*, Vol. 65, No. 1, **2013**, p. 35-43.
- Willendrup, P., E. Farhi, E. Knudsen, U. Filges, K. Lefmann; McStas: past, present and future. *Journal of Neutron Research* **17**, **2014** pp. 35-43
- Wragg, D.S., A. Gronvold, A. Voronov, P. Norby, H. Fjellvag; Combined XRD and Raman studies of coke types found in SAPO-34 after methanol and propene conversion. *Microporous and mesoporous materials* **173** 166-174 **2013**
- Ångström, J., R. Johansson, L.H. Rude, C. Gundlach, R.H. Scheicher, R. Ahuja, O. Eriksson, T.R. Jensen, M. Sahlberg; Hydrogen storage properties of the pseudo binary laves phase $(\text{Sc}_{1-x}\text{Zr}_x)(\text{Co}_{1-y}\text{Ni}_y)_2$ system. *International Journal of Hydrogen Energy*, Vol. 38, No. 23, **2013**, p. 9772-9778

DTU Mechanical Engineering, Technical University of Denmark

- Jegou, S., T.L. Christiansen, M. Klaus, C. Genzel, M.A.J. Somers; Determination of composition, residual stress and stacking fault depth profiles in expanded austenite with energy-dispersive diffraction. *Thin Solid Films*, Vol. 530, **2013**, p. 71-76
- Villa, M., M.F. Hansen, K. Pantleon, M.A.J. Somers; In-situ investigation of martensite formation in AISI 52100 bearing steel at sub-zero Celsius temperature. *Proceedings of the 2nd Mediterranean Conference on Heat Treatment and Surface Engineering*. Croatian Society for Heat Treatment and Surface Engineering, **2013**
- Villa, M., K. Pantleon, M.A.J. Somers; In situ investigation of the martensitic transformation in Fe–12 wt.%Ni–0.6 wt.%C steel at subzero temperatures. *Journal of Alloys and Compounds*, Vol. 577, No. Supplement 1, **2013**, p. S543-S548
- Wejdemann, C., H.F. Poulsen, U. Lienert, W. Pantleon; In Situ Observation of the Dislocation Structure Evolution During a Strain Path Change in Copper. *J O M*, Vol. 65, No. 1, **2013**, p. 35-43

DTU Chemistry, Technical University of Denmark

- Canton, S.E., X. Zhang, J. Zhang, T.B. van Driel, K.S. Kjaer, K. Haldrup, P. Chabera, T. Harlang, K. Suarez-Alcantara, Y. Liu, J. Pérez, A. Bordage, M. Pápai, G. Vankó, A.B. Stickrath, G. Jennings, C.A. Kurtz, M. Rovezzi, P. Glatzel, G. Smolentsev, J. Uhlig, A.O. Dohn, M. Christensen, A. Galler, W. Gawelda, C. Bressler, H.T. Lemke, K.B. Møller, M.M. Nielsen, R. Lomoth, K. Wärnmark, V. Sundström; Toward Highlighting the Ultrafast Electron Transfer Dynamics at the Optically Dark Sites of Photocatalysts. *Journal of Physical Chemistry Letters*, 4, 1972:1976, **2013**
- Frankaer, C.G., S. Mossin, K. Ståhl, P. Harris; Towards accurate structural characterization of metal centres in protein crystals: the structures of Ni and Cu T-6 bovine insulin derivatives *Acta Crystallogr. D70*, **2014**, 110-122
- Frankær, C.G., A.C. Raffalt, K. Ståhl; Strontium localisation in bone tissue studied by X-ray absorption spectroscopy. *Calcified Tissue International*. 94, **2014**, 248-257
- Georgescauld, F., L. Moynie, J. Habersetzer, L. Cervoni, I. Mocan, T. Borza, P. Harris, A. Dautant; Intersubunit Ionic Interactions Stabilize the Nucleoside Diphosphate Kinase of Mycobacterium tuberculosis. *Plos One* 8 **2013**. DOI: 10.1371/journal.pone.0057867
- Lee, J.H., M. Wulff, S. Bratos, J. Petersen, L. Guerin, J.-C. Leicknam, M. Cammarata, Q. Kong, J. Kim, K.B. Møller, H. Ihee; Filming the birth of molecules and accompanying solvent rearrangement. *Journal of the American Chemical Society*, 135, 3255:3261, **2013**
- Martic, M., I.N. Jakab-Simon, L.T. Haahr, W.R. Hagen, H.E.M. Christensen; Heterometallic [AgFe₃S₄] ferredoxin variants – synthesis, characterization and the first crystal structure of an engineered heterometallic iron-sulfur protein. *Journal of Biological Inorganic Chemistry*, **2013**, 18, 261–276

DTU Chemical Engineering, Technical University of Denmark

- Høj, M., A.D. Jensen, J.-D. Grunwaldt; Structure of alumina supported vanadia catalysts for oxidative dehydrogenation of propane prepared by flame spray pyrolysis. *Appl. Catal. A*, 451: 207-215, **2013**
- Wu, Q., L.D.L. Duchstein, G.L. Chiarello, J.M. Christensen, C.D. Damsgaard, C.F. Elkjær, J.B. Wagner, B. Temel, J.-D. Grunwaldt, A.D. Jensen; In Situ Observation of Cu–Ni Alloy Nanoparticle Formation by X-Ray Diffraction, X-Ray Absorption Spectroscopy, and Transmission Electron Microscopy: Influence of Cu/Ni Ratio. *ChemCatChem*, 6:301-310, **2014**

DTU Space, Technical University of Denmark

Fernández-Perea, M., M.-A. Descalle, R. Soufli, K.P. Ziock, J. Alameda, S.L. Baker, T.J. McCarville, V. Honkimäki, E. Ziegler, A.C. Jakobsen, F.E. Christensen, M.J. Pivovarov; Physics of Reflective Optics for the Soft Gamma-Ray Photon Energy Range. *Phys. Rev. Lett.* 111, 027404 – Published 12 July **2013**

Niels Bohr Institute, University of Copenhagen

- Bertelsen, M., H. Jacobsen, U.B. Hansen, H.H. Carlsen, K. Lefmann; Exploring performance of neutron guide systems using pinhole beam extraction. *Nucl. Instr. Meth. A* 729, 387-398, **2013**
- Blanco, J.A., B. Fåk, J. Jensen, M. Rotter, A. Hiess, D. Schmitt, P. Lejay; Phasons, amplitude modes, and spin waves in the amplitude-modulated magnetic phase of PrNi₂Si₂. *Phys. Rev. B* 87, 104411, **2013**
- Duvail, M., J.-F. Dufreche, L. Arleth, T. Zemb; Mesoscopic modelling of frustration in microemulsions. *Physical Chemistry Chemical Physics*, vol 15, nr. 19, s. 7133-7141. **2013** <http://dx.doi.org/10.1039/c3cp43981j>
- Einarsdottir, H., M.S. Nielsen, R. Miklos, R. Lametsch, R. Feidenhans'l, R. Larsen, B.K. Ersbøll; Analysis of micro-structure in raw and heat treated meat emulsions from multimodal X-ray microtomography. *Innov. Food Sci. Emger. Techn.* **2013** <http://dx.doi.org/10.1016/j.ifset.2013.11.003>
- Fischer, J., J.A. Lima, J.A. Lima Jr., P.T.C. Freire, F.E.A. Melo, R.W.A. Havenith, J. Mendes Filho, R. Broer, J. Eckert, H.N. Bordallo; Molecular flexibility and structural instabilities in crystalline L-methionine. *Biophysical Chemistry*, 180–181, 76-85, **2013**
- Gastiasoro, M.N., B.M.Andersen; Impurity bound states and disorder-induced orbital and magnetic order in the s⁺- state of Fe-based superconductors. *J. Supercond. Nov. Magn.* 26, 2651-2655, **2013**
- Gentile, L., B.F.B. Silva, S. Lages, K. Mortensen, J. Kohlbrecher, U. Olsson; Rheochaos and flow instability phenomena in a nonionic lamellar phase. *Soft Matter* 9, 1133-1140, **2013**
- Hansen, S.; Approximation of the structure factor for nonspherical hard bodies using polydisperse spheres. *J. Appl. Cryst.* 46, 1008-1016, **2013**
- Jacobsen, H., K. Lieutenant, C. Zendler, K. Lefmann; Bi-spectral extraction through elliptic neutron guides. *Nucl. Instr. Meth. A* 717, 69-76, **2013**
- Jacobsen, J., M.S. Rodrigues, M.T.F. Telling, A.L. Beraldo, S.F. Santos, L.P. Aldridge, H.N. Bordallo; Nano-scale hydrogen-bond network improves the durability of greener cements. *Sci. Rep.* 3, 2667, **2013**
- Knudsen, E.B., A. Prodi, J. Baltser, M. Thomsen, P.K. Willendrup, M. Sanchez del Rio, C. Ferrero, E. Farhi, K. Haldrup, A. Vickery, R. Feidenhans'l, K. Mortensen, M.M. Nielsen, H.F. Poulsen, S. Schmidt, K. Lefmann; McXtrace, a general software package for simulation of X-ray optics, beamlines and experiments. *J. Appl. Cryst.* 46, 679-696, **2013**
- Lefmann, K., K.H. Klenø, J.O. Birk, B.R. Hansen, S.L. Holm, E. Knudsen, K. Lieutenant, L. von Moos, M. Sales, P.K. Willendrup, K.H. Andersen; Simulation of a suite of generic long-pulse neutron instruments to optimize the time structure of the European Spallation Source. *Rev. Sci. Instr.* 84, 055106, **2013**
- Lima Jr., J.A., P.T.C. Freire, F.E.A. Melo, J. Mendes Filho, J. Fischer, R.W.A. Havenit, R. Broer, H.N. Bordallo; Using Raman Spectroscopy to understand the origin of the phase transition observed in the crystalline sulfur based amino acid L-methionine. *Vibrational Spectroscopy* 65, 132-141, **2013**

- Martins, M.L., H.N. Bordallo; Breakthrough magnetic fluid application. *Magnetics Technology International* 42-44, **2013**
- Mukherjee, S., B.M. Andersen, Z. Viskadourakis, I. Radulov, C. Panagopoulos; Bi-Quadratic magneto-electric coupling in underdoped $\text{La}_2\text{CuO}_{4+y}$. *J. Supercond. Nov. Magn.* 26, 1649-1652, **2013**
- Mukherjee, S., M.N. Gastiasoro, B.M. Andersen; Impurity-induced subgap bound states in alkali-doped iron chalcogenide superconductors. *Phys Rev B* 88, 134508, **2013**
- Mukherjee, S., M.N. Gastiasoro, P.J. Hirschfeld, B.M. Andersen; Low-energy bound states at interfaces between superconducting and block antiferromagnetic regions in $\text{KxFe}_2\text{-ySe}_2$. *Phys. Rev. B* 88, 014519, **2013**
- Pedersen, M.C., L. Arleth, K. Mortensen; WillItFit - A Framework for Fitting of Constrained Models to Small-Angle Scattering Data. *J. Appl. Cryst.* 46, 1894-1898, **2013**
- Rømer, A.T., J. Chang, N.B. Christensen, B.M. Andersen, K. Lefmann, L. Mähler, J. Gavilano, R. Gilardi, C. Niedermayer, H.M. Rønnow, A. Schneidewind, P. Link, M. Oda, M. Ido, N. Momono, J. Mesot; Glassy low-energy spin fluctuations and anisotropy gap in $\text{La}_{1.88}\text{Sr}_{0.12}\text{CuO}_4$. *Phys. Rev. B*, 87, 144513, **2013**
- Rømer, A.T., S. Graser, P.J. Hirschfeld, B.M. Andersen; Modulations of the local pairing interaction near magnetic impurities in d-wave superconductors. *J. Supercond. Nov. Magn.* 26, 1729-1732, **2013**
- Straasø, T., J. Becker, B.B. Iversen, J. Als-Nielsen; The Debye-Scherrer camera at synchrotron sources: a revisit. *J. Synchr. Rad.* 20, 98-104, **2013**
- Straasø, T., D. Mütter, H.O. Sørensen, J. Als-Nielsen; Objective algorithm to separate signal from noise in a Poisson-distributed pixel data set. *J. Appl. Cryst.* 46, 663-671, **2013**
- Tsapatsaris, N., S. Landsgesell, M.M. Koza, B. Frick, E.V. Boldyreva, H.N. Bordallo; Polymorphic drugs examined with neutron spectroscopy: Is making more stable forms really that simple? *Chemical Physics*, 427, 124-128, **2013**
- Udby, L., J. Larsen, N.B. Christensen, M. Boehm, C. Niedermayer, H.E. Mohottala, T.B.S. Jensen, R. Toft Petersen, F.C. Chou, N.H. Andersen, K. Lefmann, B.O. Wells; Direct proof of generic magnetic and superconducting phases in a series of superoxygenated high-Tc oxides. *Phys. Rev. Lett* 111, 227001, **2013**
- Vickery, A., L. Udby, N. Violini, J. Voigt, P.P. Deen, K. Lefmann; A Monte Carlo Simulation of Neutron Instrument Resolution Functions. *J. Phys. Soc. Jpn.* 82, SA037, **2013**
- Wadsäter, M., R. Barker, K. Mortensen, R. Feidenhans'l, M. Cárdenas; The Effect of Phospholipid Composition and Phase on Nanodisc films at the Solid-Liquid Interface as studied by Neutron Reflectivity. *Langmuir* 29, 2871-2880, **2013**
- Wadsäter, M., S. Maric, J.B. Simonsen, K. Mortensen, M. Cardenas; The Effect of Using Binary Mixtures of Zwitterionic and Charged Lipids on the Nanodisc Formation and Stability. *Soft Matter* 9, 2329-2337, **2013**

Dept. of Drug Design and Pharmacology, University of Copenhagen

- Assaf, Z., A.P. Larsen, R. Venskutonytė, L. Han, B. Abrahamsen, B. Nielsen, M. Gajhede, J.S. Kastrup, A.A. Jensen, D.S. Pickering, K. Frydenvang, T. Gefflaut, L. Bunch; Chemoenzymatic synthesis of new 2,4-syn-functionalized (S)-glutamate analogues and structure-activity relationship studies at ionotropic glutamate receptors and excitatory amino acid transporters. *J Med Chem.* **2013** Feb 28;56(4):1614-28. doi: 10.1021/jm301433m. Epub 2013 Feb 15. Erratum in: *J Med Chem.* 2013 Jul 25;56(14):5985
- Fiorentini, M., A. Bach, K. Strømgaard, J.S. Kastrup, M. Gajhede; Interaction partners of PSD-93 studied by X-ray crystallography and fluorescence polarization spectroscopy. *Acta Crystallogr D Biol Crystallogr.* **2013** Apr;69(Pt 4):587-94. doi: 10.1107/S0907444912051839. Epub 2013 Mar 14.
- Harpsøe, K., H. Hald, D.B. Timmermann, M.L. Jensen, T. Dyhring, E.Ø. Nielsen, D. Peters, T. Balle, M. Gajhede, J.S. Kastrup, P.K. Ahring; Molecular determinants of subtype-selective efficacies of cytosine and the novel compound NS3861 at heteromeric nicotinic acetylcholine receptors. *J Biol Chem.* **2013** Jan 25;288(4):2559-70. doi: 10.1074/jbc.M112.436337. Epub 2012 Dec 10.
- Jensen, M.H., P.O. Wahlund, K.N. Toft, J.K. Jacobsen, D.B. Steensgaard, M. van de Weert, S. Havelund, B. Vestergaard; Small angle X-ray scattering-based elucidation of the self-association mechanism of human insulin analogue lys(B29)(N(ε)ω-carboxyheptadecanoyl) des(B30). *Biochemistry.* **2013** Jan 15;52(2):282-94
- Juknaitė, L., Y. Sugamata, K. Tokiwa, Y. Ishikawa, S. Takamizawa, A. Eng, R. Sakai, D.S. Pickering, K. Frydenvang, G.T. Swanson, J.S. Kastrup, M. Oikawa; Studies on an (S)-2-amino-3-(3-hydroxy-5-methyl-4-isoxazolyl)propionic acid (AMPA) receptor antagonist IKM-159: asymmetric synthesis, neuroactivity, and structural characterization. *J Med Chem.* **2013** Mar 28;56(6):2283-93. doi: 10.1021/jm301590z. Epub 2013 Mar 13.
- Krintel, C., K. Harpsøe, L.G. Zachariassen, D. Peters, K. Frydenvang, D.S. Pickering, M. Gajhede, J.S. Kastrup; Structural analysis of the positive AMPA receptor modulators CX516 and Me-CX516 in complex with the GluA2 ligand-binding domain. *Acta Crystallogr D Biol Crystallogr.* **2013** Sep;69(Pt 9):1645-52. doi: 10.1107/S0907444913011839. Epub 2013 Aug 15.
- Kvist T., T.B. Steffensen, J.R. Greenwood, T.F. Mehrzad, K.B. Hansen, M. Gajhede, D.S. Pickering, S.F. Traynelis, J.S. Kastrup, H. Bräuner-Osborne; Crystal structure and pharmacological characterization of a novel N-methyl-D-aspartate (NMDA) receptor antagonist at the GluN1 glycine binding site. *J Biol Chem.* **2013** Nov 15;288(46):33124-35. doi: 10.1074/jbc.M113.480210. Epub 2013 Sep 26.
- Møller, M., S.S. Nielsen, S. Ramachandran, Y. Li, G. Tria, W. Streicher, M.V. Petoukhov, R.A. Cerione, R.E. Gillilan, B. Vestergaard; Small angle X-ray scattering studies of mitochondrial glutaminase C reveal extended flexible regions, and link oligomeric state with enzyme activity. *PLoS One.* **2013** Sep 30;8(9):e74783
- Nielsen, S.B., F. Macchi, S. Raccosta, A.E. Langkilde, L. Giehm, A. Kyrsting, A.S. Svane, M. Manno, G. Christiansen, N.C. Nielsen, L. Oddershede, B. Vestergaard, D.E. Otzen; Wildtype and A30P mutant alpha-synuclein form different fibril structures. *PLoS One.* **2013** Jul 4;8(7):e67713
- Nørholm, A.B., P. Francotte, L. Olsen, C. Krintel, K. Frydenvang, E. Goffin, S. Challal, L. Danober, I.

- Botez-Pop, P. Lestage, B. Pirotte, J.S. Kastrup; Synthesis, pharmacological and structural characterization, and thermodynamic aspects of GluA2-positive allosteric modulators with a 3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide scaffold. *J Med Chem.* **2013** Nov 14;56(21):8736-45. doi: 10.1021/jm4012092. Epub 2013 Nov 5.
- Skov, L.K., S. Pizzut-Serin, M. Remaud-Simeon, H.A. Ernst, M. Gajhede, O. Mirza; The structure of amylosucrase from *Deinococcus radiodurans* has an unusual open active-site topology. *Acta Crystallographica. Section F: Structural Biology and Crystallization.* Communications Online **2013**
- Ussing, C.A., C.P. Hansen, J.G. Petersen, A.A. Jensen, L.A. Rohde, P.K. Ahring, E.Ø. Nielsen, J.S. Kastrup, M. Gajhede, B. Frølund, T. Balle; Synthesis, pharmacology, and biostructural characterization of novel $\alpha 4\beta 2$ nicotinic acetylcholine receptor agonists. *J Med Chem.* **2013** Feb 14;56(3):940-51. doi: 10.1021/jm301409f. Epub 2013 Jan 22.
- Vetri, V., M. Leone, L.A. Morozova-Roche, B. Vestergaard, V. Foderà; Unlocked concanavalin A forms amyloid-like fibrils from coagulation of long-lived "crinkled" intermediates. *PLoS One.* 2013 Jul 16;8(7):e68912. doi: 10.1371/journal.pone.0068912. Print **2013**.
- Vognsen, T., I.R. Møller, O. Kristensen; Crystal Structures of the Human G3BP1 NTF2-Like Domain Visualize FxFG Nup Repeat Specificity. *PLoS One.* **2013** Dec 4;8(12):e80947. doi: 10.1371/journal.pone.0080947. eCollection 2013.

Dept. of Chemistry, University of Copenhagen

- Brown, A., L. Turner, S. Christoffersen, K.A. Andrews, T. Szesztak, Y. Zhao, S. Larsen, A.G. Craig, M.K. Higgins; Molecular Bases of Disease: Molecular Architecture of a Complex between an Adhesion Protein from the Malaria Parasite and Intracellular Adhesion Molecule 1. *J. Biol. Chem.* 288, **2013**, 5992-6003. doi: 10.1074/jbc.M112.416347
- Czene, A., E. Tóth, B. Gyurcsik, H. Otten, J.-C. Poulsen, L. Lo Leggio, S. Larsen, H.E.M. Christensen, K. Nagata; Crystallization and preliminary crystallographic analysis of an *E. coli* selected mutant of the nuclease domain of Colicin E7 metallonuclease. *Acta Cryst F* 69, 551-554, **2013** doi:10.1107/S1744309113008233
- Dreiser, J., K.S. Pedersen, A. Schnegg, K. Holldack, J. Nehrkorn, M. Sigrist, P. Tregenna-Piggott, H. Mutka, H. Weihe, V.S. Mironov, J. Bendix, O. Waldmann; Three-Axis Anisotropic Exchange Interactions in the Single-Molecule Magnets $\text{NEt}_4[\text{Mn}^{\text{III}}_2(5\text{-Brsalen})_2(\text{MeOH})_2\text{M}^{\text{III}}(\text{CN})_6]$ (M = Ru, Os). *Chem. Eur. J.* **2013**, 19, 3693–3701
- Dreiser, J., C. Piamonteze, F. Nolting, K.S. Pedersen, J. Bendix, S. Rusponi, H. Brune; XMCD Study of the Magnetic Exchange Coupling in a Fluoride-Bridged Dy-Cr Molecular Cluster. *J. Korean Phys. Soc.* **2013**, 62, 1368–1371
- Frandsen, K.H., K.K. Rasmussen, M.R. Jensen, K. Hammer, M. Pedersen, J.-C. Poulsen, L. Arleth, L. Lo Leggio; Binding of the N-terminal domain of the lactococcal bacteriophage TP901-1 CI repressor to its target DNA: a crystallography, small angle scattering and NMR study. *Biochemistry*, 52, 6892–6904, **2013**
- Heuckendorff, M., H.D. Premathilake, P. Pornsuriyasak, A.Ø. Madsen, C.M. Pedersen, M. Bols, A.V. Demchenko; Superarming of Glycosyl Donors by Combined Neighboring and Conformational Effects. *Org. Lett.*, **2013**, 15 (18), pp 4904–4907
- Knudsen, E.B., H.O. Sørensen, J.P. Wright, G. Goret, J. Kieffer; FabIO: easy access to 2D X-ray detector images in Python. *J. Appl. Cryst.* 46, **2013**, 537-539
- Langholm Jensen, J., A. Mølgaard, J.-C. N. Poulsen, M.K. Harboe, J.B. Simonsen, A.M. Lorentzen, K. Hjernø, J.M. van den Brink, K.B. Qvist, S. Larsen; Camel and bovine chymosin: the relationship between their structures and cheese-making properties. *Acta Crystallogr. Sect. D* 69, **2013**, 901-913. doi:10.1107/S0907444913003260
- Otten, H., M. Michalak, J.D. Mikkelsen, S. Larsen; The binding of zinc ions to *Emericella nidulans* endo- β -1,4-galactanase is essential for crystal formation. *Acta Crystallogr. Sect. F* 69, **2013**, 850-854 doi:10.1107/S1744309113019714
- Singh, S.K., K.S. Pedersen, M. Sigrist, C.Aa. Thuesen, M. Schau-Magnussen, H. Mutka, S. Piligkos, H. Weihe, G. Rajaraman, J. Bendix; Angular dependence of the exchange interaction in fluoride-bridged $\text{Gd}^{\text{III}}\text{--Cr}^{\text{III}}$ complexes. *Chem. Commun.* **2013**, 49, 5583–5585
- Straasø, T., D. Mütter, H.O. Sørensen, J. Als-Nielsen; An objective algorithm to separate signal from noise in a pixel data set. *J. Appl. Cryst.* 46, **2013**, 663-671
- Wadsäter, M., R. Barker, K. Mortensen, R. Feidenhans'l, M. Cárdenas; The Effect of Phospholipid Composition and Phase on Nanodisc films at the Solid-Liquid Interface as studied by Neutron Reflectivity. *Langmuir*, **2013**, 29, 2871 – 2880

Dept. of Pharmacy, University of Copenhagen

Fogh Hedegaard, S., C. Nilsson, P. Laurinmäki, S. Butcher, A. Urtti, A. Yaghmur; Aqueous dispersions of the oil-soluble anionic surfactant citrem interacting with lipids and PEGylated lipids. *RSC Adv.* **2013**, 3, 24576-24585

Nilsson, C., B. Barrios-Lopez, A. Kallinen, P. Laurinmäki, S. Butcher, M. Raki, K. Bergström, S. Weng Larsen, J. Østergaard, C. Larsen, A. Urtti, A. Airaksinen, A. Yaghmur; SPECT/CT imaging of radiolabeled cubosomes and hexosomes for potential theranostic applications. *Biomaterials* **2013**, 34, 8491-8503

Haldor Topsøe A/S

Vennestrøm, P.N.R., T.V.W. Janssens, A. Kustov, M. Grill, A. Puig-Molina, L.F. Lundegaard, R.R. Tiruvalam, P. Concepción, A. Corma; Influence of lattice stability on hydrothermal deactivation of Cu-ZSM-5 and Cu-IM-5 zeolites for selective catalytic reduction of NO_x by NH₃. *Journal of Catalysis* 309, **2014**, 477–490

Dept. of Science, Systems and Models, Roskilde University

- Nagy, G., L. Kovacs, R. Unnep, O. Zsiros, L. Almasy, L. Rosta, P. Timmins, J. Peters, D. Posselt, G. Garab; Kinetics of structural reorganizations in multilamellar photosynthetic membranes monitored by small-angle neutron scattering. *European Physical Journal E. Soft Matter*, Vol. 36, Nr. 7, 69, **2013**, s. 69-80
- Rudov, A.A., E.S. Patyukova, I.V. Neratova, P.G. Khalatur, D. Posselt, C.M. Papadakis, I.I. Potemkin; Structural Changes in Lamellar Diblock Copolymer Thin Films upon Swelling in Nonselective Solvents. *Macromolecules*, Vol. 46, Nr. 14, **2013**, s. 5786–5795
- Zhang, J., D. Posselt, A. Sepe, X. Shen, J. Perlich, D.-M. Smilgies, C.M. Papadakis; Structural Evolution of Perpendicular Lamellae in Diblock Copolymer Thin Films during Solvent Vapor Treatment Investigated by Grazing-Incidence Small-Angle X-Ray Scattering. *Macromolecular Rapid Communications*, Vol. 34, Nr. 16, **2013**, s. 1289-1295.

Dept. of Physics and Chemistry, University of Southern Denmark

- Boscia, A.L., B.W. Treece, D. Mohammadyani, J. Klein-Seetharaman, A.R. Braun, T.A. Wassenaar, B. Klösgen, S. Tristram-Nagle; X-ray structure, thermodynamics, elastic properties and MD simulations of cardiolipin/dimyristoylphosphatidylcholine mixed membranes. *Chem. Phys. Lipids* 178 (0), **2014**, 1-10
- Fragneto, G., A. Halperin, B. Klösgen, M. Sferrazza; Neutron reflectivity of supported membranes incorporating terminally anchored polymers: Protrusions vs. blisters. *The European Physical Journal E* 36(1), **2013**, 1-7