Application Form - - Danish Council for Strategic Research (DSF), March 2008

NOTE: This Form is for final applications - NOT for Phase 1 applications (prequalification)

Concerning use of the form, see: DSF's Application Guide, March 2008

0	**File number if applicable** Applicable only to applications ensuing from an approved Phase 1 application	

Items 1-11 are identical to the corresponding items on the Form for Phase 1 applications and may be copied from that Form and subsequently adjusted, if necessary.

1	**Call** *State the name of the call (one only) the application concerns*	NABIIT
2	**Theme(s)** *State the name(s) of the theme(s) the application concerns. Only themes under the selected call may be checked.*	Tværgående brug af nanoteknologi, bioteknologi, og IKT
3	**Instrument (check one option only)** *Check only instruments offered under the selected themes, cf. the call (double click the check box and then select "Checked").*	☐ **Strategic research centre** ☐ **Strategic networks** ☒ **Minor strategic research initiative** ☐ **Other:** ***enter designation***
4	**Project title (in English)** *max. 180 characters incl. spaces.*	MC-Xtrace, a simulation tool for X-ray investigations of nanostructures
5	**Project title (in Danish)** *max. 180 characters incl. spaces.*	Mc-Xtrace, et simuleringsværktøj til undersøgelser af nanostrukturer med røntgenstråling
6	**Amount applied for** *DKK*	7.917.148
7	**Applicant's name and Danish civil registration number**	Kim Lefmann 060264-0159
8	**Applicant's position and educational qualifications** *max. 39 characters incl. spaces.*	Lektor, Ph.D.
9	**Applicant's telephone no. and e-mail**	lefmann@fys.ku.dk Kontor: 3532 0476 Mobil: 2925 0476
10	**Applicant's workplace incl. address** *If the funding applied for is to be administered by another institution/company than the proposer's workplace, information about this must also be provided here.*	Niels Bohr Institutet Københavns Universitet Universitetsparken 5 2100 København Ø

11	**Scientific keywords** *Max. 5 scientific keywords to describe the research activity.*	X-ray diffraction, ray-tracing simulations, instrumentation, Small-angle scattering,bio-compatible nanostructures
12	**Project duration and commencement date** *State the estimated number of years and months and the anticipated commencement date*	4.0 years, starting 1. January 2009

13	**Popular-science project description** ***(max. 1,500 characters incl. spaces)*** *Must always be completed in Danish* Spredning af røntgenstråling er en af de mest anvendte metoder til at undersøge materialers struktur på atomar- og nano-skala. For at bygge optimale instrumenter til røntgenspredning er det nødvendigt at kende røntgenstrålingens vej gennem opstillingen med stor præcision. Det samme er tilfældet for at forstå vigtige detajler i de målte data. I dette projekt vil vi udvikle MC-Xtrace, en programpakke til udførelse af detaljerede ray-tracing simuleringer af instrumenter til røntgenspredning. Pakken er baseret på den dansk-franske pakke McStas, som er verdensførende indenfor simuleringer af den beslægtede teknik neutronspredning. Endvidere vil udviklingen basere sig på – og erstatte - det etablerede røntgen-program SHADOWS fra den førende synchrotron-røntgenkilde ESRF. Bag projektet står udviklerne af McStas og SHADOWS, samt førende danske røntgen- og bin-nano- forskere og virksomheden JJ-Xray Systems ApS. Mc-Xtrace blive udviklet med henblik på to konkrete, beslægtede opgaver: 1) Optimering af instrmenter til røntgenundersøgelser. 2) Forståelse af data fra målinger på nanostrukturer af biologisk relevans. Anvendelser af disse to typer er netop baggrunden for successen for neutronpakken McStas. Med den brede udbredelse af røntgenstråling forudses potentialet for Mc-Xtrace til langt større and McStas. Rent konkret vil anvendelsen af Mc-Xtrace i dette projekt føre til nye metoder til at studere strukturen af proteiner i vandige omgivelser.

14	**The funding applied for from the Danish Council for Strategic Research must be broken down by expense type** (as a simple summing of DSF funding across all the project's partners; see the statements on the forms for the appendices designated "dsf1"):	
	Expense type	**DKK**
	Scientific/academic salaries	5.314.554
	Technical/administrative salaries	130.000
	Equipment expenses in excess of DKK 40,000	100.000
	Operating expenses	320.000
	Overheads/admin. contributions	2.052.594
	Total DSF grant (amount must correspond to the amount stated in item 6)	**7.917.148**

15	**Is project funding being applied for from other sources?** *If so, state from which body, what amount(s) and which budget items*	No

16	**If the application is a renewed submission of one or more previously submitted applications (in revised form, if necessary), a BRIEF explanation should be given here, and file numbers must be stated in the case of applications for schemes under the Danish Agency for Science, Technology and Innovation.** -
17	**If the application is linked to other grants, a BRIEF statement must be made as to the correlation/synergy, together with key data for the other grants. File numbers must be stated if applications to the Danish Agency for Science, Technology and Innovation are involved.** -
18	**Any supplementary information.** -
19	**List of appendices** *(see requirements in the call regarding appendices).* A. Økonomi oversigt (skema dsf2) B. Specifikationer vedr. ph.d. Og post doc. Stipendier (skema dsf4) C. Specifikationer vedr. VIP og TAP løn (skema dsf5) D. Projektbeskrivelse E. CV'er for 4 hovedansøgere og 5 andre projektdeltagere F. Kommentarer til økonomiskemaer G. Økonomioversigt for hver af de 4 partnere (skema dsf1) I. Bekræftelse på samarbejde fra ESRF (Grenoble)

The applicant undertakes to notify the Danish Agency for Science, Technology and Innovation in the event of any subsequent material changes affecting the information submitted, including the amount of financing for the project or fraction thereof awarded by other sources.

The applicant hereby confirms that all the information provided herein is accurate.

Application date	21 August 2008
Applicant's signature	Kim Lefmann

Danish privacy law (Danish Act on Processing of Personal Data, *Lov om persondata*, no. 429 of 31 May 2000) accords you certain rights when information concerning you is processed electronically. We therefore ask you to note the following:

1. You have the right at your request to inspect and verify information concerning you if such information is processed electronically.
2. The Programme Commission reserves the right to obtain information about any previous and current expressions of interest and applications you may have submitted to the Scientific Research Councils, The Danish Council for Strategic Research, The Danish Council for Technology and Innovation and/or the Danish Agency for Science, Technology and Innovation, and this information may be included in the processing of your application..
3. In the event that project funding is or will be applied for from elsewhere (see item 15 of the form), the Programme Commission reserves the right to obtain information as to whether the amount has been granted.
4. The Programme Commission sends applications for external assessment in the following instances: If the council/commission/committee lacks expert knowledge in a given application, where a total of more than DKK 10m is applied for, or if a member of a council, a commission or a committee is the principal applicant or an associate and a total of more than DKK 1m is being applied for or if the Commission otherwise finds it appropriate.
5. If the application is approved in whole or in part, details of the principal applicant's title, name, place of employment, the names of the project partners, the project's title and duration, key figures for the grant and the size of the grant will be published in the Danish Research Database (http://www.forskningsdatabasen.dk) and on the Danish Agency for Science, Technology and Innovation's website (http://www.fi.dk) and in Danish Council for Strategic Research's publications. The popular science description of the project may be published in the same places.
6. Where relevant, in connection with the awarding of a grant, a requirement may be made for the collected data material to be submitted to Dansk Data Arkiv (DDA) in its documented state.

Samlet budget og finansieringsoversigt

Det Strategiske Forskningsråd
Skema dsf2, marts 2008

Projekttitel	**Mc-Xtrace – a simulation tool for X-ray investigations of nanostructures**

	Institution/virksomhed *Tilføj/slet om nødvendigt linier*	Udgiftsbudget	Finansieringsbidrag		
		A Partnerens udgiftsbudget (DKK)	**B** Partnerens andel af den søgte bevilling fra DSF (DKK)	**D** Partnerens egen dækning af egne udgifter (DKK)	**E** Partnerens øvrige bidrag til det samlede projekt (DKK)
Projekt-partnere	Niels Bohr Institutet, KU	4,655,550	2,935,516	1,077,900	-
	Afdelingen for Materialeforskning, Risø-DTU	3,766,844	2,806,816	960,029	-
	JJ X-ray Systems ApS	450,000	-	450,000	-
	Institut for Grundvidenskab, KU-Life	3,082,846	2,174,815	908,031	-
Andre finansie-ringskilder					
	ESRF, Grenoble	-	-	-	642,134
I alt		**11,955,240**	**7,917,147**	**3,395,960**	**642,134**

Dato og hovedansøgers underskrift	19/8-08
Dato, underskrift og stempel for den institution, der skal administrere bevillingen	19/8-2008 Professor John Renner Hansen Institutleder Niels Bohr Institutet, Københavns Universitet Blegdamsvej 17, 2100 København Ø Tel: +45 3532 5292 - Fax: +45 3532 5217 Email: head@nbi.dk - www.nbi.ku.dk

Samlet budget og finansieringsoversigt

Det Strategiske Forskningsråd
Skema dsf2, marts 2008

Se DSF's ansøgningsvejledning af marts 2008 vedr. udfyldelse af skemaet

Projekttitel	McXtrace – a simulation tool for X-ray investigations of nanostructures

Én linie pr. person *Tilføj/slet om nødvendigt linier*	A	B	C	D	E
	Samlet længde af deltagelse i projektet	Løn og uddannelsestilskud knyttet til tidsforbruget anført i kolonne A (ekskl. overhead)	Del af beløbet anført i kolonne B, der søges dækket af DSF	Del af beløbet anført i kolonne B, der ***ikke*** søges dækket af DSF	Oplysninger om hvem, der dækker omkostningerne, nævnt i kolonne D
	Antal måneder	*DKK*	*DKK*	*DKK*	*Tekst*
Ph.d.-stipendier					
Ph.D. 1, NBI	36	1,360,974	1,360,974	0	
Ph.D. 2, ~~NBI~~ KU-Life	36	1,360,975	1,360,975	0	
Sum ph.d.	**72**	**2,721,949**	**2,721,949**	**0**	
Post.doc.-stipendier					
Post doc 1, NBI	36	1,426,964	713,482	713,482	KU og ESRF
post doc 2, Risø	36	1,371,040	1,156,829	214,211	Risø-DTU
Sum post.doc.	**72**	**2,798,004**	**1,870,311**	**927,693**	

Dato og hovedansøgers underskrift	Dato, underskrift og stempel fra den institution, der skal administrere bevillingen
19/8-08	Professor John Hemmingsen Institutleder Niels Bohr Institutet, Københavns Universitet Blegdamsvej 17, 2100 København Ø Tel: +45 3532 5292 - Fax: +45 3532 5217 Email: head@nbi.dk - www.nbi.ku.dk 19/8-2008

I venstre kolonne identificeres, på hver sin linie, de personer, der indgår i projektet via ph.d.- eller post.doc.-stipendier. Informationen kan f.eks. opstilles som følger: "ph.d.-/post.doc.-nr., navn (hvis det kendes) og ansættelsessted (dvs. i hvilket delbudget, omkostningen optræder)". Desuden kan anføres hvilke workpackages eller inden for hvilket fagligt felt, vedkommende skal arbejde

I kolonne A anføres den samlede længde af den tid, personen nævnt i venstre kolonne, arbejder på projektet. Der skal normalt ikke ske fradrag for ferie eller undervisningsforpligtelse. Eksempel: For en ph.d.-studerende, der arbejder 100% på projektet i et 3-årigt forløb, anføres 36 måneder. For en fuldtidsansat post.doc., der anvender 75% af sin tid på projektet i 2 år, anføres 18 måneder

Specifikationer vedr. ph.d.- og post.doc.-stipendier

Det Strategiske Forskningsråd

Skema dsf4, marts 2008

I kolonne B anføres sum af løn/feriepenge mm. og (for ph.d.'er) uddannelsestilskud for tiden anført i kolonne A. ***Beløbet skal være eksklusive overhead***

I kolonne C og D opdeles beløbet i kolonne B på finansieringskilder

I kolonne E anføres navnet på den kilde, der finansierer omkostningerne anført i kolonne D

Se i øvrigt DSF's ansøgningsvejledning af marts 2008

Specifikationer vedr. VIP- og TAP-løn i projektbudgettet

Det Strategiske Forskningsråd
Skema dsf5, marts 2008

Projekttitel	**MC-Xtrace, a tool for simulating nanostructure X-ray experiments**

Titel, navn, ansættelsessted - én linie pr. person *Tilføj/slet om nødvendigt linier*	A Anvendt løntakst	B Effektiv arbejdstid i projektet	C Samlede løn-omkostninger knyttet til tids-forbruget anført i kolonne B (ekskl.overhead/ adm. bidrag)	D Del af beløbet anført i kolonne C, der søges dækket af DSF	E Del af beløbet anført i kolonne C, der ***ikke*** søges dækket af DSF
	DKK. pr. måned eller pr. time (jf. vejledningen)	*Antal måneder eller timer*	*DKK*	*DKK*	*DKK*
VIP (ekskl. ph.d./post.doc.)					
Lektor, Kim Lefmann, NBI	50702	4	202,808	0	202,808
Professor, Robert Feidenhans'l, NBI	61732	4	246,928	0	246,928
Professor, Kell Mortensen, KU-Life	61732	6	370,392	0	370,392
CEO, Karsten Johnsen, JJ-Xray systems	600	750	450,000	0	450,000
Professor, Martin Meedom Nielsen, NBI		4	(dækkes via Grundforskningsfonden og tæller ikke)		
Professor Henning Friis Poulsen, Risø-DTU		4	(dækkes via Grundforskningsfonden og tæller ikke)		
Seniorforsker, Søren Schmidt, Risø-DTU	545127 pr. År	1,25	681,409	681,409	0
Udvikler, Peter Willendrup, Risø-DTU	448717 pr. År	0,50	224,359	0	224,359
Seniorforsker, Lawrence Marguiles, Risø	545127 pr. År	0,50	272,563	0	272,563
Sum VIP			**2,448,459**	**681,409**	**1,767,050**
TAP					
Laborant, Marianne Lund Jensen, KU-Life	30000	4	120,000	60,000	60,000
Elektroniktekniker, Klavs Hilden, KU-Life	35000	4	140,000	70,000	70,000
Sum TAP			**260,000**	**130,000**	**130,000**

Dato og hovedansøgers underskrift	Dato, underskrift og stempel for den institution, der skal administrere bevillingen
19/8-08	19/8-2008 Professor John Renner Hansen Institutleder Niels Bohr Institutet, Københavns Universitet Blegdamsvej 17, 2100 København Ø Tel: +45 3532 5202 - Fax: +45 3532 5217 Email: head@nbi.dk - www.nbi.ku.dk

OBS: *Skemaet skal ikke omfatte de ph.d.- og post.doc.-stipendiater, der er anført på skema dsf4*

I venstre kolonne identificeres, på hver sin linie, de personer, der indgår i projektet. Alle projektdeltagere medtages, uanset om der søges lønmidler til dem. Er personnavnet ikke kendt kan f.eks. skrives "laboratorietekniker", "AC-fuldmægtig" etc.

I kolonne A anføres løntaksten (gennemsnit) for personen nævnt i venstre kolonne - Husk at anføre enheden DKK/md. eller DKK/time

Specifikationer vedr. VIP- og TAP-løn i projektbudgettet

Det Strategiske Forskningsråd
Skema dsf5, marts 2008

I kolonne B anføres den samlede længde af den tid, personen nævnt i venstre kolonne, arbejder på projektet. Anfør enhed måneder eller timer

I kolonne C anføres lønomkostningerne svarende til tiden anført i kolonne B. ***Beløbet skal være eksklusive overhead/ administrationsbidrag***

I kolonne D og E opdeles beløbet i kolonne C på finansieringskilder

Se i øvrigt DSF's ansøgningsvejledning af marts 2008

Appendix D, Project description

Summary

X-ray scattering is one of the most widely used probes of atomic- and nanoscale structure of materials and molecules in solid state as well as in solution. For the optimal design and construction of instrumentation for X-ray scattering, it is necessary to exactly determine the path of the X-ray beam through the experimental set-up. The same type of knowledge is also needed to correctly interpret fine details of the measured data.

In the project at hand, we will develop a new tool Mc-Xtrace, a software package to perform detailed ray-tracing simulations of X-ray scattering instruments and employ it to develop a highly sofisticated small angle X-ray scattering setup. The potential of the new instrument will be demonstrated by a detailed structure determination at the nano scale of new synthetic protein assemblies called nano discs.

The package will be based on the Danish-French McStas package, a world leading package in the related field of neutron scattering simulation. Furthermore, the development will be based on the established X-ray software SHADOW, based at the leading European synchrotron radiation source ESRF, and is intended to replace it as the standard of the international community in x-ray scattering Developers of the McStas and SHADOW packages, leading Danish X-ray scientists, and the Danish company JJ X-Ray Systems ApS will participate in the software project. The package will give JJ X-Ray Systems ApS a unique advantage for optimising their instrumentation.

The first fully developed use of Mc-Xtrace will be in helping design and optimisation of a Small Angle X-ray Scattering instrument (SAXS). The instrument will be used for analyzing data in studies of nanodisc-assemblies, giving both novel insight into nanodiscs, and an important tool for validating the Mc-Xtrace. The SAXS instrument will be constructed by JJ X-Ray Systems ApS, and experts from KU-life will provide samples and insight into nanoscale structural biology for benchmark experiments.

In neutron scattering simulations, McStas has achieved great results by solving similar types of problems, and since use of X-ray scattering is much more widespread than neutron scattering, Mc-Xtrace has an even larger potential than McStas.

The insight gained from virtual experiment simulations of instruments and nanodisc samples will help provide an important supplementary technique to current state of the art protein crystallography methods. Hence, the project combines methods within IT and nanoscience to obtain new insight within the fields of structural biology and soft matter in an interdisciplinary manner.

Project aim

Scientific aims:

- We will merge McStas, the leading simulation code for neutron scattering, with the X-ray simulation program SHADOW to create a state-of-the-art simulation tool for X-ray scattering, available to the X-ray scattering community as a whole.
- A SAXS instrument will be constructed by JJ X-Ray Systems ApS, optimised for study of nanostructures using the developed simulation tools.
- The developed software will be applied to studies of nanodisc assemblies by SAXS, improving methods for advanced data treatment and analysis, potentially providing a supplementary technique to current state of the art protein crystallography methods.

Commercial aims:

- Provide JJ X-Ray System ApS and its customers with an industry-unique software tool
- Optimize and characterize a second-generation SAXS instrument from JJ X-Ray Systems ApS.

Society aims:

- New insight in biological nano-scale issues, specifically nano-disc assemblies, could solve a broad range of problems, relevant to biology, medicine etc.

Expected main results of the project

The expected results and consequences of the Mc-Xtrace project are:

1. A newly developed, effective simulation code will be available for the international X-ray community and provide the first implementation of a complete, virtual experiment in X-ray scattering.
2. Improvement of methods for advanced data treatment and analysis in SAXS in general, targeting specific nano- and bio-scientific experimental challenges, plus related optimised scientific output from SAXS for nano- and bioscience.
3. JJ X-Ray Systems and its customers will benefit from being first with a currently industry-unique software tool.
4. As part of the project, the developed code will be verified experimentally, using a JJ X-Ray Systems developed SAXS machine, and the ESRF beamlines ID-09B and ID-11.
5. New analytical software will be available for treating the solution structure of complex biological systems.
6. Detailed insight will be obtained about the possibility of using nanodiscs as templates for studying membrane proteins, membrane protein complexes, and their dynamics in natural environments.

Project background and idea (hypothesis)

Modern instruments for X-ray scattering in general, consist of a large number of beam-optical components. Hence, an accurate analytical description of the instrument characteristics (e.g. measurement resolution) is often impossible, although the effect

of each component is known accurately. As a consequence, much X-ray equipment is being designed on the basis of trial-and-error, combined with experience and only rather primitive calculations to predict the performances.

A useful way to perform a calculation of instrument performance is through ray-tracing simulations of photons through the instrument. These simulations are in-principle correct, but are difficult to program and debug. For this purpose, a number of well-tested simulation packages exists, the most renowned being the ESRF code SHADOW [shadow].

However, SHADOW is aging and built on old IT technology. Hence, it has been agreed with the ESRF to port the functionality of SHADOW into the world leading ray-tracing package McStas [mcstas]. McStas is developed in Denmark and France, and is designed to simulate neutron scattering instruments. However, neutron- and X-ray instruments are strikingly similar, enabling a re-cycling of major part of the McStas efforts.

With the use of modern IT, simulations have gained enormously in performance, opening a whole new field of opportunities. Topics, which have recently been exploited within neutron scattering simulation, include the use of computer clusters and general multi-parameter optimization algorithms. The most promising results come from the concept of virtual experiments, which denotes the simulation of a complete experiment from source to detector. This has found use in a large number of applications in neutron scattering [lefmann08]:

- Design of instruments through virtual experiments
- Test of data analysis software
- Preparation of experiments
- On-the-fly diagnostics of running experiments
- Aid in analysis of complex data (e.g. multiple scattering, background)
- Teaching and training of students and novice users

The present project will open all these opportunities also for X-ray scattering science.

As part of the project, we will apply our developed virtual experiment techniques to the study of nanodisc assemblies by SAXS, facilitating a supplementary technique to current state-of-the-art protein crystallography methods.

Project novelty, effect, and relevance

The idea to develop Mc-Xtrace was spawned through requests from the ESRF and the X-ray scattering community. Hence, there is a current need for this software, which has the potential to be highly used by scientists within all areas of X-ray science.

Small-angle X-ray scattering (SAXS) is currently undergoing a large expansion, and many such laboratory systems and synchrotron beamlines are being installed each year. Hence, the ability to design and fully optimise these systems and predict their properties is essential. This project will address these important questions, for the benefit of both Danish science and industry.

Within the project, we will further develop advanced simulation-based analysis programs for scattering data from complex biomolecules, in particular from nanodiscs

and -ensembles. The nanodisc concept has great potential, and we foresee utilization as templates for studying membrane proteins in near-physiological realistic environments. This will enable us to elucidate relatively high-resolution structures of a wide range of membrane proteins which cannot be crystallized. Further, and even more important, it will be possible to study the dynamical association to other biomolecules, using time-resolved X-ray scattering, to bring detailed insight into the biological function. The foreseen results of this project will be of interest to a wide range of research and industry related to biology and soft matter studies.

It should be added that in the recent SFR publication on ”innovationsaccelererende forskningsplatforme”, scientific instrumentation (including X-ray instrumentation) was one of the selected 10 topics.

Project method and results

In the project, we will develop the package Mc-Xtrace and make it functional for use in nano- and nano-bioscience. The project will essentially be based on three pillars: A) Development of the Mc-Xtrace infrastructure, B) Use of Mc-Xtrace in connection with the construction of laboratory X-ray equipment and synchrotron beamlines, e.g. a small-angle X-ray (SAXS) instrument, C) Use of Mc-Xtrace for the assistance in and interpretation of SAXS studies of a bio-compatible nanodiscs. The three pillars are strongly connected, with A) being the most labour intensive. Below, we describe the planned development/research methods and expected results within each pillar.

A) The Mc-Xtrace package will be developed on the basis of the knowledge from SHADOW [shadow] within the IT infrastructure of the existing neutron package McStas [mcstas].

For clarity, we first outline the internal organization of McStas. Here, the simulations are performed in three layers:

1. the upper layer is the instrument description, which specifies the geometry of the components of a particular instrument.
2. the middle layer is the component description, which specifies the effect of a particular type of component on an X-ray beam.
3. the lower layer is the kernel, which contains a compiler for the instrument/ component files, handles the internal flow of the simulations, displays simulation results etc.

In McStas – and in Mc-Xtrace – the user or the instrument responsible scientist will write the instrument file and use it to perform the simulations, e.g. from a graphical user interface. In contrast, most components will be developed and tested by the Mc-Xtrace project group, while some specialized components will be contributed by expert users and other collaborators. The kernel will be maintained by the Mc-Xtrace project group only.

In the present project, only few changes to the McStas kernel is needed, accounting for the different motion of neutrons and X-rays. Much more work is needed at the component level. A large neutron component library exists in McStas and X-ray components are available in SHADOW, however they need to be ported from FORTRAN to ANSI-c. This situation will be analyzed in detail to identify which components should be contained in a starting package, from where code could

possibly be re-used, and how the components should be developed and tested.

Since ray-tracing is a tool of geometrical optics, particular care is taken to analyze the use of ray-tracing for simulating wave properties of X-rays. One simple example is scattering from the edge of slits, while a more complex situation is the scattering from multi-pinhole arrays. To ensure correctness of the Mc-Xtrace simulations, while maintaining the speed of ray-tracing (compared to full wavefront propagation methods), it is important to design and implement a suitable heuristical method for these types of problems.

B) A very important part of the Mc-Xtrace project is the interplay between simulations and experimental results. On one hand, experiments will be used to test the simulation code; on the other hand, simulations will be used as a tool to optimize the geometry of an instrument and to help analyzing experimental data (the latter is presented under C)

We will use experimental results from laboratory equipment at Copenhagen University, Risø DTU, and JJ X-Ray Systems ApS to validate central components within Mc-Xtrace, in particular source descriptions for laboratory X-ray sources. In addition, synchrotron-related components will be validated through simulations and experiments at the ESRF beamlines ID-09B and ID-11.

We will use Mc-Xtrace to predict optimize the performance of a suite of instruments. One example will be the ID-09B beam line in connection with set-ups for time-resolved studies.
This will have obvious value in the long term for possible redesign of beamline parameters, and in the short term for improved methods for separating the instrument function from recorded scattering data. The latter is of crucial importance in time resolved measurements, where, even at world leading facilities such as the ID09B, the available X-ray fluxes typically are 3 orders of magnitude smaller than usual at synchrotron sources, and satisfactory data quality correspondingly challenging to achieve. An improved description of the instrument response function, will enable us to minimize the effects of the instrument induced smearing of intensity and scattering angle measurements. An important class of samples for time resolved X-ray structural investigations, molecular systems in solution, are measured in a geometry very similar to SAXS. Experience developed for either experiment type will be easily transferred to the other.

Another example will be the JJ X-Ray Systems second generation SAXS instrument, where the trade-off between resolution and intensity will be studied in order to help obtaining an automated selection of experimental configuration for non-expert users. This will be performed in the three modes of operation: standard SAXS, grazing-incidence SAXS, and reflectivity.

C) The project will include practical applications of Mc-Xtrace, which are scientifically interesting in their own right. We will perform SAXS studies on the solution structure of nanodiscs, nanodisc assemblies and nanodisc complexes.

Nanodiscs are self-assembled nanostructures composed of phospholipids encircled by a genetically engineered membrane scaffold protein (MSP), as shown schematically

in fig. 1. Such nanodiscs can be dispersed in water and are thus amenable for solution studies of their *structure, dynamics* and *function* by state-of-the-art techniques, like SAXS.

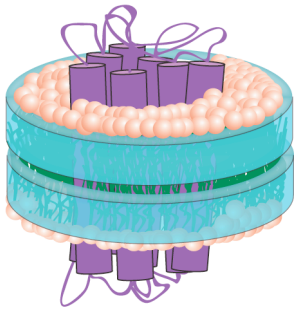

Figure 1: Nanodiscs with trans-membrane proteins

The experimental studies focus on the reconstitution of membrane bound proteins, structurally confined in water-soluble nanodiscs. We expect that further refinement of the nanodiscs' chemistry will allow self-assembly into macroscopic two- and/or three dimensionally ordered assemblies, opening the possibility for using small-angle scattering to obtain relatively high resolution of protein structures, in much more realistic environments than when using single crystal diffraction.

Based on modern software programs for modeling the structure of complex biomolecular assemblies, we will setup realistic 'nanodisc samples' for virtual scattering experiments using Mc-Xtrace. By systematic varying the modelsystem, we will be able in detail to validate the limitations of real experiments, using laboratory X-ray scattering experiments and different high-resolutiuon synchrotron source based facilities.

An important question in this project concerns the instrumental confinements in studying such complexes. The combination of experimental and simulation studies are necessary to elucidate the effect that instrumental and sample conditions have on the quality of the obtained parameters. For optimal output and utilization of advanced small-angle scattering facilities, it is of fundamental importance to understand in detail the limiting factors for e.g. signal-to-noise ratio that the sample and instrument provides. Examples of this are natural molecular flexibility and dispersity in size and aggregation numbers, instrumental smearing by limited collimation, detector resolutions, multiple scattering between sample and surroundings, etc. Both experimental studies and simulations will include studies based on 'standard' laboratory-based SAXS instrumentation such as the JJ X-Ray Systems equipment, and on the most advanced high-resolution synchrotron based SAXS facilities.

In the project, the simulations will be used for the development and test of advanced software for analyzing the SAXS data on nanodisc complexes, by analyzing both simulated and experimental data and by including directly information on the experimental resolution through virtual experiments.

An example of a specific complex system, utilizing the nanodiscs concept is a project concerning the structure and function of cytochrome P450 enzymes. This is a collaboration with B.L. Møller, Plant Biochemistry, KU-Life, and T. Bjørnholm, Nano Science Center, KU. Cytochrome P450 enzymes are powerful oxidation catalysts that activate molecular oxygen and insert on oxygen atom in a typically

lipophilic endogenous or xenobiotic substrate. Their functions span from detoxification reactions in the human liver to synthesis of complex bioactive natural products in plants like the cyanogenic glucoside dhurrin. The dhurrin metabolon is composed of a varity of sub-components with known chemical structure [nielsen08]. Using the software tools of this project, we aim to reconstitute dhurrin metabolon in nanodiscs and use combined SAXS and biochemical techniques to investigate and determine the interacting domains facilitating efficient channelling of intermediates. Understanding of the assembly and regulation of cytochrome P450 metabolons will provide clues on how to design plants as green factories of desired high-value bioactive components and leads to the design of nano machines that inactivate toxic components and xenobiotics in the human body.

New advanced analysis programs will be developed with the attempt to get insight into the solution structure of complex biological molecular assemblies. The new programs will be based on codes from both own existing software packages, and external sources.

The progress of each of these pillars in this project will benefit the others. Thus the utilizations in B) and C) needs a working prototype of Mc-Xtrace A), while the essential testing and demonstration of the package (A) comes through practical use (B and C). B) and C) are interconnected both through the actual use of SAXS for nano-structural research and data analysis, and by the common competence in the practical use of Mc-Xtrace, built up during the project.

Project plan

The project can be divided into a series of subtasks. For most of these, we have appointed one or two participanta, the first one listed as primary responsible. In general, Risø DTU is responsible for the kernel level and parts of the component level, NBI has responsibilities on the component level and on the virtual experiment level, KU-Life is responsible for virtual and real SAXS experiments, and JJ X-Ray Systems contributes on the component and instrument simulation level. Two tasks are common workpackages for all participants, component development and virtual experiment tools.

In total, we have identified 16 subtasks, which are presented in the Gantt chart below. The tasks and task responsibles are:

1. (NBI) Validation of Mc-Xtrace components at the ESRF beamline ID-09B, at the NBI laboratory, and at JJ X-Ray Systems
2. (NBI+Risø DTU) Porting the SHADOW functionality to Mc-Xtrace
3. (NBI+Risø DTU) Analysis of particle-wave propagation problems
4. (NBI) Applying Mc-Xtrace for teaching purposes
5. (Risø) Develop basic kernel features for Mc-Xtrace
7. (Risø DTU) Validation of Mc-Xtrace components at the ESRF beamline ID-11
8. (Risø DTU) Construction of websites and other IT infrastructure
9. (Risø DTU) Construction of web portal for virtual experiments
10. (Risø DTU+NBI) Release of Mc-Xtrace for public use

11. (Life) Procuding nanodisc samples
12. (Life) Performing SAXS experiments on nanodiscs
13. (JJ) Developing second generation SAXS instrument
14. (JJ) Optimizing instrument design using Mc-Xtrace
15. (All) Development of components for Mc-Xtrace
16. (All) Development of virtual experiment tools for SAXS

Task	Partner	2009				2010				2011				2012			
		jan	apr	jul	okt	jan	apr	jul	okt	jan	apr	jul	okt	jan	apr	jul	okt
1	NBI																
2	NBI+Risø DTU																
3	NBI+Risø DTU																
4	NBI																
5	Risø DTU																
6	Risø DTU																
7	Risø DTU																
8	Risø DTU																
9	Risø DTU+NBI																
10	Life																
11	Life																
12	Life																
13	JJ																
14	JJ																
15	All																
16	All																

Milestones will consist of the end result of each task in the Gantt chart and are thus not listed explicitly.

As one of the main goals of the project is the realisation of an effective X-ray simulation code, the interaction between X-ray scientists and simulation experts is essential. The staff primarily involved in the design and implementation of this code will form the “core” project group, composed by

- Kim Lefmann, Copenhagen University
- Robert Feidenhans’l, Copenhagen University
- Peter Willendrup, Risø DTU
- Søren Schmidt, Risø DTU

The rest of the applicant list will form an “inner shell” of people providing input to the project, and surrounding research environments at all participating institutions will form an “outer shell”.

The core project group and the formal board mentioned elsewhere will be jointly responsible for supervising the time plan and redistribute ressources when necessary.

The resources will be allocated for each institution in the following way (as detailed in the economy forms):

- NBI: 1 Ph.D. student and 1 post. doc. full time for 3 years, plus input from 3 senior VIP (10% each) + access to equipment

- Risø DTU: 1 post doc full time and 1 senior VIP half time for 3 years, plus input from 3 senior VIP (10-15% each) + access to computer ressources
- KU-Life: 1 Ph.D. student 3 years, plus input from 1 senior VIP (10%) and 2 TAP (10% each) + access to equipment
- JJ X-Ray Systems ApS: 1 senior developer (10%) + access to equipment

Computing resources will be applied for through the Danish Centre for Scientific Computing. Smaller runs will be performed on a multi-processor, multi-core computer, purchased through the project (price approx. 100.000 DKK).

International dimension of the project

Mc-Xtrace will supersede the present X-ray package SHADOW, which has been developed at the ESRF, Grenoble. The experience accumulated in this process makes ESRF a vital collaborator in the project. Further, McStas is itself developed in collaboration with ILL, Grenoble.

The generality of the McStas-package has facilitated its use for optimizing new instrument designs at neutron scattering facilities worldwide, with active contributions from the user community. A similar X-ray package has the potential for use at X-ray facilities all over the world. A project web portal will be set up to ease communication with the international X-ray community. Thus the project opens possibilities for Danish scientists for worldwide collaborations. For example, the ESRF upgrade program includes complete redesign of several beamlines, where the Mc-Xtrace software tool would be extremely useful.

International activities planned within the project include stationing one post doc at the ESRF for 1 year to transfer the knowledge from SHADOW. In addition, test experiments will be performed at a number of beamlines at international facilities, in particular ESRF.

The project will make scientists from Danish universities and industry major players in advanced instrument simulation on the highest international level, as McStas has done it for neutrons. We foresee that such simulation systems will be most important for future design of not only experimental facilities, but also on the direct user interface. Danish scientists will have significant impact on the important facilities XFEL being built in Hamburg, and the neutron facility ESS, which is expected to be initiated in Europe within the next 1-2 years, likely hosted in Lund in Sweden..

Legal and ethical aspects

The Mc-Xtrace package will be published on an open-source Gnu Public Licence (GPL), since its predecessor McStas is under this licence.

The proposed scientific and IT development tasks give rise to no other legal or ethical concerns.

Publication and outreach strategy

Foremost, this project deals with making the package Mc-Xtrace available to the international community. This will be done through a web portal, in analogy with the neutron package McStas [mcstas]. This portal will include a demonstration of the use of X-rays in the form of a virtual experiment to be controlled though the portal.

The results of this project, i.e. the development of the package, the results of the instrument simulations, and the data on nanodiscs, will be presented at conferences and through refereed publications. Also popular articles are planned, targeted on the broad community of X-ray users.

Simulations have proven to be an excellent tool for teaching and training in beamline science, because it provides the students a deeper understanding of the instruments and opens for virtual experiment and analysis of the virtual data. We will use Mc-Xtrace in the teaching of X-ray scattering techniques at KU and DTU. The applicants have pioneered this field through the KU course in neutron scattering, which has be taught since 2005 and recently won the NBI teaching award.

Innovation

Since the Mc-Xtrace package will be open source (GPL), there are no patent possibilities in the software itself.

However, the use of Mc-Xtrace for the design and optimization of new instrument solutions bear the possibilities for patenting. The same is the case for data analysis algorithms and programs, supported and tested by Mc-Xtrace.

Patent issues will be discussed in the board of the project, and the necessary measures will be taken to protect IPR when possible. The participation of an industrial partner eases the selection of results worth protecting.

Partners

This project aims at combining existing Danish research and industrial competences in areas of bio- and nano-science, scientific computing and technical industry, for increased scientific, innovative and industrial output.

Niels Bohr Institute, KU has a long tradition for developing and utilizing instruments and software for X-ray and neutron scattering. In particular, Robert Feidenhans'l is chairman of the board of the European Synchrotron Radiation Facility ESRF, Martin M. Nielsen leads the X-ray based Center for Molecular Movies, and Kim Lefmann is the co-founder and project leader of the simulation package McStas. In addition, NBI is the home for the Danish instrument center for neutron and synchrotron X-ray scattering, DANSCATT.

Kim Lefmann will be the daily responsible for the NBI activities, which will be based development of the X-ray functionality of the McStas components with Risø DTU, including testing against experiments at the JJ-X-ray SAXS insturment and the ID-

09B beamline (ESRF). NBI has the primary responsibility of porting the knowledge from SHADOW and thus the contact to ESRF. The conceptual problem of including wave propagation in ray-tracing methods will be studied. Finally, NBI will develop the Mc-Xtrace teaching platform and are responsible for the contact to virtual experiments at KU-Life.

Materials Research Department, Risø DTU has a long tradition for hardware and software for neutron and X-ray science, and is the place where McStas was initiated. The department hosts the X-ray based Center for Metal Structures in 4D (M4D), lead by Henning Friis Poulsen and with Lawrence Marguiles and Søren Schmidt as central participants in the centre. Peter Willendrup is responsible for the kernel development and daily support of McStas.

The M4D centre has valuable experience from earlier projects, in terms of in-house, specialised simulation codes for the ESRF ID-11 instrument, suitable for comparison with the newly developed, general Mc-Xtrace code. Few X-ray instruments have as complex arrangement of components as ID-11, providing a counterpart to the comparatively simpler geometry and setup of SAXS instruments. M4D also has experience in detector simulation codes, which can also become a valuable input for Mc-Xtrace.

Søren Schmidt has a wide range of important competences, including X-ray physics, algorithms and data analysis. Currently, Søren is employed full time by M4D, but we believe that his skills are essential for the success of the Mc-Xtrace project, and that a transfer of funds must be made to ensure his participation.

Peter Willendrup will be the daily leader of the Risø DTU activities, which will include the modifications of the McStas kernel to X-ray use, and co-development/testing of the X-ray component library with NBI. In addition, Risø DTU will assist NBI to test Mc-Xtrace on JJ X-Ray Systems instruments and by simulation of the ESRF beamline ID-11.

Institute of Basic Science, KU-Life has a large group specialized in structural nano-biosystems studied by scattering methods, in particular SAXS. The group leader, Kell Mortensen, is an internationally renowned scientist and expert in small-angle scattering.

Kell Mortensen will be responsible for the daily KU-Life activities, which consist of testing Mc-Xtrace in combination with SAXS experiments on a particular system: nano-discs, in collaboration with NBI. Hereby, the concept of virtual experiments within X-rays will be elucidated, in analogy with the neutron scattering case.

JJ X-Ray Systems ApS is a Danish company with world leading expertise in the design and construction of X-ray instruments, including SAXS. The CEO, Karsten Joensen, has decades of experience within X-ray instrumentation.

The company will provide input on instrument and component design and hence guide the development of Mc-Xtrace with Risø DTU and NBI. Further, X-ray instruments from JJ X-Ray Systems ApS will be used as a testing platform for the simulation package. In return, the company will gain competences in using a leading

simulation tool for optimization and data analysis.

Project leadership

Board. The overall project progress will be overseen by a board, consisting of one member from each of the 4 partners, in close collaboration with the core project group, as mentioned in the project plan. The board will meet bi-monthly, with one annual meeting at ESRF to strengthen this collaboration. The board and core group will jointly have the power to terminate parts of the project and to redistribute funds, in agreement with DSF.

Partners and observers. Each board member has the responsibility of the daily progress at his own institute/company, as sketched under "Partners". The leading synchrotron X-ray facility ESRF will be an observer on the board.

Collaborators. The project will be strongly connected with the M4D center at Risø DTU and the Center for Molecular Movies at KU and DTU. Further, the project will collaborate with all Danish X-ray scattering groups through the national center DANSCATT. International partners include ESRF and Hasylab (D), which has large interest in instrumentation from X-ray scattering for the large construction project of the XFEL (X-ray free-electron laser).

Teaching/Training. The package Mc-Xtrace will be used directly in the education at NBI and DTU. On the M.Sc. level, the package will be used as a teaching tool at the popular X-ray course at NBI, in analogy with the use of McStas for teaching neutron scattering. M.Sc training will further come via contributions to M.Sc. projects. On the Ph.D. Level, the teaching effort will be centered around the two students employed by the project, but will also have more widespread effects through the scientific possibilities it can offer for the large number of students presently working in the field of X-ray scattering.

The whole Mc-Xtrace project will result in an increased level of knowledge of X-ray instrumentation, in particular training of students and post docs. This will lead to strategic advantages for JJ X-Ray Systems ApS.

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Appendix E, Participant CV´s

The following pages contain CV´s of the project participants.

CURRICULUM VITAE for Kim Lefmann

Professionel address:

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Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark
Email: lefmann@fys.ku.dk, *Phone: (+45) 3532 0476 Mobile: (+45) 2925 0476*

Civil status:

Born	6. Feb. 1964
Married to	Anne Katrine Lefmann
Children	Sidsel 1996; Helene 2000
Private address	Grævlingestien 31c, DK-2880 Bagsværd

Academic titles and experience:

Associate Professor, Niels Bohr Institute, University of Copenhagen	2008-
Adjoint Professor, Niels Bohr Institute, University of Copenhagen	2006-2008
Senior Scientist, Risø National Laboratory, Dept. Materials Physics and Chemistry	2000-2008
Scientist, Risø National Laboratory, Dept. Materials Physics and Chemistry	1996-2000
Post doc, Low Temperature Laboratory, Helsinki University of Techonology	1995-1996
Ph.D. degree in Solid State Physics, Niels Bohr Institute, University of Copenhagen	1995
Guest student, Hahn-Meitner Institut, Berlin	1993
Ph.D. student, Risø National Laboratory, Dept. Solid State Physics	1992-1995
M.Sc. in Solid State Physics, Niels Bohr Institute, University of Copenhagen	1991
B.Sc. in Physics AND Computer Science, University of Copenhagen	1988

Membership of committees and boards:

Member of the selection panel for neutron instruments at NIST (Washington DC)	2008-
Member of the selection panel for neutron instruments at FRM-2 (München, D)	2008-
Member of the selection committee for Jülich neutron instruments at FRM-2, SNS, ILL	2007-
Member of the Neutron Committee, Int. Union of Crystallography (IUCr) www.iucr.org	2005-2011
Board Member EU Initiative on neutrons and muons, NMI3, www.neutron-eu.net	2004-
Chairman of the Solid State Physics Division, Danish Physical Society	2004-
Board Member, Danish Physical Society, www.nbi.dk/dfs	2004-
Board Member of Solid State Physics Division, Danish Physical Society	2002-
Member of the Science committee for ESS-Scandinavia	2002-2007
Board Member Danish Neutron Scattering Society, www.danssk.risoe.dk	1999-
Member of the Alan Mackintosh award committee	2002-2004
Board Member of the organisation ESS-Scandinavia, www.ess-scandinavia.org	2000-2002

Other relevant information in brief:

Author	81 refereed papers	11 popular papers
	35 reports and manuals	14 teaching notes and material
Organizer	6 conferences and workshops	
Total grants	24.6 Mkr, acquired and administrated	
Referee	for 9 international journals	
Presentations	> 40 (invited at international conferences and research institutions)	
Lecturer	and developer of 4 theoretical, 3 experimental, and 1 combined University courses	
Teacher	of further 5 theoretical and 1 experimental University courses	
Supervisor	for 9 post docs, 8 Ph.D. students, 11 M.Sc. students, and 15 project students	

Research interests

- Correlated electron systems (Quantum magnetism, Quantum phase transitions, High-Tc supercond.)
- Magnetism on the nanoscale (Nanoparticles, Phase transitions)
- Instrumentation (Neutron scattering, Low temperature equipment)

SELECTED PUBLICATION LIST for Kim Lefmann since 1999:

- P.L.W. Tregenna-Piggott, F. Juryani, P. Christiansen, P. Willendrup, **K. Lefmann**, *Reduction of data from inverted-geometry time-of-flight instruments*, accepted for J. Neutr. Res. (2008)
- M. Christensen et al.: *Direct Evidence of the Rattler Effect in Thermoelectric Materials*, accepted for Nature Materials (2008)
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DK-2000 Frederiksberg
Denmark

Date of birth: 27 September 1973, Copenhagen
Partner: Ellen Askholm
Children: Emil (1998), Carla (2000), Elmer (2004)

Education:

- 1995 B.Sc. (Math., Physics) University of Copenhagen/RISØ, thesis: "Neutrondiffraktion og magnetiske strukturer."
- 2000 M.Sc. (Physics) University of Copenhagen, thesis: "Point-spread Functions in Tomography using Filtered Back-projection Reconstruction"

Employment:

- 1998-1999 Teacher of physics, Skt. Annæ Gymnasium
- 1999 Software developer at Neurobiology Research Unit, Rigshospitalet (modelling and visualisation of human brain scans)
- 2000-2002 Research assistant at Neurobiology Research Unit, Rigshospitalet (modelling and visualisation of human brain scans)
- 2002- Development engineer, Materials Resarch Department, RISØ (day to day software project manager for McStas)

Main software projects:

- Simulation package for parameter significance in tomographic imaging
- d3view - 3D visualisation package for brain images
- MARS - Multiple Algorithms for Registration of Scans - image registration framework
- McStas - versions 1.7, 1.8, 1.9, 1.9.1, 1.10, 1.11, and 1.12 of the neutron ray tracing package

Teaching: Involved in University of Copenhagen course "Neutronspredning teori, simulering og praksis" 2005,2006,2007,2008

Research Interests: Scattering physics, Scientific computing, Modelling, Software Usability and Efficiency.

Books:

- **Willendrup P**. Farhi E. Lefmann K. *User and Programmers Guide to the Neutron Ray-Tracing Package McStas*, Version 1.12 (Risø-R-1416(rev.ed.)(EN), ISBN 978–87–550–3679–6)
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- **P. Willendrup**, L. Pinborg, S. Hasselbalch, K.H. Adams, K. Stahr, G.M. Knudsen, and C.Svarer. *Assessment of the precision in co-registration of structural MR-images and PET-images with localized binding*, in ICS 1265, Pages 275-280 Elsevier, 2004
- **P. Willendrup**, C. Svarer, S.G. Hasselbalch, G.M. Knudsen. *Comparison of Coregistration Techniques for Neuroreceptor PET images*. Society of Nuclear Medicine. Society of Nuclear Medicine, 2002.
- **P. Willendrup**, C. Svarer, S.G. Hasselbalch, G.M. Knudsen. *Precision of Coregistration Techniques for F18-Altanserin PET Images.* NeuroImage, 2002: S85.
- **P. Willendrup**, C. Svarer, L.G. Hanson, O.B. Paulson *A simple approach to combined inhomogenity correction and tissue segmentation of MR MPRAGE images*. J Cereb Blood Flow Metab 2002;21(suppl.1):S580

Kell Mortensen **CV 2008**
Professor, Head of Biophysics, Dept. Basic Sciences, University of Copenhagen
E-mail kell@life.ku.dk. Web: http://www.dina.kvl.dk/~kell/

Date and Place of birth: Febr. 21, 1952, Rønne, Denmark

1981 Ph.D.	Technical University of Denmark, Physics Lab. III.
1977 M.Sc.	Technical University of Denmark, Electro Physics

Career/Employment

2007-	Professor at KU, Head of Biophysics Group at KU-LIFE
2000-2007	Head of Program Polymer Analysis and Structure, Risø,
1995-2007	Research Professor, SNF/Risø. Denmark
1984-1995	Scientist / Senior Scientist, Dept. Solid State Physics, Risø.
1982-1984	SNF-Senior Fellowship, DTU and Risø, Denmark
1981	Project Scientist, Danish National Bank and DTU,
1980-1981	IBM-World Trade Fellow, IBM TJ Watson Res Center,
1977-1979	DTU-Fellowship, Phys. Lab. III, DTU,Lyngby,Denmark

Specialization

Main field: Bio- and Polymer Physics, Small-Angle Neutron and X-Ray Scattering
Research projecs: Molecular Self-Assembly, structure and dynamics., NanoDiscs,

Honors, Awards, Fellowships, include

SNF Research Professor Award 1995; SNF SeniorFellowship 1982-84; SNF Fellowship 1981; IBM-World Trade Fellowship 1980

Boards, Committees, include

Graduate Schools: Faculty of Life Sciences, KU, 2007- (chairman); *Polymer Science*, 2003-; *Biophysics*, 1996-2001
Research Foundation*: The Danish National Research Foundation* (DG) 1999-2008
Societies*: The Danish National Committee for Crystallography*, 2009- ; *The Danish Neutron Scattering Society* 1998-; Chairman 2003-; *FNU-Instrument Centre for Neutron Scattering* 2003-; *European Neutron Scattering Association* 2003-; *Eu. Spallation Source, Scand.* 2000-
SAC committees at International Large-Scale Facilities:
ESRF, Grenoble FR, 2008-; *NIST*, USA, 2006-; *FRM2*, Germany, 2006-
PSI, Switzerland, 2004-; *FZJ*, Germany 2001-2004
SAC committees: *Journal of Macromolecular Science - Physics* (Marcel Dekker)
ESRF, Grenoble FR, 2008; *Council for Natural Sciences*, Finland, 2002-2008; *ESS Large Scale Structures* 1995-1996; *ESS Soft Matter*, 2000 – 2003; *ESS Instrumental Task Group on Small Angle Scattering*, 2000 - 2003

Publications (http://www.dina.kvl.dk/~kell/kell-publ.pdf)

Papers in refereed journals and books:	310 (incl. 5Nature, 1Science, 27PRL, 6EPL)
Books (Ed):	3
Popular articles:	16
Invited talks, scientific meetings:	more than 100

Citations (http://www.dina.kvl.dk/~kell/kell-citations.pdf)

Paper cited more than 9156 (ISI Web of Science, Sept 2007), h-index 51.0.

Organization of Meetings/Schools, include since 2004:

European Conference on Neutron Scattering, Lund SE, June 2007
Joint Scandinavian Neutron Scattering Meeting, SE, Oct. 2005. (co-Chair)
Symposium on Polymer Conetworks, Gels, Membranes Prague Sept. 2005 (Adv)
19th Conf. European Colloid and Interface, Geilo, Norway, Sept. 2005 (Adv)
2nd Scandinavian Symp. on Small-angle Scattering, Lyngby Feb. 2005 (Co Chair)
B Lebech Symposium and DANSSK-Annual meeting, Roskilde Sept. 2004 (Chair)

Peer reviewed Publications, since 2004:

- Kell Mortensen, Walther Batsberg, and Søren Hvidt. Effects of PEO-PPO diblock impurities on the cubic structure of aqueous PEO-PPO-PEO Pluronics micelles: fcc and bcc ordered structures. *Macromolecules*, **41**, 1720–1727, 2008.
- Kell Mortensen, Urs Gasser, Selmiye Alkan Gursel, and Gunther G. Scherer. Structural Characterization of Radiation Grafted Block Copolymer Films, using SANS Technique. *J Polymer Science B. Polymer Physics*, **46**, 1660–1668, 2008.
- S.C.M. Teixeira, et al. New sources and instrumentation for neutrons in biology. *Chemical Physics* **345**, 133-155, 2008., and *Chemical Physics* **345**, 170-170, 2008.
- Christine M Papadakis, R Ivanova, K Ludtke, Kell Mortensen, PK Pranzas, R Jordan, Micellar structure of amphiphilic poly(2-oxazoline) diblock copolymers, *J Appl Cryst*., **40**, 361–362, 2007.
- Lise Arleth, Birgitta Svensson, Kell Mortensen, Jan Skov Pedersen, Ulf Olsson. A Block Copolymer Microemulsion With Solvent Induced Segregation. *Langmuir*, **23**, 2117, 2007.
- Brian Lohse, Mario T Ivanov, Jens W Andreasen, Robert Vestber, Søren Hvilsted, Rolf H Berg, P S Ramanujam, Craig J Hawker, Kell Moartensen. Self-Assembling Uracil-PAMAM Dendrimer Systems. *Macromolecules*, **40**, 1779–1781, 2007.
- Torben Ishøy, Kell Mortensen. Lamellar-to-Cubic Phase Change in Phospholipid Bilayer Systems Incorporated with Block Copolymers - DMPC and PEO-PPO-PEO (P85). *Langmuir*, **21**, 1766–1775, 2005.
- Ruya Eskimergen, Kell Mortensen, Martin M Vigild, Shear Instability of a Gyroid Diblock Copolymer, *Macromolecules*, **38**, 1286–1291, 2005.
- Christine M Papadakis, Frank Rittig, Kristoffer Almdal, Kell Mortensen, Petr Stepanek, Collective dynamics and self-diffusion in a diblock copolymer melt in the body-centered cubic phase, *Eur Phys J, E* **15**, 359–370, 2004.
- Kell Mortensen, Three-Dimensional Crystallographic Determination of the Cubic bcc Morphologies of Shear aligned Block Copolymer Systems. *J. Polymer Science Polymer Physics,* **42**, 3095–3101, 2004.
- Pavel Strunz, Kell Mortensen, Stefan Janssen, SANS-II at SINQ. Installation of the former Risø-SANS facility, *Physica* B, **350**, E783–E786, 2004.
- Elisabeth Theunissen, N Overbergh, Harry Reynaers, S Antoun, R Jerome, Kell Mortensen, Silica reinforced triblock copolymer gels. Polymer, 45, 1857, 2004.
- Martin E. Vigild, Kell Mortensen, Ruya Eskimergen. SANS, SAXS, rheology and birefringence - Strength and weaknesses in probing phase behavior of a diblock copolymer, *Physica*, B **350**, E885–E888, 2004.

POPULAR ARTICLES, since 2004

- NH Andersen, K Lefmann, B Lebech, K Mortensen. Neutroner. *Kvant* **2007**, 3.
- Kell Mortensen, Jan S Pedersen. Neutrons and Soft Matter. *Kvant* **2007**, 28, 2007.
- Martin E. Vigild, Kell Mortensen. Neutrons and Polymers. *Kvant* **2007**, 26.
- Kell Mortensen. ICNS: SANS and Reflec,. *Neutron News* **17**, 14, 2006.
- Martin E. Vigild, Sokol Ndoni, and Kell Mortensen. The gyroid phase of a diblock copolymers - nano-porous materials. *Swiss Neutron News*, **24,** 26, 2004.
- Martin E. Vigild, Sokol Ndoni, and Kell Mortensen. Selvorganiserende polymerer – skabeloner til nanoporøse materialer. *Dansk Kemi*, **85,** 32–34, 2004.

Personal Details for Karsten Joensen, JJ X-Ray Systems ApS.

Name:	Karsten Joensen		
Nationality:	Danish	Address:	Gl. Skovlundevej 54 2740 Skovlunde Denmark
Born:	June 9, 1966 Gentofte, Denmark		
Age:	42	Telephone:	+45 3537 0770 (Home) +45 4776 3003 (Work) +45 4776 3009 (Fax)
Languages:	Danish (Mother Tongue) English (Mother Tongue) French (Quasi-Fluent) German (Falteringly)	E-mail:	karsten.joensen@jjxray.dk

Family Status: Married with French Canadian/Italian Lilianna Milani (in Denmark since 1995, works as upholsterer for Fritz Hansen, Allerød Denmark)

Children: One Daughter: Lauraine Joensen (born 1998)

Academic Experience:

1974-1981	Primary and Secondary School at Bahrain International School, Manama, Bahrain
1981-1982	Secondary School, Rosenlundskolen, Skovlunde, Denmark
1982-1985	Mathematics and Physics direction atNørre Gymnasium, Brønshøj, Denmark
1985-1992	University of Copenhagen, Niels Bohr Institute of Astrophysics, Physics and Geology. Physics Major (Material Science), Math Minor.
1992	Master of Science (M.Sc.) awarded based on thesis performed at the Danish Space Research Institute, Lyngby, Denmark. Topic: X-Ray Detectors and Analysis of Silica Aerogels (nanoparticles) by Small Angle X-Ray Scattering
1992	6-months Fellowship for study at Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachussetts, USA. Topic: Theoretical Framework for High Energy Broadband Multilayers for X-Ray Astrophysics Instrumentation
1992-1995	3 year Pre-Doctoral Fellowship at Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachussetts, USA. Topic: Designing, Fabrication and Characterization of Multilayers for Broad-Band Hard X-Ray Astrophysics Instrumentation.

1995	Awarded Ph.D. Degree based on work at Harvard-Smithsonian Center for Astrophysics. Degree awarded by Niels Bohr Institute.
1995-1997	Research Adjunct at the Experimental Physics. Built up Experimental X-Ray group under Prof. Jens Als-Nielsen. Commissioned two high intensity x-ray facilities at Hasylab synchrotron facility Germany.
1999-2000	Participating in Part-Time Executive MBA Program (Master of Business Administration) at the Copenhagen Business School
2000	Awarded MBA-degree: MBA-Thesis on "Becoming a star-performer in the Analytical X-Ray Industry". Focusing on improving the innovative process
2001-2004	External Advisor for Ph.D-student Henrik Jensen, Aalborg University, Dept. of Applied Chemistry. Topic: "New Process for Nanoparticle Production"
2002-2008	External Advisor for various MBA-strategic projects at the Copenhagen Business School. Around. Around 20 half-year projects.

Work Experience:

1995-1997	Research Adjunct at the Experimental Physics Group at the Ørsted Laboratory, University of Copenhagen. Built up Experimental X-Ray group under Prof. Jens Als-Nielsen. Commissioned two high intensity x-ray facilities at Hasylab synchrotron facility, Hamburg Germany.
1997-2001	Self-employed Research Liaison, primarily facilitating interaction between the R&D divisions of the Michigan-based company Osmic Inc. and their European customers (companies and individuals). Working out of Copenhagen and Skive, Denmark.
2001-2002	Vice-President, Research and Intellectual Property Rights in the incubator company Giantcode A/S, Klokkerholm, Denmark. Responsible for Internal Research Group (8 people) and Full Patent Portfolio.
2002-2004	Head of Sales and Marketing, JJ X-Ray Aps, a 4-person company that produces and sells custom components and instrument to X-Ray Scientists all around the world
2004-2008	Director and Owner of JJ X-Ray Systems ApS, a spin-off of JJ X-Ray Aps, that sells complete scientific instruments for niche markets

Curriculum vitae for Robert Feidenhans'l (August 2008)

Name:	Robert Krarup Feidenhans'l.	.Born	June 29 1958 in Haderslev.
Address:	Møllehusvej 64, 4000 Roskilde.	Phone (privat)	+45 46357869
E-mail:	robert@fys.ku.dk	Phone (work)	+45 35320397

Academic background:

January 83 Master degree in Physics and Mathematics. The master thesis project had the title 'High energy ion scattering investigations of the clean and oxygen covered Cu(110) surface'.

January 86 Awarded the A. Angelo prize.

June 86 Received the Ph.D. degree in Physics at the Institute of Physics, University of Aarhus.

Professional career

July 86 Employed as staff scientist at the Department of Solid State Physics, Risø.

March 93 Program leader for the program 'Surfaces and Interfaces' at Risø.

June 01 Head of Department of the Materials Research Department at Risø

January 05 Professor in X-ray Physics at the Niels Bohr Institute, Copenhagen University

March 07 Vice institute leader for research at the Niels Bohr Institute

Membership of committees etc:

Chairman for the National Committee for Crystallography (1998 - 2007)

Member of the 'Forschungsbeirat Synchrotronstrahlung' HASYLAB, DESY(1995 - 1998)

Member of the Program Advisory Committee at MAXLAB, Lund, Sweden (1998 -)

Director of DANSYNC from 2004

Chairman of the ESRF Council from 2006-2009, Vicehairman 2002-2005

Member of the program commitee for the IUCr congress in Glasgow August 1999

Co-organizer of several meetings and summerschool, e.g. International Conference on Solid Films and Surfaces ICSFS-9, Copenhagen 1998, and the Nordic Summerschool on Synchrotron Radiation 1997, 2001, 2004.

Chairman of the sub-committee for technological foresight of nano materials 2004

Vice Chairman of the Gordon Conference on X-rays Physics in 2003, chairman for the conference in 2005

Chairman of the Ph.D. Committee at the Physics Graduate School at the Niels Bohr Institute (2005 -)

Member of the Academic Council of the Faculty of Science, Copenhagen University (2006-)

Chairman of the Ph.D. Committee at the Faculty of Sciences, Copenhagen University (2007-)

Publications:

About 110 publications within surface and interface science in international, refereed journals resulting in about 2750 citations as of end of 2007.

1 patent application, was not continued

3-4 invited talks yearly at conferences, summerschools or research institutions (not during my time as Head of Department at Risø)

Educational activities:

Have been supervising about 15 master students and 6 Ph.D. students.

Currently supervising about 10 Ph.D. students, 4 master students and 4 bachelor students.

Is responsible for the courses Introduction to Solid State Physics, Experimental X-ray Physics and Structural Tools in NanoScience, all 7.5 ECTS courses.

Brief Curriculum Vitae, Martin Meedom Nielsen, August 2008

Born June 23, 1967 in Aarhus, Denmark. Danish Citizen.
Married, 3 children. Home address: Dronning Sofies Vej 109, DK-4000 Roskilde, Denmark. Private email: martin.meedom@gmail.com

Education

1996: Ph.D. in physics from Aarhus University. Thesis: "Structures of Alkali Covered Aluminium Surfaces Studied by Low Energy Electron Diffraction".
1994: M.Sc. in physics from Aarhus University.

Professional experience

2005 – Present: Professor, Director of the Danish National Research Foundations Centre for Molecular Movies, Niels Bohr Institute, University of Copenhagen
2000 – 2005: Senior scientist, the Danish Polymer Centre, Risø Natl. Lab.
1997 – 2000: Post Doc., the Dept. of Cond. Mat. Phys. and Chem., Risø Natl Lab.
1996 – 1997: Post Doc, IGV, Forshungszentrum Jülich, Germany.
1993 – 1996: Ph.D. student at Inst. of Physics and Astronomy, Aarhus University.

Honours

"Rene Descartes Prize" 2000 of the European Commission.

Scientific publications

56 papers in peer-reviewed journals and 2 submitted. Front page of Nature Materials, Dec. 2006. Referee for Nature Materials, Advanced Materials, Phys Rev, and others.

Research

Structure-property relationships in materials, X-ray scattering techniques and methods. Major achievements include the co-discovery of substitutional adsorption of alkali metals on metal surfaces (Phys. Rev. Lett. **69**, 1532 (1992), and Phys. Rev. Lett. **72**, 3370 (1994)), demonstration of the relationship between microstructure and charge carrier mobility in organic field effect transistors (Nature, **401**, 685 (1999)), the first evidence for molecular epitaxy as the controlling mechanism for alignment of molecules on patterned substrates (J. Am. Chem. Soc., **125**, 2252 (2003), and Adv. Mater., **15**, 495 (2003)), and use of polymer blends to optimise device structure (Nature Materials **5**, 950 (2006)).

Teaching

Supervising or has supervised 4 MSc students, 6 PhD students and 6 post docs

External funding 2001-2008 (personal share)

European sources 1 M€. Danish sources 4.5 M€ (including an ESF coordinated grant and a grant from the Danish National Research Foundation).

Selected publications 2008-2004, relevant to the application

1. G.F. Velardez, H.T. Lemke, D.W. Breiby, M.M. Nielsen, K.B. Møller, and N.E. Henriksen, *Theoretical Investigation of Perylene Dimers and Excimers and Their Signatures in X-Ray Diffraction,* J. Phys. Chem, published on web august (2008)

2. D.W. Breiby, O. Bunk, J.W. Andreasen, H.T. Lemke and M.M. Nielsen, *Simulating X-ray Diffraction of Textured Films*, J. Appl. Cryst, **41**, 262-271 (2008).

3. S. Goffri, C. Müller, N. Stingelin-Stutzmann, D.W. Breiby, C.P. Radano, J.W. Andreasen, R. Thompson, R.A.J. Jannsen, M.M. Nielsen, P. Smith and H. Sirringhaus, *Multi-component semiconducting polymer systems with low crystallization-induced percolation threshold*, Nature Materials, **5**, 950 (2006). Also the front page of this issue

4. D.W. Breiby, O. Bunk, W. Pisula, T. I. Sølling, A. Tracz, T. Pakula, K. Müllen, and M. M. Nielsen, *The Structure of Zone-cast HBC-$C_{12}H_{25}$ Films,* J. Am. Chem. Soc., **127**, 11288-11293 (2005).

5. O. Bunk and M.M. Nielsen, *Angle calculations for a z-axis / (2S+2D) hybrid diffractometer.* J. Appl. Cryst., **37**, 216-222 (2004).

21 August 2008

CURRICULUM VITAE

Name:	**Søren Schmidt**
Address:	Risø National Laboratory Materials Research Department Building 228, P.O. Box 49 DK-4000 Roskilde Denmark Phone direct: +45 46 77 5826 Fax: +45 46 77 5758 E-mail: soeren.schmidt@risoe.dk
Home Address	Ringstedgade 8, 4th, DK-2100 Ø Copenhagen, Denmark
Date of Birth	30 April 1970
Marital Status	Married to Margarita Iniakhina Schmidt
Child	Katharina Anastasia, born in 2003.
Academic Degrees	M.Sc. (cand. scient.) in Physics at University of Copenhagen, 1996. Thesis: *Anomalous Couplings in WW->lvlv at LEP-II* Ph.D. in Physics at University of Copenhagen, 2000. Thesis: *Second Level Trigger studies at the HERA-B experiment*.

Employments

1996	Research assistant at Niels Bohr Institute (NBI), 3 months.
1997-2000	Ph.D. stipendiary at NBI.
2000-2002	Post. Doc. at the Materials Research Department, Risø
2002-30. April 2005	Scientist in Center for Fundamental Research: Metal Structures in Four Dimensions.
1. May 2005 -	Senior Scientist in Center for Fundamental Research: Metal Structures in Four Dimensions.

Scientific Production

31 papers in international journals, 7 invited/keynote presentations at international conferences, 16 papers in proceedings of international conferences, 1 book chapter and 1 paper at a Danish conference.

Selected publications

1. *S. Schmidt, S.F. Nielsen, C. Gundlach, L. Margulies, X. Huang, D. Juul Jensen*, Watching the Growth of Bulk Grains During Recrystallization of Deformed Metals, *Science* (2004), **305**, 229–232.
2. S. Schmidt, U.L. Olsen, H.F. Poulsen, H.O. Sørensen, E.M. Lauridsen, L. Margulies, C. Maurice, D. Juul Jensen, *Direct observation of grain growth in Al-0.1% Mn*, Scripta Mater., 59 (2008), 491-494

Scientific Interests

Reconstruction algorithms for synchrotron x-ray data, Recrystallization in metals.

Lawrence Margulies

EDUCATION

Iowa State University, Ames, IA
Ph.D., Materials Science and Engineering, 1999

Carleton College, Northfield, MN
B.A., Physics, 1992

PUBLICATIONS

Schmidt, S., Olsen, U.L., Poulsen, H.F., Soerensen, H.O., Lauridsen, E.M., Margulies, L., Maurice, C., Juul Jensen, D., "Direct observation of 3-D grain growth in Al-0.1% Mn," SCRIPTA MATERIALIA, 59: 491-494 2008

Lauridsen, EM; Schmidt, S; Nielsen, SF; Margulies, L; Poulsen, HF; Jensen, DJ, "Non-destructive characterization of recrystallization kinetics using three-dimensional X-ray diffraction microscopy," SCRIPTA MATERIALIA, 55 (1): 51-56 2006

Jensen, DJ; Lauridsen, EM; Margulies, L; Poulsen, HF; Schmidt, S; Soerensen, HO; Vaughan, GMB, "X-ray Microscopy in Four Dimensions," MATERIALS TODAY, 9(1-2): 18-25 2006

Larsen, AW; Poulsen, HF; Margulies, L; Gundlach, C; Xing, QF; Huang, XX; Jensen, DJ, "Nucleation of recrystallization observed in situ in the bulk of a deformed metal," SCRIPTA MATERIALIA, 53 (5): 553-557 2005

Lienert, U; Han, TS; Almer, J; Dawson, PR; Leffers, T; Margulies, L; Nielsen, SF; Poulsen, HF; Schmidt, S, "Investigating the effect of grain interaction during plastic deformation of copper," ACTA MATERIALIA, 52 (15): 4461-4467 2004

Offerman, SE; van Dijk, NH; Sietsma, J; Lauridsen, EM; Margulies, L; Grigull, S; Poulsen, HF; van der Zwaag, S, "Solid-state phase transformations involving solute partitioning: modeling and measuring on the level of individual grains," ACTA MATERIALIA, 52 (16): 4757-4766 2004

Schmidt, S; Nielsen, SF; Gundlach, C; Margulies, L; Huang, X; Jensen, DJ, " Watching the growth of bulk grains during recrystallization of deformed metals," SCIENCE, 305 (5681): 229-232 2004

Winther, G; Margulies, L; Schmidt, S; Poulsen, HF, "Lattice rotations of individual bulk grains Part II: correlation with initial orientation and model comparison," ACTA MATERIALIA, 52 (10): 2863-2872 2004

Gundlach, C; Pantleon, W; Lauridsen, EM; Margulies, L; Doherty, RD; Poulsen, HF, "Direct observation of subgrain evolution during recovery of cold-rolled aluminium," SCRIPTA MATERIALIA, 50 (4): 477-481 2004

Poulsen, HF; Margulies, L; Schmidt, S; Winther, G, "Lattice rotations of individual bulk grains - Part I: 3D X-ray characterization," ACTA MATERIALIA, 51 (13): 3821-3830 AUG 1 2003

Appendix F, Kommentarer til økonomiskemaer

Der er i ansøgningen anvendt overhead efter de nye takster, 35%.

Lønudgifter er beregnet ud fra KUs standardtal. Der er medregnet anciennitetsstigning og en forventet lønstigning over projektperioden på 12% (d.v.s. Et gennemsnitstillæg på 6%). Feriepenge er eksplicit medregnet i månedslønnen, hvilket vil sige, at en årsløn er 10,615 månedslønninger, med 6 ugers ferie. Det antages, at nye Ph.D. Studerende ikke afholder ferie første år, d.v.s. 12 månedslønninger. Takterne er

ph.d. Studerende, 1. år	30.232 / mnd. + 80.000 / år for taxameter	= 442.784 / år
ph.d. Studerende, 2. år	30.948 / mnd. + 80.000 / år for taxameter	= 408.513 / år
ph.d. Studerende, 3. år	33.221 / mnd. + 80.000 / år for taxameter	= 432.641 / år
Post doc, trin 6	40.360 / mnd.	= 428.421 / år
Post doc, trin 8	42.272 / mnd.	= 448.717 / år
Lektor stand. tillæg	45.702 / mnd. + 60.000 / år	= 545.127 / år
Professor, ramme 37	61.732 / mnd.	= 655.285 / år

Medfinanciering via løn for fast personale konteres ikke for Martin Meedom Nielsen og Henning Friis Poulsen, da deres løn allerede er dækket af Danmarks Grundforskningsfond, hhv. Center for Molecular Movies (CMM) og Metal Structures in 4D (M4D).

Løn for TAP personale for KU-Life regnes som 4 måneder á 30.000 kr. og 4 måneder á 35.000 kr, ligeligt fordelt på medfinanciering og SFR.

Der ansøges som lønmidler til VIP Søren Schmidt, idet han besidder kompetencer der er essentielle for projektets succes, se brødtekst. Lønmidlerne beløber sig i alt til 1,25 årsværk.

Endvidere regnes afskrivning på ekssiterende apparatur, 50.000 kr/år, med som medfinanciering for KU-Life.

Som fælles computer facilitet indkøbes en multi-processor, multi-core maskine, opstillet på Risø-DTU. Pris, ca. 100.000 DKK.

Beløb for drift dækker rejser, konference, og (for KU-Life) kemikalier. Driftsudgifterne bliver minimeres ved at rejser til eksperimenter dækkes af den nationale instrumentcenter DANSCATT.

Økonomioversigt vedr. hver partners deltagelse i projektet

Det Strategiske Forskningsråd
Skema dsf1, marts 2008

Projekttitel	**MCXtrace – a simulation tool for X-ray investigations of nanostructures**
Partner (Institution/virksomhedsnavn)	Niels Bohr Institutet, Københavns Universitet
Anfør CVR-nr. eller (for udenlandske enheder) hjemland	29979812
For private virksomheder: Er virksomheden en SMV[1)] eller en stor virksomhed? Skriv: "SMV" eller "Stor"	

Alle beløb anføres i DKK

A: Udgiftsbudget	
VIP-løn	3,348,556
TAP-løn	
Apparatur over 40.000 DKK	0
Drift	100,000
Evt. overhead/adm.bidrag	1,206,995
Sum udgiftsbudget	**4,655,550**

B: DSF-bevilling	
VIP-løn	2,074,457
TAP-løn	
Apparatur over 40.000 DKK	0
Drift	100,000
Evt. overhead/adm.bidrag	761,060
Sum DSF bevilling	**2,935,516**

C: Tilskud fra anden side	
VIP-løn	475,655
TAP-løn	
Apparatur over 40.000 DKK	
Drift	
Evt. overhead/adm.bidrag	166,479
Sum tilskud fra anden side	**642,134**

D: Egendækning	
VIP-løn	798,444
TAP-løn	
Apparatur over 40.000 DKK	
Drift	
Evt. overhead/adm.bidrag	279,456
Sum egendækning	**1,077,900**

E: Øvrige bidrag til det samlede projekt	
Anfør beløb der overføres til anden partner	

OBS:

Summen af beløbene under pkt. B, C og D skal svare til beløbene under pkt. A

Summen af beløbene i pkt. D og E svarer til partnerens samlede medfinansiering af projektet

Dokumentation for tilskud fra eksterne kilder skal vedlægges

Overhead/administrationsbidrag anført i afsnit B og D skal - for danske enheder - svare til de takster, der fremgår af opslag/ansøgningsvejledning

"VIP-løn" inkluderer både ph.d./post.doc. og øvrig VIP-løn (posterne specificeres på hhv. skema dsf4 og dsf5)

Se i øvrigt DSF's ansøgningsvejledning af marts 2008, hvor der også findes eksempler

[1)] "SMV" står for "små og mellemstore virksomheder". Se vejledningen om definitionen af en SMV

Professor John Renner Hansen
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Niels Bohr Institutet, Københavns Universitet
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Email: head@nbi.dk - www.nbi.ku.dk

Dato og partnerens underskrift og stempel 19/8-2008

Økonomioversigt vedr. hver partners deltagelse i projektet

Det Strategiske Forskningsråd
Skema dsf1, marts 2008

Projekttitel	**MCXtrace – a simulation tool for X-ray investigations of nanostructures**
Partner (Institution/virksomhedsnavn)	Afdeling for Materialeforskning, Risø-DTU
Anfør CVR-nr. eller (for udenlandske enheder) hjemland	DK 30060946
For private virksomheder: Er virksomheden en SMV[1)] eller en stor virksomhed? Skriv: "SMV" eller "Stor"	

Alle beløb anføres i DKK

A: Udgiftsbudget	
VIP-løn	2,590,255
TAP-løn	0
Apparatur over 40.000 DKK	100,000
Drift	100,000
Evt. overhead/adm.bidrag	976,589
Sum udgiftsbudget	**3,766,844**

B: DSF-bevilling	
VIP-løn	1,879,123
TAP-løn	
Apparatur over 40.000 DKK	100,000
Drift	100,000
Evt. overhead/adm.bidrag	727,693
Sum DSF bevilling	**2,806,816**

C: Tilskud fra anden side	
VIP-løn	
TAP-løn	
Apparatur over 40.000 DKK	
Drift	
Evt. overhead/adm.bidrag	0
Sum tilskud fra anden side	**0**

D: Egendækning	
VIP-løn	711,133
TAP-løn	0
Apparatur over 40.000 DKK	
Drift	
Evt. overhead/adm.bidrag	248,896
Sum egendækning	**960,029**

E: Øvrige bidrag til det samlede projekt	
Anfør beløb der overføres til anden partner	

OBS:

Summen af beløbene under pkt. B, C og D skal svare til beløbene under pkt. A

Summen af beløbene i pkt. D og E svarer til partnerens samlede medfinansiering af projektet

Dokumentation for tilskud fra eksterne kilder skal vedlægges

Overhead/administrationsbidrag anført i afsnit B og D skal - for danske enheder - svare til de takster, der fremgår af opslag/ansøgningsvejledning

"VIP-løn" inkluderer både ph.d./post.doc. og øvrig VIP-løn (posterne specificeres på hhv. skema dsf4 og dsf5)

Se i øvrigt DSF's ansøgningsvejledning af marts 2008, hvor der også findes eksempler

[1)] "SMV" står for "små og mellemstore virksomheder". Se vejledningen om definitionen af en SMV

Dato og partnerens underskrift og stempel

Risø National Laboratory
for Sustainable Energy
Technical University of Denmark-DTU
Building 101, P.O. Box 49
DK-4000 Roskilde
Denmark

Financial summary of each partner's commitment to the project

The Danish Council for Strategic Research
Form dsf1, march 2008

Project title	**Mc-Xtrace – a simulation tool for X-ray investigations of nanostructures**
Partner (institution/company name)	Institut for Grundvidenskab og Miljø, Københavns Universitet
Enter CVR-no. or (for foreign entities) country of domicile	29979812
For private-sector enterprises: If the enterprise is an SME[1)] or a large enterprise, enter: "SME" or "Large"	

All amounts must be stated in DKK

A: Expenditure budget	
Scientific/academic salaries	1.753.590
Technical/administrative salaries	260.000
Equipment expenses in excess of DKK 40,000	0
Operating expenses	270.000
Overheads/admin. contributions	799.256
Total expenditure budget	**3.082.846**

B: DSF grant	
Scientific/academic salaries	1.360.974
Technical/administrative salaries	130.000
Equipment expenses in excess of DKK 40,000	0
Operating expenses	120.000
Overheads/admin. contributions 35%	563.841
Total DSF grant	**2.174.815**

C: Funding from other sources	
Scientific/academic salaries	0
Technical/administrative salaries	0
Equipment expenses in excess of DKK 40,000	0
Operating expenses	0
Overheads/admin. contributions 35%	0
Total funding from other sources	**0**

D: Self-financing	
Scientific/academic salaries	392.616
Technical/administrative salaries	130.000
Equipment expenses in excess of DKK 40,000	0
Operating expenses	150.000
Overheads/admin. contributions 35%	235.415
Total self-financing	**908.031**

E: Other contributions to the overall project	
Amount transferred to other partner	

NOTE:

The total of the amounts under items B, C and D must tally with the amounts under item A.

The total of the amounts in items D and E corresponds to the partner's total co-financing of the project.

Documentation for funding from external sources must be appended.

Overheads/admin. contributions under items B and D must - for Danish entities - tally with the rates set out in the call/Application Guide

Scientific/academic salaries include both PhD and postdoctoral salaries and other scientific/academic salaries specify items on Forms dsf4 and dsf5, respectively)

See further examples in DSF's Application Guide, March 2008.

[1)] See the Application Guide for the definition of SMEs (small and medium-sized enterprises).

Date and partner's signature and stamp

Susanne Sørensen
Head of Department
Department of Natural Sciences
40 Thorvaldsensvej . DK-1871 Frb. C, Denmark

19/8.08

FACULTY OF LIFE SCIENCES
UNIVERSITY OF COPENHAGEN

BUDGETKONTORET
DET BIOVIDENSKABELIGE FAKULTET
KØBENHAVNS UNIVERSITET

18/8-2008

Økonomioversigt vedr. hver partners deltagelse i projektet

Det Strategiske Forskningsråd
Skema dsf1, marts 2008

Projekttitel	**MCXtrace – a simulation tool for X-ray investigations of nanostructures**
Partner (Institution/virksomhedsnavn)	JJ X-ray systems ApS
Anfør CVR-nr. eller (for udenlandske enheder) hjemland	27647790
For private virksomheder: Er virksomheden en SMV[1)] eller en stor virksomhed? Skriv: "SMV" eller "Stor"	SMV

Alle beløb anføres i DKK

A: Udgiftsbudget	
VIP-løn	450,000
TAP-løn	
Apparatur over 40.000 DKK	
Drift	
Evt. overhead/adm.bidrag	0
Sum udgiftsbudget	**450,000**

B: DSF-bevilling	
VIP-løn	
TAP-løn	
Apparatur over 40.000 DKK	
Drift	
Evt. overhead/adm.bidrag	
Sum DSF bevilling	**0**

C: Tilskud fra anden side	
VIP-løn	
TAP-løn	
Apparatur over 40.000 DKK	
Drift	
Evt. overhead/adm.bidrag	
Sum tilskud fra anden side	**0**

D: Egendækning	
VIP-løn	450,000
TAP-løn	
Apparatur over 40.000 DKK	
Drift	
Evt. overhead/adm.bidrag	0
Sum egendækning	**450,000**

E: Øvrige bidrag til det samlede projekt	
Anfør beløb der overføres til anden partner	

OBS:

Summen af beløbene under pkt. B, C og D skal svare til beløbene under pkt. A

Summen af beløbene i pkt. D og E svarer til partnerens samlede medfinansiering af projektet

Dokumentation for tilskud fra eksterne kilder skal vedlægges

Overhead/administrationsbidrag anført i afsnit B og D skal - for danske enheder - svare til de takster, der fremgår af opslag/ansøgningsvejledning

"VIP-løn" inkluderer både ph.d./post.doc. og øvrig VIP-løn (posterne specificeres på hhv. skema dsf4 og dsf5)

Se i øvrigt DSF's ansøgningsvejledning af marts 2008, hvor der også findes eksempler

[1)] "SMV" står for "små og mellemstore virksomheder". Se vejledningen om definitionen af en SMV

Dato og partnerens underskrift og stempel

19/8-2008

JJ X-Ray Systems
Gl.Skovlundevej 54
2740 Skovlunde
Denmark

Appendix I, ESRF Collaboration Agreement

The following document confirms ESRF contribution to the project.

EUROPEAN SYNCHROTRON RADIATION FACILITY
INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

Prof. Sine Larsen
Director of Research
Tel : +33 (0) 4 76 88 21 81
: +33 (0) 4 76 88 20 14 (secretary)
Fax : +33 (0) 4 76 88 21 60
Email: slarsen@esrf.fr

Dr. Kim Lefmann
Associate Professor
Niels Bohr Institute
University of Copenhagen

Ref: SL/ED 08/29

August 19, 2008

Dear Dr. Lefmann,

As part of a collaboration between the University of Copenhagen and the ESRF on the

"Development of an efficient and flexible ray-tracing tool suitable for X-ray nano-focusing and imaging optics"

I can confirm that the ESRF is willing to finance one year's salary for a post-doc working at the ESRF on the project.

Yours sincerely,

Sine Larsen

Sine Larsen