SNSS-19

2015 Annual Meeting of the Swedish Neutron Scattering Society

KTH, Royal Institute of Technology, 26-28 May 2015, Stockholm, Sweden

Välkommen till KTH och Stockholm!

SNSS is an organisation open to all those who are using, or interested in the use of, neutron scattering and imaging techniques. The membership fee has been maintained at 0 SEK since the foundation of the society and there are currently about 150 members. SNSS is also affiliated to the European Neutron Scattering Association (ENSA).

One of the main tasks of SNSS is to encourage and support new users to join the Swedish neutron science community. This task has clearly become even more important lately thanks to the current development and construction of the European Spallation Source (ESS) in Lund. This opens up great opportunities for performing world leading neutron science by Swedish researchers and industry.

Thank you all for joining this meeting and hereby helping us to strengthen the Swedish neutron science community!

For SNSS and the local organizing
committee of SNSS-19

Asst. Prof. Dr. Martin Månsson
KTH Royal Institute of Technology

KTH
VETENSKAP
OCH KONST

Our Partners:

EUROPEAN SPALLATION SOURCE

Vetenskapsrådet

SWEDISH FOUNDATION *for* STRATEGIC RESEARCH

THE NOBEL COMMITTEE FOR PHYSICS
THE ROYAL SWEDISH ACADEMY OF SCIENCES

SOME PRACTICAL INFORMATION

KTH/ESS kick-off colloquium "Science Using Neutrons"

Time: 26/5 kl. 15:00 – 19:00

Place: KTH Main Campus Valhallavägen
Lecture room E2
Lindstedtsvägen 3, floor 3
Stockholm
http://www.kth.se/places/room/A43:03/1337

SNSS-19 Annual Meeting

Time: 27-28/5

Place: KTH Main Campus Valhallavägen
Lecture room K2
Teknikringen 28, ground floor *("officially" named floor 05)*
Stockholm
http://www.kth.se/places/room/A43:15/571

Closest subway station for KTH is "Tekniska Högskolan", using the "red" subway line.
(please note that the color of the actual trains does not mean anything!)

When you arrive at KTH, please use the map(s) on the following pages.

Contact Person

Martin Månsson, condmat@kth.se
Tel. +46-(0)8-790 4094
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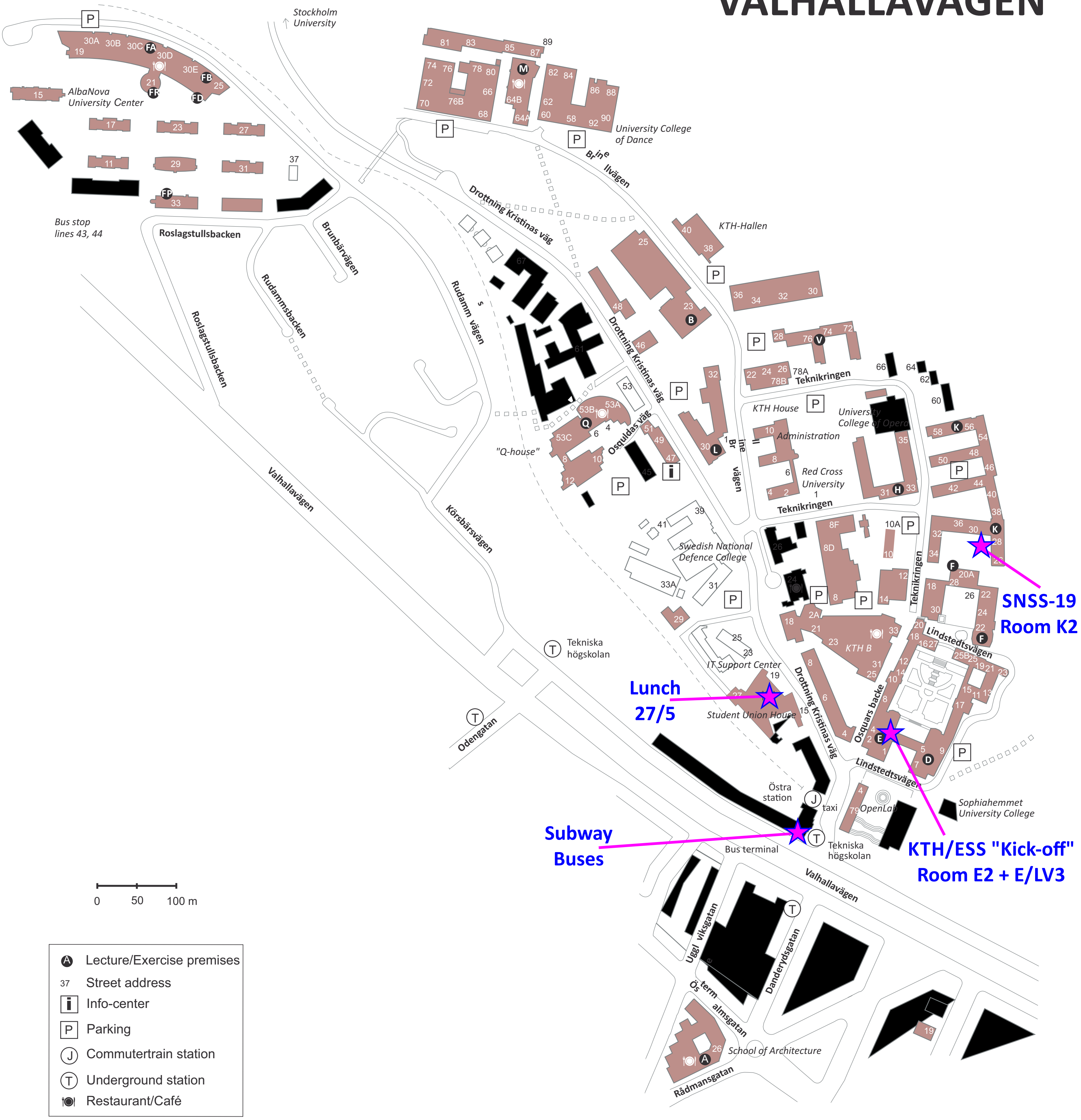
KTH
MAIN CAMPUS
VALHALLAVÄGEN



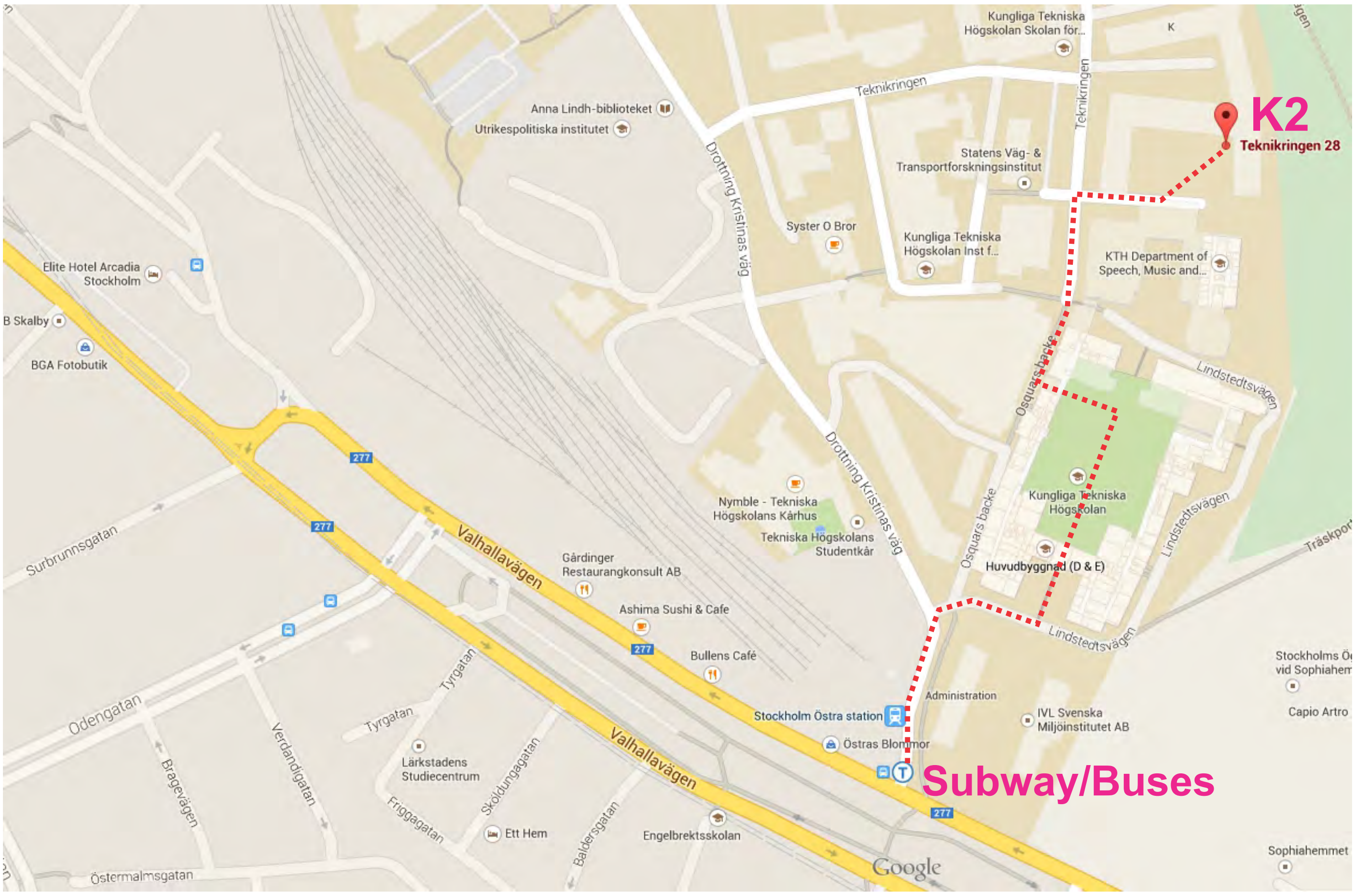
SNSS-19
Room K2

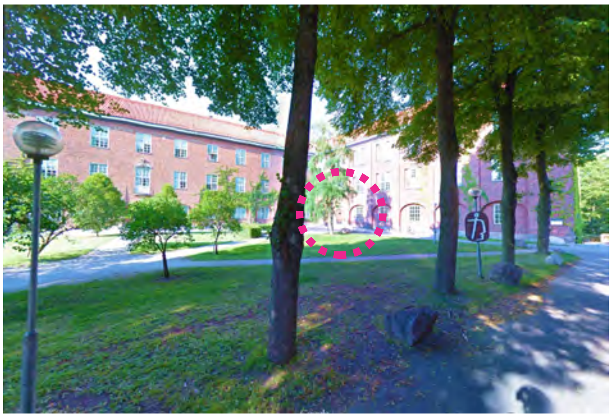
Lunch
27/5

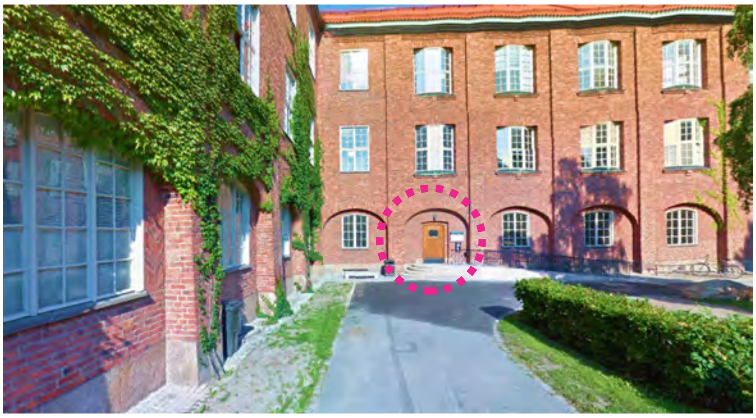
Subway
Buses

KTH/ESS "Kick-off"
Room E2 + E/LV3

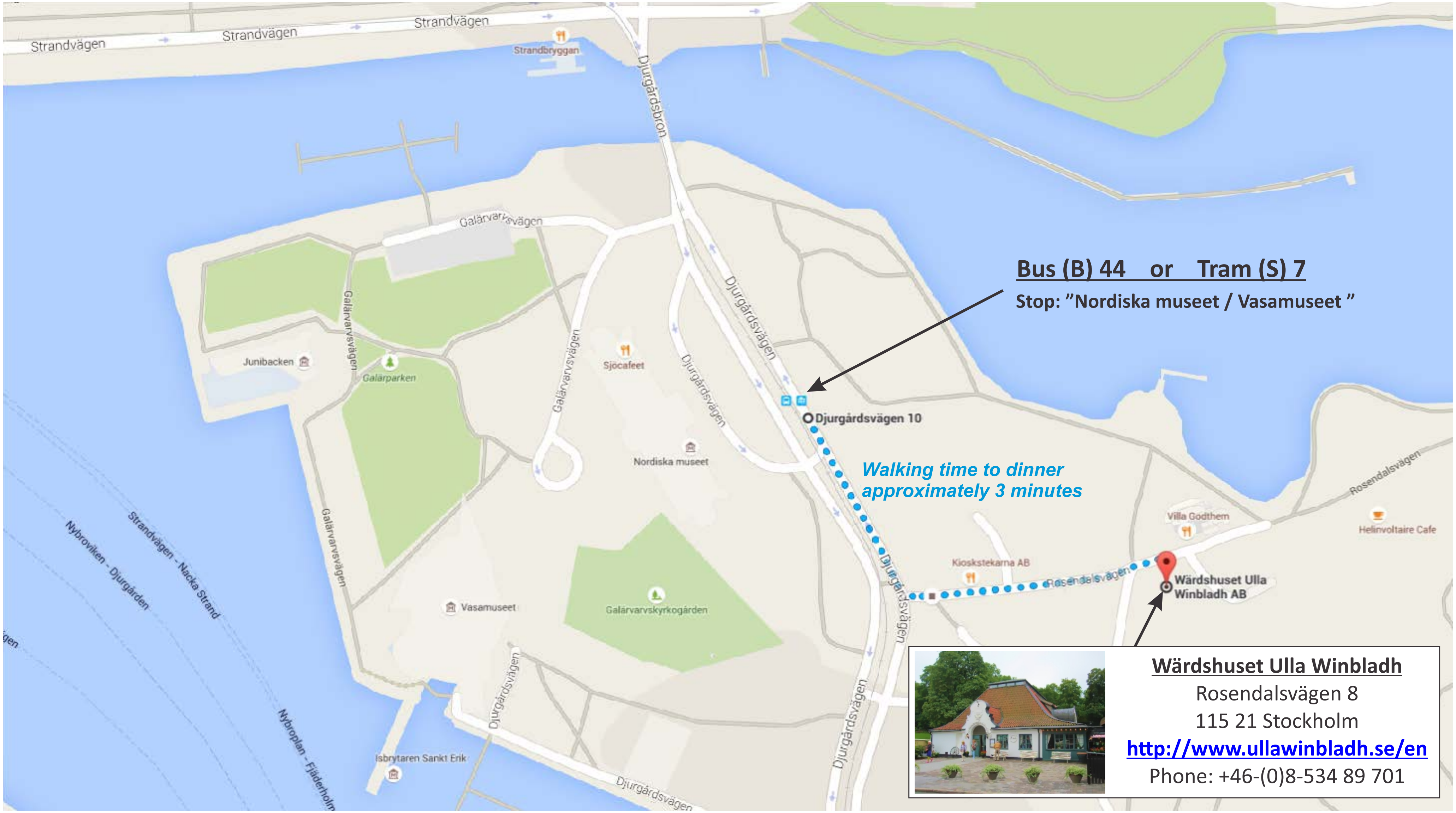
Conference Venue: KTH Main Campus
Lecture Room K2
Teknikringen 28







"DINNER-MAP"



Bus (B) 44 or Tram (S) 7

Stop: "Nordiska museet / Vasamuseet "

Walking time to dinner approximately 3 minutes

Wärdshuset Ulla Winbladh
Rosendalsvägen 8
115 21 Stockholm
http://www.ullawinbladh.se/en
Phone: +46-(0)8-534 89 701

Science Using Neutrons

An ESS / KTH colloquium
on life, materials and energy science, kicking off
the annual meeting of the Swedish Neutron Scattering Society.

May 26th 15:00 - 19:00 at KTH, room E2

15:00 **Neutrons for Green and Safe Energy Materials**
Assistant Professor Martin Månsson
Royal Institute of Technology, Sweden

15:35 **Hydrogen Dynamics in our Daily Life**
Associate Professor Heloisa N. Bordallo
Niels Bohr Institute, University of Copenhagen, Denmark

16:10 **Visions for Studies of Biomolecules at ESS**
Professor Poul Nissen
Nordic-EMBL Partnership for Molecular Medicine, Aarhus University, Denmark

17:00 - 19:00 **Neutron Mingle**
Please join us for light food and drinks, at KTH , Ljusgården E/LV3.

KTH
VETENSKAP
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Welcome!

No registration necessary.

ess

More info: http://www.snss.se/2015

Swedish Neutron Scattering Society
Annual Meeting of the Swedish Neutron Scattering Society SNSS-19
KTH Royal Institute of Technology, Stockholm, Sweden, 27-28 May, 2015

SNSS-19 PROGRAM

Location:	KTH Royal Institute of Technology Lecture Hall K2 Teknikringen 28	Stockholm Sweden

27 May, 2015

Time	Topic	Speaker
Intro Session		
09:00 – 10:00	**Basic Introduction to Neutron Science**	Asst. Prof. Martin Månsson, KTH
10:00 – 10:30	Coffee Break & Registration / Poster Session	
10:30 – 10:45	**SNSS Welcome and Practical Info**	Asst. Prof. Martin Månsson, KTH Prof. Maths Karlsson, CTH
10:45 – 11:00	**Research at KTH**	**Vice President Prof. Arne Johansson** KTH Royal Institute of Technology Sweden
11:00 – 11:30	**ESS Status & Update**	**Prof. Dimitri Argyriou** European Spallation Source (ESS) Sweden
11:30 – 12:00	**T.B.A**	**Swedish Research Council (VR)**
12:00 – 13:30	Lunch @ THS Nymble	
Versatile Neutrons: from Swedish Steel to Soft Cells		
13:30 – 14:10	**Neutrons for Imaging / Tomography and Diffraction** **Invited Talk**	**Dr. Anders Kaestner** Paul Scherrer Institute (PSI) Switzerland
14:10 – 14:30	**Neutrons for Better Roads** *Towards understanding the breaking of bitumen emulsions using neutrons computed tomography and radiography*	Abdullah Khan, KTH
14:30 – 14:45	**Neutrons for Stronger Steel?** *Thermal surface free energy and stress of iron*	Dr. Stephan Schönecker, KTH
14:45 – 15:00	**Measuring slow dynamics at ESS**	Dr. Melissa Sharp, ESS
15:00 – 15:20	**Contrasts in Neutron Scattering** **Invited Talk** Playing with contrast variation in soft matter beyond classical studies in 4-components systems	**Dr. Fabrice Cousin** Laboratoire léon Brillouin France
15:20 – 15:35	***Neutrons for Life*** *Biomimetic surfaces for membrane bound protein structural and functional studies*	Prof. Marité Cárdenas, MAH
15:35 – 16:00	Coffee Break / Poster Session	
Neutron Science and Industry		
16:00 – 16:30	**Industrious Neutrons** **Invited Talk** *Engaging with Industry at* **ISIS**	**Dr. Christopher Frost** ISIS Facility, Rutherford Appleton Laboratory UK
16:30 – 17:00	**Neutron & Industry @ Oak Ridge National Laboratory** **Invited Talk** *Neutron scattering at ORNL to support materials science and engineering research*	**Dr. Andrew Payzant** SNS, Oak Ridge National Laboratory USA
17:00 – 17:30	**Invited Talk** **Industry at Paul Scherrer Institute**	**Dr. Giorgio Travaglini** Paul Scherrer Institute (PSI) Switzerland
19:00 – 22:00	Dinner @ Ulla Winblad on Djurgården	

28 May, 2015

Time	Topic	Speaker
Energy Materials		
08:30 – 09:00	**Dynamical studies of hydrogen in materials for energy applications**	Prof. Maths Karlsson, CTH
09:00 – 09:20	**Invited Talk** **Neutrons and materials for energy** A focus on clathrate hydrates	**Prof. Arnaud Desmedt** CNRS / University of Bordeaux France
09:20 – 09:35	***Neutrons for Solar Cells*** *Structure and cation orientation in the perovskite photovoltaic methyl ammonium lead iodide between 100 and 350 K*	Dr. Paul F. Henry, ESS
09:35 – 09:50	**Neutrons for Energy Storage** *In operando measurements of Li-ion batteries*	Dr. William Brant, UU
09:50 – 10:20	Coffee Break / Poster Session	
A Neutrons view of Magnetic Materials		
10:20 – 10:50	**Inelastic Neutron Scattering for Magnetism** **Invited Talk**	**Prof. Bella Lake** Helmholtz Zentrum Berlin für Materialien & Energy Germany
10:50 – 11:30	**Magnetic & Superconducting Nano-phases** **Invited Talk** *Static and Elastic Properties of Superconducting Vortex Lattices and Skyrmion Lattices in Chiral Magnets Studied by Time Resolved Neutron Scattering*	**Dr. Sebastian Mühlbauer** Heinz Maier-Leibnitz Zentrum Garching (MLZ) Germany
11:30 – 11:45	**Neutrons for Future Refrigerators** *Magnetocaloric Hydrides of NdGa and GdGa*	Dr. Jonas Ångström, UU
11:45 – 13:00	Lunch / ***General Assembly of the SNSS members***	
The Neutron Spin		
13:00 – 13:45	**Polarizing the Neutron Spin** **Invited Talk** *Longitudinal and Spherical Neutron Polarimetry: Applications and Examples*	**Dr. Bertrand Roessli** Paul Scherrer Institute (PSI) Switzerland
13:45 – 14:05	**Frustrated Magnetism** **Invited Talk** *Anisotropy-tuned magnetic order in pyrochlore iridates*	**Dr. Virginie Simonet** Institut Néel France
14:05 – 14:20	**Order in Spin Ice**	Prof. Patrik Henelius, KTH
14:20 – 14:40	**Swedish Instrument Development** *The New Super ADAM – Swedish neutron reflectometer at ILL*	Dr. Alexei Vorobiev, ILL/UU
14:40 – 14:45	**Closing Remarks**	Martin Månsson
14:45 – …	Coffee Break / Poster Session	
FR – SWE		
14:45 – …	**France – Sweden** **Collaborations Panel discussion**	

POSTER SESSION

P1
Atomic and magnetic structure and magnetocaloric properties of $AlFe_2B_2$
Johan Cedervall *et al.*
Uppsala University

P2
Local coordination and vibrational properties of protons in proton conducting perovskite oxides
Laura Mazzei *et al.*
Chalmers Technical University

P3
Neutrons for Green & Safe Energy Materials: Sodium Based Energy Storage
Martin Månsson *et al.*
KTH Royal Institute of Technology

P4
Random-Singlet State in Antiferromagnetic Heisenberg Spin Chain Compound $BaCu_2(Si_{0.5}Ge_{0.5})_2O_7$ Studied by Inelastic Neutron Scattering
Martin Månsson *et al.*
KTH Royal Institute of Technology

P5
Introducing High Entropy Alloys
Samrand Shafeie *et al.*
Chalmers Technical University

P6
GISANS from solid-liquid boundaries
Max Wolff *et al.*
Uppsala University

BOOK OF ABSTRACTS

Swedish Neutron Scattering Society
Abstract submitted to the 2015 Annual Meeting of the Swedish Neutron Scattering Society SNSS-19
KTH Royal Institute of Technology, Stockholm, Sweden, 27-28 May, 2015

INVITED TALK

Neutron Imaging and Diffraction

Anders Kaestner, Steven Peetermans, Christian Grünzweig, and Eberhard Lehmann
Neutron Imaging and Activation Group
Laboratory for Neutron Scattering and Imaging
Paul Scherrer Institut, CH5232 Villigen PSI, Switzerland

Neutron imaging is a versatile experiment method operating in the spatial domain and mainly using the using neutrons transmitted through the sample to produce high resolution radiographs with pixel sizes down to about 10 microns. With neutron computed tomography (CT) it is possible to reconstruct 3D volumes describing the spatial material distribution of the sample. Radiography and CT are together the most common acquisition techniques and the resolution in space, time, and energy can be varied to meet the requirements from a wide user community. Scattering is often the dominant interaction mechanism between samples and neutrons; therefore we have added several instrument options measure the neutrons not reaching the detector through direct transmission. Energy selection makes contrast enhancement through Bragg edge imaging possible. ICON [1] and BOA [2] at the Swiss Spallation neutron Source provide for energy selective imaging using velocity selectors and crystal monchromators. A further option using the time of flight principle will be implemented at the new imaging beamline ODIN [3] at ESS which will provide higher energy resolution and faster acquisition. Grating interferometry provides the additional information of differential phase and dark field. The latter is related to ultra small angle neutron scattering. Recently the option to place an additional imaging detector on a position off the direct beam has made it possible to acquire images representing the neutrons diffracted from single crystal samples or samples with few crystals [4]. With this technique it is possible to make a 3D reconstruction of the crystal orientations in the sample.

We will give an overview of experiment methods available at a state of the art neutron-imaging instrument and show a selection of examples of applications.

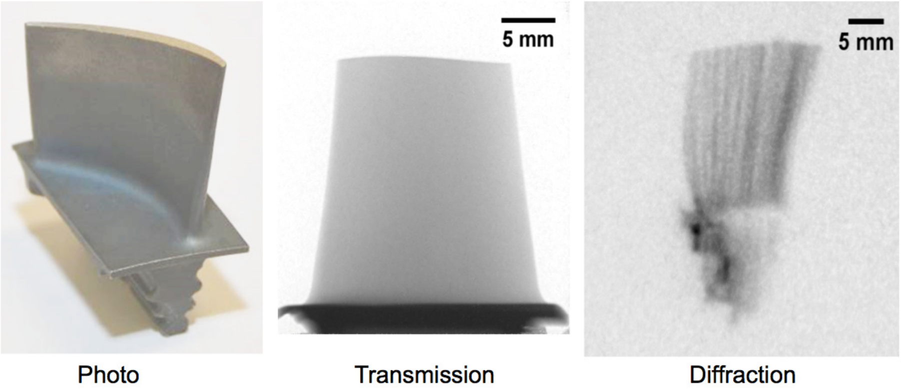

Figure 1: A single crystal turbine blade. A neutron transmission image (middle) shows a homogeneous sample while the diffracted neutrons registered from the side indicate inhomogeneities in the sample.

REFERENCES

[1] A. Kaestner et al, "The ICON beamline - A facility for cold neutron imaging at SINQ" *Nucl. Instrum. Methods Phys. Res., Sect. A,* vol. 659, no. 1, pp. 387-393, 2011.

[2] M. Morgano et al., "Neutron imaging options at the BOA beamline at Paul Scherrer Institut" *Nucl. Instrum. Methods Phys. Res., Sect. A,* vol. 754, pp. 46-56, 2014.

[3] M. Strobl, "The Scope of the Imaging Instrument Project ODIN at ESS" *Physics Procedia,* Accepted for publication, 2015.

[4] S. Peetermans and E. H. Lehmann, "A Double Detector Set-up for Simultaneous Transmission and Diffraction Neutron Imaging" *Physics Procedia,* vol. 43, pp. 179-185, 2013.

CONTRIBUTED TALK

Towards understanding the breaking of bitumen emulsions using neutrons computed tomography and radiography

Abdullah Khan[1], Anders Kaestner[2], Stephen Hall[3], Per Redelius[4], Niki Kringos[1]
[1] *KTH Royal Institute of Technology, Dept. of Civil and Architectural Engineering, 10044 Stockholm, Sweden*
[2] *Neutron Imaging and Activation Group, Paul Scherrer Institute, PSI West, 5232 Villigen, Switzerland*
[2] *Lund University, Dept. of Solid Mechanics, ESS AB, 22100 Lund, Sweden*
[4] *Nynas Bitumen AB, 14982 Nynäshamn*, Sweden

Emulsions are among the most important colloids in everyday life and have a variety of usage in different fields, though the main focus of this work is bitumen emulsions for road pavement and their maintenance. In the current study, cationic bitumen emulsions were investigated under a neutron beam at ICON & NEUTRA beam stations at PSI Switzerland to perform time series experiments using computed tomography and radiography. In these experiments, different bitumen emulsion recipes were used with slow and fast setting. After mixing emulsions with aggregates, structural changes were observed with different time projections. The evaporation of the water phase could also be traced with the movement of air bubbles in time series experiments. It was observed that bitumen phase density changes at the binder aggregate interface with time as water evaporates and viscosity of the binder builds up. In the continuation of this work, more parameters will be investigated and clear linking to material properties to improve the emulsions can be made.

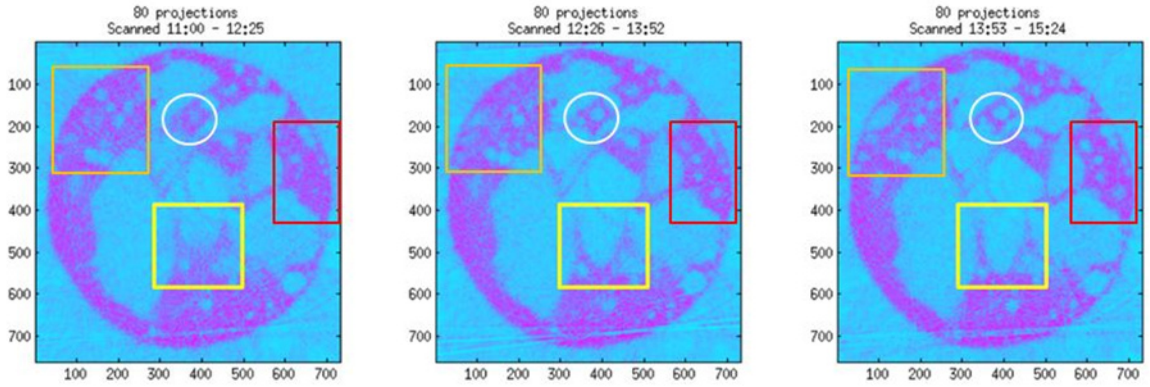

Figure: Phase density changes at bitumen-aggregates interface with time
(CTs as a sequence over time to help unguided observer to understand the slices)

REFERENCES

[1] Khan A., Kaestner A., Redelius P., Kringos N., WCNR-10 (10th World Conference on Neutrons Radiography), October 5-10, 2014, Grindelwald Switzerland
[2] Khan A, Redelius P, Kringos N., Paper 933, ISAP 2014, Raleigh NC, USA
[3] Anderson I.S., McGreevy R., Bilheux H.Z., “Neutron Scattering Applications and Techniques”, Springer 2009, XVI

CONTRIBUTED TALK

Thermal surface free energy and stress of iron

Stephan Schönecker[1], Xiaoqing Li[1], Börje Johansson[1,2], Se Kyun Kwon[3], Levente Vitos[1,2,4]
[1] *Applied Materials Physics, Department of Materials Science and Engineering, KTH- Royal Institute of Technology, Stockholm SE-10044, Sweden*
[2] *Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75120, Uppsala, Sweden*
[3] *Graduate Institute of Ferrous Technology, Pohang University of Science and Technology, Pohang 790-784, Korea*
[4] *Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest H-1525, P.O. Box 49, Hungary*

Absolute values of surface energy and surface stress of solids are hardly accessible by experiment. Here, we investigate the temperature dependence of both parameters for the (001) and (110) surface facets of body-centered cubic Fe from first-principles modeling taking into account vibrational, electronic, and magnetic degrees of freedom. The monotonic decrease of the surface energies of both facets with increasing temperature is mostly due to lattice vibrations and magnetic disorder. The surface stresses exhibit nonmonotonic behaviors resulting in a strongly temperature dependent excess surface stress and surface stress anisotropy.

Seizing the opportunity, I will also briefly summarize our research activities in the *Applied Materials Physics group* at KTH headed by Levente Vitos [1].

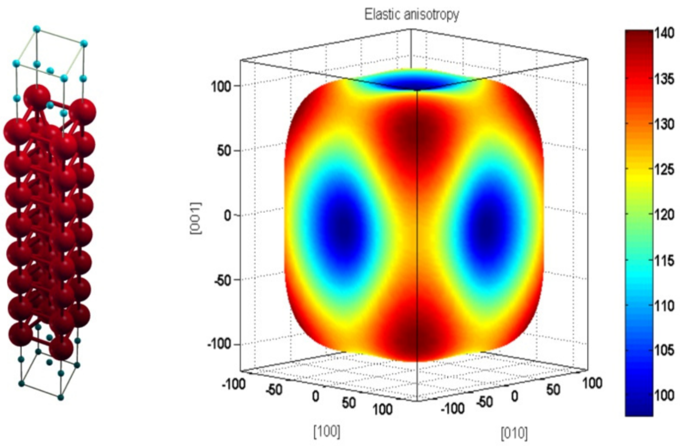

Figure: (Left) Slab model of a (100) surface facet of a bcc metal and (Right) Elastic anisotropy of high entropy alloy.

REFERENCES

[1] https://www.kth.se/en/itm/inst/mse/organisation/avdelning/tillampadmaterialfysik/research-1.427073

CONTRIBUTED TALK

Opportunities for measuring slow dynamics at ESS

Melissa A. Sharp[1]
[1] *European Spallation Source (ESS), Lund, Sweden*

Neutron spin-echo spectroscopy is the neutron technique with the highest energy resolution for probing the dynamics of materials. At the European Spallation Source it is currently planned to have 2 NSE spectrometers in the full suite of instruments: one instrument optimised for the highest resolution and one for a wide angular coverage. They would thus be complementary and allow for a broad range of science within soft matter, biology, energy materials and magnetism, and provide good complementarity to the chopper and backscattering spectrometers **[1]**.

Here I will present the planned NSE spectrometers and provide an example of a recent NSE study of the domain motions in a protein that would benefit from this new world-leading source **[2]**.

REFERENCES

[1] ESS Technical Design Report, 2013
[2] L. Hong, M.A. Sharp, S. Poblete et al; Biophysical Journal, 107, 393, 2014

INVITED TALK

Playing with contrast variation in soft matter beyond classical studies in 4-components systems

Fabrice Cousin[1]
[1] *Laboratoire Léon Brillouin (LLB), CEA Saclay, France*

The possibility to play with contrast by a clever choice of the Scattering Length Densities (SLD) of components has been the cornerstone of the success of structural studies in Soft Matter by neutron scattering methods (SANS or reflectometry) for decades. Such "contrast variations" methods are usually declined with two philosophies: (i) to create some contrasts in binary systems where it does not exist, e g by deuteration, for instance in polymer melts or (ii) to adjust the contrast of a component of a ternary system to those of another in order to "match" it, simplifying the system to a two-components one from neutron point of view.

Although very efficient, such contrast variations are usually restricted systems containing at maximum 3 components. However, if one aims at probing specifically the structure of a given species in a 4-components system, contrast variation remains powerful if the system is craftily designed with respect to neutrons, with three of the components having a close SLD, very different from those of the component to be characterized. We will illustrate it by showing two examples representative of soft matter systems : - the localization of counter-ions in complexes of proteins and polyelectrolyte of opposite charges in aqueous solution **[1]** and - the determination of the conformation of polymeric chains in nanocomposite made of polymeric melts reinforced by nanoparticles, grafted or not by a polymeric shell **[2]**.

REFERENCES

[1] J.Gummel, F.Cousin, F.Boué, J. Am. Chem. Soc.), 2007, 129(18), 5806-5807.
[2] A.-S. Robbes, F. Cousin, F. Meneau, F. Dalmas, R. Schweins, D. Gigmes, J. Jestin Macromolecules, 2012, 45, 9220–9231.

CONTRIBUTED TALK

Biomimetic surfaces for membrane bound protein structural and functional studies

Marité Cárdenas[1,2], Tomas Laursen[3], Birger Lindberg Moller[3,] Robert Barker[4]
[1]*Nano-Science Center and Institute of Chemistry, Faculty of Science, University of Copenhagen, DK-2200 Copenhagen, Denmark*
[2]*Biomedical Science Department, Health and Society, Malmö University, 20506, Malmö, Sweden*
[3]*Plant Biochemistry Laboratory, Department of Plant and Environmental Science, Faculty of Science, University of Copenhagen, DK-1871 Frederiksberg C, Denmark*
[4]*Institut Laue Langevin, 6 rue Jules Horowitz – BP 156, 38042 Grenoble Cedex 9, France*

The interest in biomimetic membrane development has increased lately, in part due to the consensus that lipid function goes beyond cell compartmentalization: Lipids are not only the main barrier to reach the cell but also they can regulate membrane protein function. The exact lipid composition of each type of cell is complex and varies significantly depending on the type of cell and/or organism. The complexity in lipid composition can be taken down into two basic physical chemical aspects: charge and fluidity. These two properties should cover non-specific aspects of biomolecular interactions with the cell membrane. This is of particularly important for membrane bound and transmembrane proteins, since they only exist in a fully functional environment in the lipid bilayer. Thus, a major challenge is the need to use biomimetic surfaces for in situ studies on the effects of protein function/structure in a native like environment. In this talk I will present the efforts done in my group to develop biomimetic systems to study lipid effects on membrane protein structure.

INVITED TALK

Industrious Neutrons: Engaging with Industry at ISIS

Christopher Frost[1]
[1] *ISIS Facility, Rutherford Appleton Laboratory, Harwell Oxford, UK*

Following its discovery by Chadwick in 1932 the neutron has increasingly become a vital probe of condensed matter providing an often unique view into the atomic scale world of materials and their properties. The scientific community has, since the advent nuclear reactors and more recently accelerator driven spallation sources, been developing a wide variety of techniques and instrumentation to exploit the neutron's properties extending the areas of science and technology where the neutrons can make a significant impact.

This talk will focus on the impact that the neutron can have in the industrial world where the neutron's capabilities are perhaps less well known, but which can benefit enormously from progress the scientific community has made and the unique insights it can provide. The model used for industrial access to the UK's ISIS neutron and muon facility will be examined and brief case studies presented. The talk will encompass key aspects such as confidentially, assessment of proposals, how outcomes should drive and influence the process and how certain industries are clearly able to exploit and benefit from the investment made in neutron science in the UK and Europe.

Science & Technology Facilities Council
ISIS

Figure 1: ISIS Neutron facility at the STFC Rutherford Appleton Laboratory, near Oxford in the United Kingdom.

REFERENCES

[1] http://www.isis.stfc.ac.uk/

INVITED TALK

Neutron scattering at ORNL to support materials science and engineering research

E. Andrew Payzant
Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

High-flux neutron sources have limited availability and, while perceived as primarily serving the condensed matter physics community, support a significant and growing effort in "materials science and engineering", including neutron imaging and tomography, small angle neutron scattering, and spatially-resolved neutron diffraction for study of microstructure and mechanics in metals, alloys, and ceramics. While there are x-ray based analogs for these techniques, neutrons provide important advantages in many systems that make them either a complementary, or sometimes unique, characterization probe. These characterization needs are presently met at HFIR with the CG-1D Imaging, the CG-2 GP-SANS, and the HB-2B Residual Stress instruments, and at the Spallation Neutron Source by BL-7 VULCAN (SNS), and the planned imaging beamline BL-9 VENUS. This presentation will provide an overview of the present capabilities of the neutron facilities at Oak Ridge, with a focus on applications to industry. Recent changes include improved modes of access and enhanced instrument capabilities. Selected research projects will be highlighted, relevant to study of advanced materials for industry.

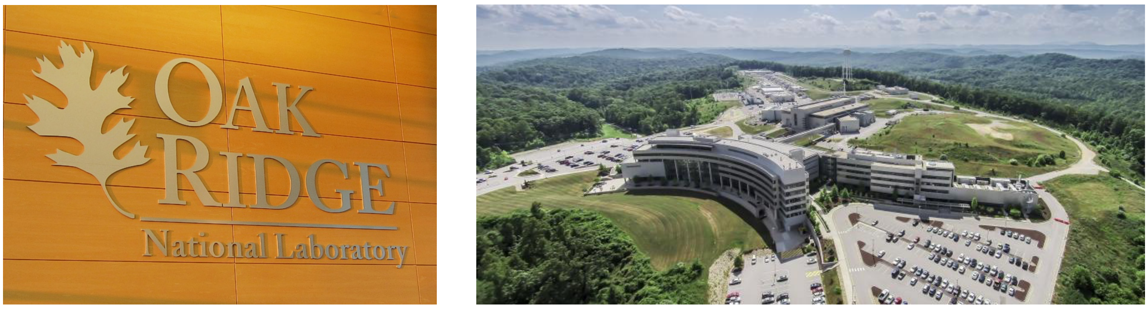

Figure: Neutron Sciences at ORNL, US-TN, is home to the High Flux Isotope Reactor (HFIR) as well as the Spallation Neutron Source (SNS).

REFERENCES
[1] https://neutrons.ornl.gov/

INVITED TALK

Industry at Paul Scherrer Institute

Giorgio Travaglini
Paul Scherrer Institute, Villigen PSI, Switzerland

The Paul Scherrer Institute, PSI, is the largest research centre for natural and engineering sciences within Switzerland. With more than 1900 employees, PSI performs world-class research in three main subject areas: Matter and Material; Energy and the Environment; and Human Health. By conducting fundamental and applied research, PSI works on long-term solutions for major challenges facing society, industry and science.

PSI develops, constructs and operates large scale research facilities such as the Swiss Light Source SLS, the Spallation Source SINQ and the Muon Source SμS. The new and powerful large scale facility SwissFEL (Free Electron Laser) is currently under construction and will be commissioned in 2016. The combination of these facilities is worldwide unique. PSI's facilities generate neutrons, muons and synchrotron light and are used for PSI's own research as well as for industry and other institutions. Even today the industrial utilization rate is more than 10%. More than 2400 external users benefit from access to PSI infrastructure.

One important pillar of PSI's mission is the Technology Transfer. PSI has a broad range of knowhow, technologies and processes and makes them available for industry: companies use PSI-technologies for example to implement business cases and to enter new markets with innovative products. PSI also has a lot of long-term research collaborations with industrial partner.

With its new innovation park "PARK innovAARE", PSI intends to strategically strengthen the transfer of technologies and knowhow to industry. PARK innovAARE is part of the Swiss Innovation Park, which currently consist of four locations: Zürich, Lausanne, Canton of Basel and Canton of Aargau (PARK innovAARE). The general concept of Swiss Innovation Park is to bring together research and business activities at one place in order to intensify the collaborations between industry and research and to generate strategic competitive advantages and innovations. Derived from PSI's research spectrum, PARK innovAARE focuses on four innovation fields: Accelerator Technologies, Human Health, Materials & Processes and Energy. PSI's innovation park is realized directly next to PSI. Companies that are located at PARK innovAARE will benefit from this close proximity to PSI with its large scale facilities, technologies and knowhow.

Figure: Paul Scherrer Institute (PSI), Villigen, Switzerland

REFERENCES
[1] http://www.psi.ch

INVITED TALK

Dynamical studies of hydrogen in materials for energy applications

Maths Karlsson[1]
[1]*Department of Applied Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden.*

Understanding the fundamental properties, such as atomic-scale structure and dynamics, of materials of relevance for alternative energy technologies is crucial in addressing the global challenge of cleaner sources of energy. In this presentation I aim to demonstrate the usefulness of neutron scattering for dynamical studies of proton conducting oxides. Currently, the main interest in these materials comes from their promise as electrolytes in future electrochemical devices and particularly through their use as electrolytes in next-generation, intermediate-temperature, fuel cells. However, the realization of such devices depends critically on the development of new, more highly proton conducting oxides. Such a development depends on increasing the current understanding of proton conduction in oxides and for this purpose neutron scattering, in particular inelastic and quasielastic methods, is an important means [1,2]. The aim with this presentation is to introduce briefly the non-specialist to the basic principles of dynamical studies using neutron scattering, and to exemplify with recent studies on proton conducting oxides. Examples of hydrogen dynamics in other classes of energy relevant materials, such as alkali silanides [3], will also be included in the presentation.

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INVITED TALK

Neutron and materials for energy: focus on clathrate hydrates

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Clathrate hydrates are nanoporous crystalline materials made of a network of hydrogen-bonded water molecules (forming host cages) that is stabilized by the presence of foreign guest molecules. The natural existence of large quantities of hydrocarbon hydrates in deep oceans and permafrost is certainly at the origin of numerous applications **[1]** in the broad areas of energy and environmental sciences and technologies (e.g. gas storage such as hydrogen **[2]**). At a fundamental level, their nanostructuration confers on these materials specific properties (e.g. super-protonic conductivity **[3]**, "glass-like" thermal conductivity **[4]**, etc…) for which the host-guest interactions play a key role **[5]**. These interactions occur on broad energy range (from van der Waals to ionic interactions) and thus require the use of multi-technique approach combining theoretical and numerical approaches, in which neutron scattering brings unvaluable information **[6]**. This talk will review the dynamical properties of clathrate hydrates, ranging from intramolecular vibrations to Brownian relaxations; it illustrates the contribution of neutron scattering in the understanding of the underlying factors governing specific chemical-physics properties relevant to energy area.

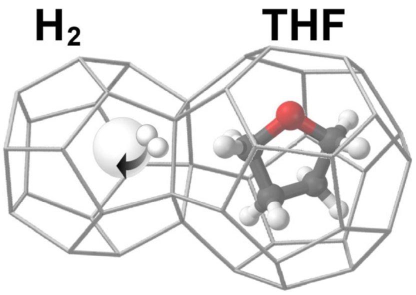

Fig. 1: Water cages of a mixed tetrahydrofuran clathrate hydrates confining hydrogen molecules.

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CONTRIBUTED TALK

Structure and cation orientation in the perovskite photovoltaic methyl ammonium lead iodide between 100 and 350 K

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The hybrid perovskite phase methylammonium lead iodide ($MAPbI_3$) has attracted increasing amounts of scientific attention since its identification as a highly efficient and low cost photovoltaic material. [1] Device efficiencies have rapidly risen to 17.9%, [2] while significant questions still remain regarding the device physics, especially the dynamic response under working conditions, [3] and also the fundamental structural properties of the material as a bulk solid and dynamically in operando. Full structural definition of the phases of $MAPbI_3$ has been hindered by the inherent complexity of the hybrid perovskite, with disorder in both organic and inorganic components observed in the higher temperature phases, [4] and the inherent limitations of X-ray diffraction techniques; these include an inability to distinguish the near isoelectronic atoms carbon and nitrogen, and difficulty in locating the light atom positions in the presence of the heavy atoms, Pb and I. The high temperature phase (>327 K) is cubic [5], the intermediate phase ($165 < T < 327$ K) tetragonal [6] and the low temperature phase orthorhombic [7]. However, the hydrogen positions and the orientation of the methylammonium cation remain unclear.

In this work we have investigated the full structure of $[CH_3NH_3]PbI_3$ using neutron powder diffraction on a **fully hydrogenous** sample. This has provided key information on light atom positions in this heavy metal compound and distinguished carbon and nitrogen, due to their contrasting scattering lengths. Investigation of hydrogenous samples also has the advantage of avoiding isotope effects, which can markedly change phase behaviour in ammonium and alkylammonium compounds while also providing a strong contrast between carbon, nitrogen, and hydrogen due to the latter's negative scattering length.

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CONTRIBUTED TALK

Understanding the link between lithium position and structural flexibility in defect perovskite lithium ion conductors

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As lithium ion batteries continue their rapid development towards power sources for electric vehicles, there is a growing need for batteries which can be rapidly recharged. Some of fastest lithium ion conductors are defect perovskites based off of the composition $Li_{0.34}La_{0.51}TiO_{2.94}$ (LLT), which exhibit bulk conductivities one order of magnitude less than currently used liquid electrolytes [1,2]. It is thought that one of the reasons for the high ionic conductivity in defect perovskites is the concerted motion of lithium hopping between vacant sites and dynamic octahedral rotations.

The connection between lithium position and dynamic octahedral rotations was explored in the cubic defect perovskite $Li_{0.18}Sr_{0.66}Ti_{0.5}Nb_{0.5}O_3$. Using a combination of *ex situ* and *in operando* X-ray and neutron diffraction methods the lithium position at different lithium compositions was tracked and linked to structural changes observed during electrochemical cycling. At room temperature the lithium ions are disordered within the as-synthesised material. After cooling to 4 K the lithium appears to order to a position within the *A*-site cavity which is off-set from the Ti/NbO$_6$ octahedral face. However, once more than one lithium ion is inserted per vacant site, the lithium migrates into the oxygen window between vacant sites. *In operando* diffraction studies revealed the rate of unit cell expansion increases by 54(1)% once the lithium occupancy per vacant site exceeds this composition (figure). As the rate of unit cell expansion is directly linked to the extent of dynamic octahedral rotations, the sudden jump in cell expansion was concluded to be due to a damping of the octahedral rotations. Using *in operando* neutron diffraction experiments, the damping of octahedral rotation was observed as a reversible reduction in oxygen atomic displacement parameters.

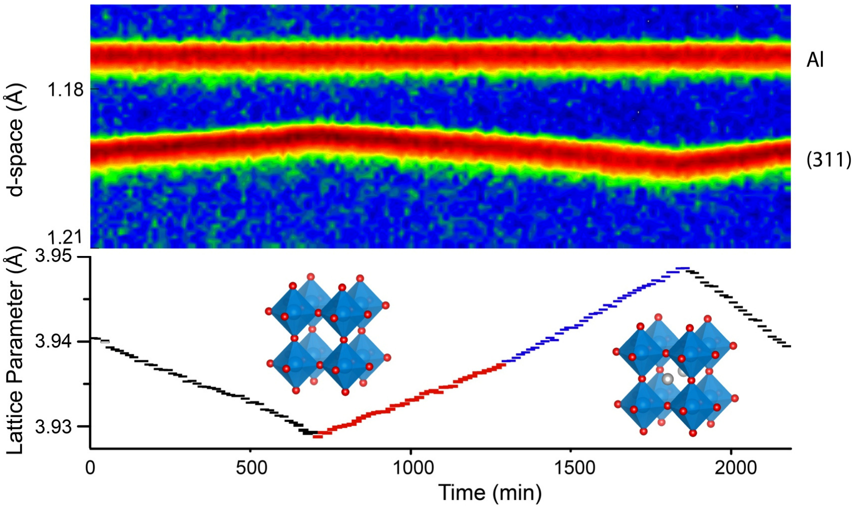

Fig. 1: *In operando* neutron diffraction data (top) and unit cell parameter (bottom) as a function of time.

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INVITED TALK

Inelastic Neutron Scattering for Magnetism

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Neutron scattering is the ideal technique to study magnetic excitations because it is well-matched to them on both time and length scales and is thus able provide measurements of the excitation spectrum as a function of energy and wavevector across the full Brillouin. Furthermore it directly and quantitatively measures the dynamical structure factor – a quantity easily calculated making comparison to theories relatively simple. Convention magnetic excitations such as spin-waves have been well-studied, they are routinely measured using neutron scattering and used to extract the exchange interactions of the system by comparison to spin-wave theory. More recently neutron scattering is being used to study quantum magnets where quantum fluctuations are strong and give rise unconventional ground states and exotic excitations different from spin-waves. Quantum fluctuations arise in low dimensional magnets where magnetic ions with low spin value are coupled by antiferromagnetic interactions into low-dimensional structures, they are also enhanced in frustrated magnets where the interactions compete with each other and/or with local anisotropies. It is possible to make model materials engineered to exhibit specific quantum features which can then be investigated using neutron scattering. This talk will start by giving examples of neutron scattering measurements from typical conventional and quantum magnets. Then a new frustrated magnet will be presented which consists of kagome layers of spin-1/2 ions formed from alternating ferromagnetic and antiferromagnetic triangles. The kagome layers are themselves coupled into bilayers by ferromagnetic interactions. Despite having predominantly ferromagnetic interactions and no measureable anisotropy, this system fails to develop long-range magnetic order down to the lowest temperatures. Inelastic neutron scattering reveals that the excitations are diffuse at all wavevectors, energies and temperatures, while muon spectroscopy shows slow relaxation suggesting a spin liquid ground state. Possible origins of this behavior will be discussed.

INVITED TALK

Static and Elastic Properties of Superconducting Vortex Lattices and Skyrmion Lattices in Chiral Magnets Studied by Time Resolved Neutron Scattering

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Both superconducting vortex (VL) **[1,2]** and skyrmion lattices (SKL) in chiral magnets **[3]** can be regarded as macroscopic lattices, formed by topological entities. Analogous to condensed matter, a large variety of phases is also observed for vortex-matter (VM) and Skyrmion matter, resembling the particle like character and reflecting the underlying physical properties. Moreover, both VL and SKL represent ideal model systems for questions of general importance as topological stability and decay.

The elastic matrix $\Phi_{\alpha\beta}$ of a VL describes the energy of a distorted VL. We report direct measurements of the VL tilt modulus c_{44} in ultra-pure bulk Niobium using time-resolved stroboscopic SANS **[2]**. With its low GL parameter κ situated at the border of type-I superconductivity, Niobium is ideally suited as a model system for studies of VM. By a periodic tilting of the magnetic field, we induce a relaxation process of the VL which shows increasing stiffness with increasing magnetic field and reduced damping with increasing temperature and agrees well with calculations performed within a diffusion model.

Skyrmion lines can be seen as magnetic whirls – sharing strong similarities with vortices of type II superconductors where the particle-like character of the Skyrmions is reflected in the integer winding number of their magnetization **[3]**. As for superconducting VM, SKL melting transitions, Skyrmion liquids and Skyrmion glass phases are expected to exist in the various B20 materials. Due to their topology, SKLs provide an excellent showcase for the investigation of topological phase conversion **[4]**. A further consequence of the special topological properties of Skyrmions is called emergent electrodynamics: While moving through the SKL, conduction electrons collect a Berry´s phase in real space which leads to a very efficient coupling of transport current and magnetic structure. This leads to considerable spin transfer torque effects at current densities as low as 10^6 A/m^2 **[5]**.

Similar to our study on VLs, we present recent time-resolved SANS experiments on the elasticity of the SKL in MnSi, exploiting the technique TISANE. Our study paves the way how to access directly VL and SKL melting as well as their current induced motion and dynamic properties in bulk samples. Finally, we present the planned implementation of TISANE at the new SANS-1 instrument at FRM II, Munich.

*Work in collaboration with: J. Kindervater, T. Adams, A. Chacon, F. Jonietz, A. Bauer, A. Neubauer, W. Wünzer, R. Georgii, M. Janoschek, S. Dunsiger, P. Böni, C. Pfleiderer, M. Garst, K. Everschor-Sitte, C. Schütte, J. Waizner, S. Buhrandt, A. Rosch, P.Milde, L. Eng, J. Seidel, H. Berger, E. M. Forgan, M. Laver, E. H. Brandt, U. Keiderling, A. Wiedenmann

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CONTRIBUTED TALK

Magnetocaloric Hydrides of NdGa and GdGa

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ReGa (Re= most rare-earth elements) form Zintl-phase compounds that crystallise in the CrB-type structure.[1,2] Many of these compounds are potential magneto-caloric materials.[3] We are investigating the structures and properties of the hydrides of NdGa and GdGa.

Fourier-difference maps from neutron diffraction data of $NdGaD_x$ indicates that hydrogen (deuterium) atoms are located in two types sites (see figure): a Nd_4 tetrahedral site (indicating a interstitial hydride) and a Nd_3Ga tetrahedral site (indicating a possible covalent bond).

Multiple results indicate that these compounds are hydrogenated in two steps, possibly corresponding to ReGaH and $ReGaH_2$. The nature of the Gd-H bond and the properties of the hydrides of the two Zintl phases are still being investigated using theoretical calculations and other techniques.

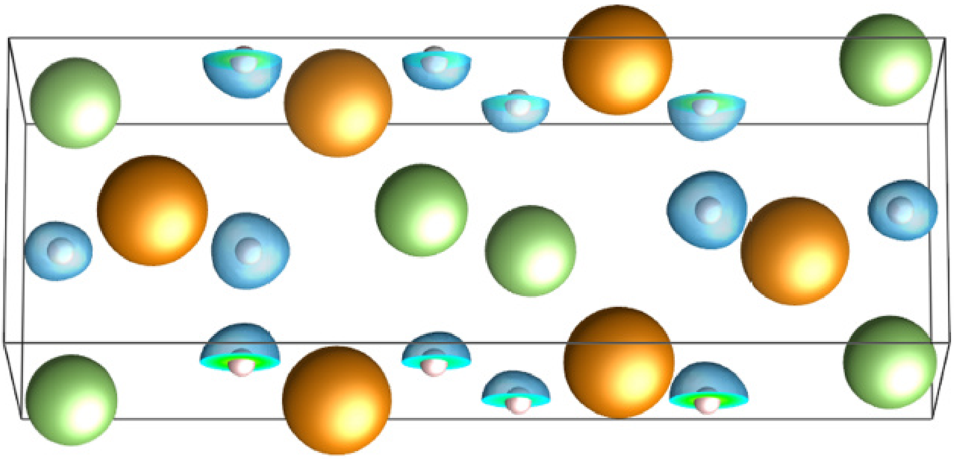

Figure 1: Approximate structure of $NdGaD_x$. Deuterium atoms (white) were located by Fourier difference map (neutron scattering densities are shown in blue). Nd atoms are shown as orange sphere and Ga atoms as green spheres.

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Swedish Neutron Scattering Society
Abstract submitted to the 2015 Annual Meeting of the Swedish Neutron Scattering Society SNSS-19
KTH Royal Institute of Technology, Stockholm, Sweden, 27-28 May, 2015

INVITED TALK

Longitudinal and Spherical Neutron Polarimetry: Applications and Examples

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The techniques of longitudinal [1] and spherical [2] polarized neutron scattering are presented with emphasis on applications. Examples of the usefulness of the method in inelastic neutron scattering are given like the separation of magnetic from nuclear scattering or the measurement of the polarisation of magnetic excitations. Finally spherical neutron polarimetry is explained. Application of the technique to complex magnetic structure determination is described and it is discussed how the population of the different types of magnetic domains can be determined. In particular it will be shown how an electric field can modify the population of the chiral domains in multiferroics [3, 4].

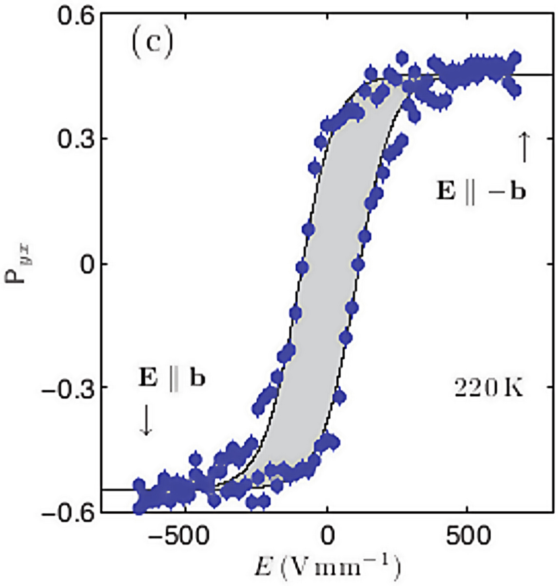

Fig. 1: Dependence of the population of chiral domains in CuO during an electric field sweep (from [4])

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INVITED TALK

Anisotropy-tuned magnetic order in pyrochlore iridates

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I will present our study of a family of materials, prone to magnetic frustration, and in which a strong spin-orbit coupling is inherent to the presence of magnetic Ir^{4+}. Attention of the condensed matter community was indeed recently attracted by the iridates. Due to the interplay between a strong spin-orbit coupling, crystalline electric field and moderate electronic interactions, the Ir^{4+} ions could be close to a new spin-orbitronic state with $J_{eff} = 1/2$, up to a local distortion of the Ir^{4+} environment.

In the pyrochlores $R_2Ir_2O_7$ (R = rare-earth element), the Ir^{4+} 5d electrons might then stabilize unprecedented electronic phases like Weyl semi-metal [1]. Both the rare-earth and the Ir atoms lie on interpenetrated pyrochlore lattices. We have studied $Er_2Ir_2O_7$ and $Tb_2Ir_2O_7$ by magnetization measurements and neutron diffraction. I will explain how the contrasting behaviors of the Er and Tb compounds result from the competition between the Ir molecular field and the different single-ion anisotropy of the rare-earths on which it is acting. Additionally, our study strongly supports the all-in/all-out iridium magnetic order and suggests new routes to study magnetic frustration in pyrochlores [2].

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CONTRIBUTED TALK

Order in Spin Ice

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The spin ice family of materials is one of the foremost realizations of a frustrated system displaying a macroscopic ground state degeneracy down to very low temperatures. With the strongest interactions frustrated, small perturbations may eventually cause non-trivial and exotic ordering, which would be hidden in an unfrustrated system. In this study we find that $Dy_2Ti_2O_7$, a member of the spin ice family, is a prime example of this phenomenology. We calculate the phase diagram determined by weak further neighbor interactions. Although no ordered state has been experimentally observed we find that the neutron scattering structure factor, already at $T = 1$ K, is a sensitive probe of the likely eventual order at $T \approx 0.1$K.

CONTRIBUTED TALK

The New Super ADAM – Swedish neutron reflectometer at ILL

Alexei Vorobiev, Anton Devishvili, Gunnar Palsson, Max Wolff, and Björgvin Hjörvarsson
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The Super ADAM reflectometer – a part of Collaborative Research Group at ILL – is modern competitive neutron research platform, which is destined primarily for Swedish use (70% of total beam time). Super ADAM has a large variety of incident beam optics including two monochromators, large experimental area and modular design, which allows unrivalled flexibility in use. Through its high resolution and polarization (up to 99.7%) Super ADAM excels in reflectivity measurements on magnetic thin films and multilayers. The high-flux option (relaxed resolution) for soft matter studies is currently under commissioning. A major upgrade of the reflectometer was started in October 2013 in connection to the ILL H5 program, in which the whole guide system of Super ADAM was renewed and optimized. All optical elements in the casemate starting from the monochromator were upgraded. Furthermore, the instrument was moved to a new location, closer to the reactor. This yielded significant increase in flux but also allowing for a large experimental area as well as for significant improvements. Upgraded Super ADAM was the first instrument accessible to external users in the renovated ILL22 guide hall (the 19th of November 2014). The feedback from users is extremely positive which explicitly underlines the excellent performance of the new instrument. Here we describe its performance and give examples of recent results, highlighting the possibilities provided for the users of the instrument.

Figure 1: The New Super ADAM reflectometer

[1] https://www.ill.eu/?id=13616
[2] http://material.fysik.uu.se/SuperAdam/SuperAdam.html

POSTER PRESENTATION

Atomic and magnetic structure and magnetocaloric properties of $AlFe_2B_2$

Johan Cedervall[1], Mikael Andersson[2], Tapati Sarkar[2], Erna Delczeg[3], Lennart Häggström[3], Tore Eriksson[3], Per Nordblad[2], Martin Sahlberg[1]
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The use of magnetic cooling in refrigerators as a replacement for conventional gas cooling devices could lead to lower power consumption and less hazardous materials in the life cycle of the refrigerator. Recently, a new class of materials based on layered AlM2B2 (M = Fe, Mn, Cr) was proposed as a candidate compound for magnetocaloric applications [1].

Here we report a detailed study on the synthesis and magnetic properties of AlFe2B2. Single phase samples were prepared using high-temperature synthesis methods gaining high quality samples. Magnetic and crystallographic properties were studied with powder diffraction, Mössbauer spectroscopy and magnetic measurements. The study shows that AlFe2B2 is a ferromagnetic compound with a magnetic transition at Tc=285K. The saturation magnetization at 10K is 60 Am2kg-1 and ΔSm(5T)=-4.5JK-1kg-1 around room temperature.

Mössbauer spectroscopy confirms a ferromagnetic substance and shows good agreement with the magnetic measurements. Theoretical calculations were carried out using the spin polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) method. Applying the scalar relativistic full potential (fully relativistic) approach a magnetic moment of 2.67 (2.36) µB/f.u. was found. The Curie temperature was estimated to 250 K using a Monte Carlo method implemented in the UppASD code.

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Swedish Neutron Scattering Society
Abstract submitted to the 2015 Annual Meeting of the Swedish Neutron Scattering Society SNSS-19
KTH Royal Institute of Technology, Stockholm, Sweden, 27-28 May, 2015

POSTER PRESENTATION

Local coordination and vibrational properties of protons in proton conducting perovskite oxides.

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One of the major challenges in material science is, nowadays, the development of cleaner and more sustainable source of energy. The hydrogen fuel cell represents, in this respect, one of the most promising, yet challenging, clean energy technologies. In particular, intermediate temperature fuel cells technology (~200-500 °C) is attracting considerable interest due to their potential use as both stationary and mobile energy production devices [1]. The performance of these devises depends crucially on the properties of their components, as for example the proton conductivity of the electrolyte material. Targeted conductivities exceed 10^{-2} Scm^{-1} and in this respect acceptor doped perovskite type oxides, such as In doped $BaZrO_3$, have emerged as most promising [2]. However, the conductivity of even the best electrolytes available today remains to be too low for operation in the intermediate temperature range [2]. The further development of fuel cell technology depends critically on the development of new materials with higher conductivity. The understanding of the behavior of protons in the most promising materials is, therefore, a crucial requirement in order to achieve this goal.

In order to obtain details about the vibrational spectrum of protons and proton sites in acceptor doped perovskite oxides, we have investigated the local coordination and vibrational properties of protons in the proton conducting perovskite $BaZr_{0.5}In_{0.5}O_3H_{0.5}$, by means of inelastic neutron scattering (INS) and infrared (IR) spectroscopy. We observed, in agreement with previous works on similar systems [3,4], a broad range of O-H stretch vibrations, which can be related to symmetrical and asymmetrical local proton environments, respectively [3]. An example of these local proton environments is given in Figure1. On the basis of the study of the INS spectrum and its Q-dependence, we assigned to fundamental modes or combination of O-H vibrations the observed bands in the vibrational spectrum of $BaZr_{0.5}In_{0.5}O_3H_{0.5}$. Some of these bands appear to be a common feature in several acceptor doped perovskite oxides and their nature has been subject of debate [3,4]. In particular, a key result of our study is the identification of fundamental O-H stretching vibrations at really low energy (2000-2400 cm^{-1}). The presence of such a low-energy modes is an indication of the presence of proton sites characterized by very strong hydrogen bonding between the proton and neighboring oxygen [3]. According to previous studies based on first-principles calculations [3] highly hydrogen-bonded configurations arise in correspondence to "extreme" local proton environments, such as in the vicinity of several protons and/or oxygen vacancies.

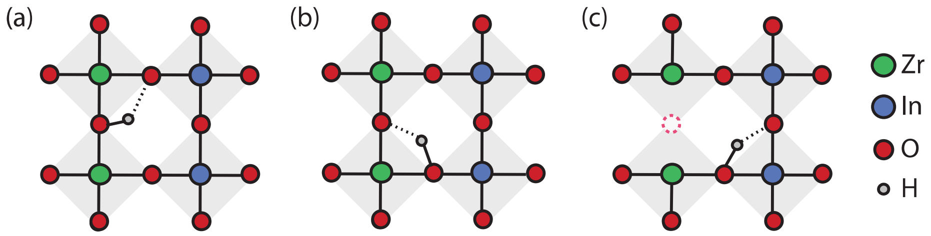

Figure 1: Schematic representation of symmetrical **(a)** asymmetrical **(b,c)** proton environments .

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Swedish Neutron Scattering Society
Abstract submitted to the 2015 Annual Meeting of the Swedish Neutron Scattering Society SNSS-19
KTH Royal Institute of Technology, Stockholm, Sweden, 27-28 May, 2015

POSTER PRESENTATION

Neutrons for Green & Safe Energy Materials

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While Li-ion batteries are considered the main candidate for mobile applications, compounds based on lithium's heavier cousin, sodium (Na) have also started to receive a lot of attention lately. One reason is that our Li-reserves are limited and to realize future electric vehicles we might have to reconsider the Li-ion technology. Na has indeed many advantages over Li *e.g.* Na is one of the most abundant elements in nature (earth's crust as well as in normal seawater of our great oceans), which makes it about 5 times cheaper than Li. Further, Na-ion batteries are also much less toxic and easier to recycle. In many ways the Na_xCoO_2 compound is a Na-analog of the most common Li-ion battery electrode material Li_xCoO_2. Hence, understanding Na-ion diffusion mechanisms in Na_xCoO_2 would seem a logical first step. Consequently, we have conducted extensive studies of this compound using muon spin rotation/relaxation (μ^+SR) **[1,2]**, neutron powder diffraction (NPD) **[3]** and quasi-elastic neutron scattering (QENS) **[4]** as a function of temperature, chemical composition and pressure/strain. Our results show unique details of the diffusion processes in these compounds. One example is how the Na-ion diffusion paths evolve from quasi-1D to fully 2D as a function of temperature and that this evolution is directly linked to subtle structural changes that unlock the diffusion channels. Further, we also reveal an intriguing new possibility to enhance/tune the ion diffusion rate by pressure/strain on an atomic level **[5]**. This allows us to reconsider several previously discarded material candidates for future energy applications. It also clearly shows the power of performing energy related materials science using large-scale experimental facilities. The increased understanding of ion diffusion mechanisms allows us to contemplate and actively consider future possibilities for solid state engineering of energy related materials with improved functional properties.

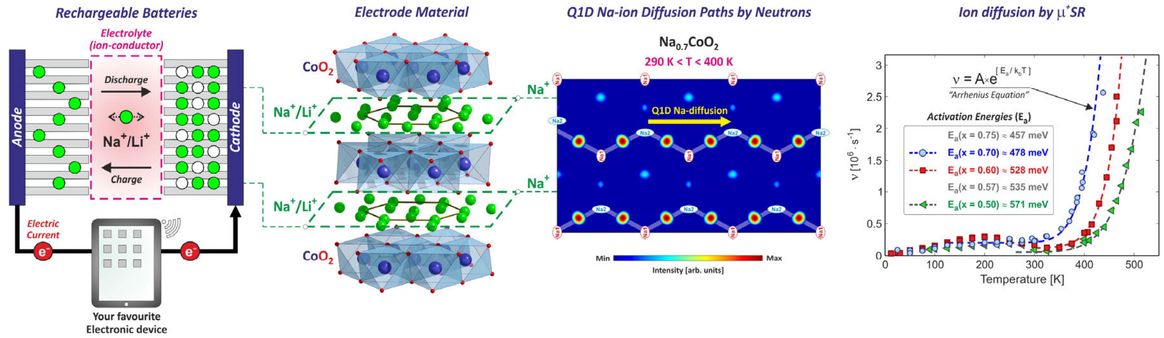

FIG. 1: **(a)** Working principle for a rechargeable battery **(b)** Layered electrode material **(c)** Novel Q1D diffusion channels in Na_xCoO_2 **(d)** Activation energies (E_a) for Na-ion diffusion extracted from our μ^+SR experiments.

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POSTER PRESENTATION

Random-Singlet State in Antiferromagnetic Heisenberg Spin Chain Compound $BaCu_2(Si_{0.5}Ge_{0.5})_2O_7$ Studied by Inelastic Neutron Scattering

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Several compounds are known as quasi-one-dimensional (Q1D) AF Heisenberg systems with random bond strengths. However, the title compound, $BaCu_2(Si_{0.5}Ge_{0.5})_2O_7$ has been celebrated as an almost ideal realization of the random AF Heisenberg spin (S=½) chain for more than 10 years [1]. Despite several attempts, there is up until now no direct spectroscopical evidence of the famous random–singlet state (RSS) in this material. Earlier inelastic neutron scattering (INS) results instead reflected typical AF Heisenberg spin chain behavior with average interactions $\langle J \rangle = 37$ meV [2]. Recent bulk magnetization data was compared to results of extensive Quantum Monte Carlo (QMC) simulations [3], which showed that the behavior of this material agrees with the theoretical model for a RSS at all temperatures $T \geq 2$ K. Further, QMC simulations also offer an explanation to why the RSS was not detected by previous neutron studies. At low temperatures, the deviation from the disorder–free Heisenberg AF chain (i.e. the linear behavior) only occurs for low magnetic fields; below a few Tesla. Such fields should correspond to neutron energy transfers of only fractions of a single meV. For example, at 2 K, the RSS should appear below $H_c \approx 6$ T, which is equivalent to $\omega \approx 0.3$ meV. Hence, the dominant part of the effective interactions binding the spins is less than 1% of the nearest–neighbor exchange integral, an energy range ignored by previous studies [2].

In this study we have performed an inelastic INS study of $BaCu_2(Si_{0.5}Ge_{0.5})_2O_7$ using the backscattering spectrometer OSIRIS at ISIS/UK. This setup gives a 25 μeV resolution, which allowed us to study magnetic excitations down to at least $\omega \approx 0.1$ meV for a temperature range $T = 1.7 – 25$ K. In similarity to the previous high-energy INS investigations, also our high-resolution data clearly display vertical streaks of scattering at the 1D AF zone centers, $l = \pm 1$, for all measured temperatures. To investigate the energy and temperature scaling of the spin correlations, the dynamic structure factor $S(q,\omega)$ was extracted from fits to a series of constant-energy cuts for different temperatures. The result was compared to an approximate scaling function for a Luttinger spin liquid, showing a clear deviation for low excitation energies and elevated temperatures, well in line with our simulations. To the best of our knowledge, this is the first clear spectroscopic evidence of the RSS [4]. Further theoretical work is now needed to parameterize and understand this intriguing phase.

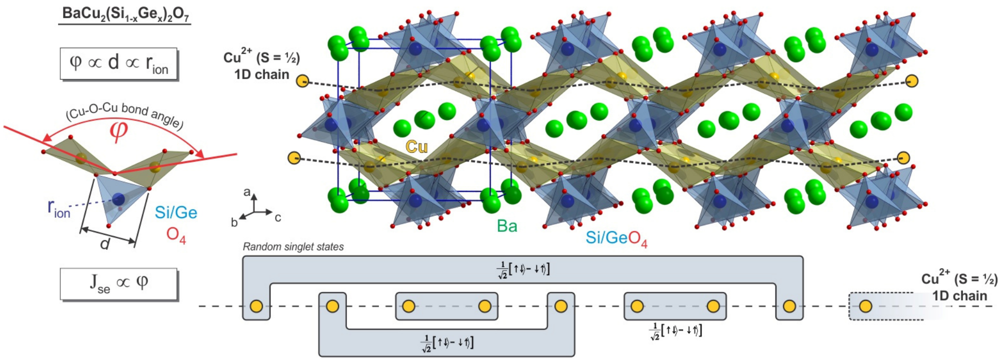

FIG. 1: Crystal-structure of $BaCu_2(Si_{1-x}Ge_x)_2O_7$ showing the 1D Cu^{2+}-chains and a schematic view of an RSS.

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POSTER PRESENTATION

Introducing High Entropy Alloys

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The development of new materials with improved properties is an important societal challenge. Among the metals, the most common way to improve the properties (e.g., mechanical, electrical, magnetic etc.) has been through alloying with a second or third element. **[1]** Alloying often works well to a certain limit (e.g., until the classical Hume-Rothery rules are broken and solid solution is no longer maintained), and has been successfully used since the early use of metals. However, with further technologically advanced applications arising, there is also a need for novel materials that can deliver new and improved properties.

High entropy alloys (HEAs), or equiatomic multi-component alloys have recently been reported as new types of complex alloys with improved properties. Theoretically, HEAs should be able to maintain solid solution for higher concentrations of alloying elements through the increased entropic contribution (e.g., >5 different elements at concentrations ~5-35 at%). **[1]** Due to the immense number of combinations and concentrations for HEAs, a great challenge currently lies in achieving a more accurate way of predicting solid solutions for new compositions (apart from combining binary and ternary phase diagrams). Additionally, once an accurate prediction route is established, it will be possible to design entirely new alloys with desired electronic and microstructural properties for advanced electronic, mechanical and magnetic applications.

Due to the relatively new area of research, few neutron scattering studies **[2]** have been made on HEAs, and will therefore present new and interesting opportunities for the neutron scattering society.

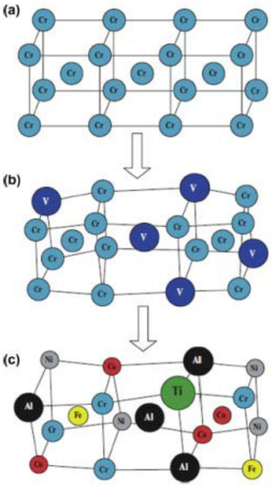

Figure 1: Schematic illustration of **(a)** metal, **(b)** binary alloy and **(c)** HEA [1]

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POSTER PRESENTATION

GISANS from solid-liquid boundaries

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Neutrons are characterized by a weak interaction, resulting in a high penetration power, for many engineering materials. This property is combined with a relatively large scattering power for light elements. These facts make neutrons an ideal probe for the study of buried liquid interfaces. In particular, the finite angle of total external reflection at the interfaces between many solids and deuterated liquid opens unique possibilities for the study of the near surface structure of fluids in contact with a solid wall.

In this presentation neutron small angle scattering applied under grazing incidence beam geometry (for the scattering geometry see **Figure 1**) will be introduced and the peculiarities will be discussed. An overview over recent results of self assembled polymers, colloids as well as magnetic particles will be given.

The scientific challenges and opportunities will be discussed on the example of a model system of a micellar aqueous three block polymer solution in contact to silicon wafers with distinct terminations **[2]**. Emphasis will be on exploiting the broad spectrum of incident wavelength at time of flight instruments for depth **[3]** as well as time **[4]** resolved experiments.

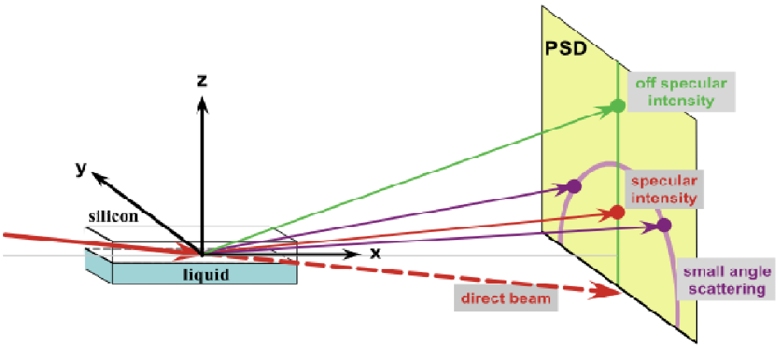

Fig. 1: Scattering geometry for gracing incidence scattering experiments from the solid-liquid boundary **[1]**.

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Swedish Neutron Scattering Society

Annual Meeting of the Swedish Neutron Scattering Society SNSS-19
KTH Royal Institute of Technology, Stockholm, Sweden, 27-28 May, 2015

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