# 10th MaMaSELF Status Meeting 2018


# Report of Contributions

https://indico.frm2.tum.de/e/112

Contribution ID: **1** Type: **Main Lecture**

# Swiss Neutron Scattering at SINQ and at ESS

will arrive later.

**Primary author:** SCHEFER, Jürg (Paul Scherrer Institut)

Contribution ID: **2** Type: **Student contribution**

# Lead free piezoelectric thin films and powders

Piezoelectric materials are nowadays intensively used in numerous fields of modern society (sensors, energy harvesters from vibrations, etc.). The research work focuses on tetragonal tungsten bronze (TTB) phases that have received little attention until now compared to perovskite phases, although TTB structures have diverse properties (e.g. nonlinear optic, pyroelectric, and piezoelectric) as a result of their compositional flexibility. The project involves the synthesis of powders by various methods like solid state reaction, flux method, seeding etc. and the synthesis of thin films and nanorods films by pulsed laser deposition (PLD) with an emphasis on compositional, microstructural and orientation control. It also includes the study of the impact of parameters (targets composition, laser energy and frequency, substrates, ⋯), on morphology and growth of thin films and nanorods. The samples are characterized by X-ray diffraction, scanning electron microscopy, energy dispersive X-ray spectroscopy.

**Primary authors:** Ms KHANCHANDANI, Heena (MaMaSELF Masters student); Dr DEMANGE, Valerie (CNRS Researcher)

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **3** Type: **Student contribution**

# Magnetic Nanoparticles in Polymer Matrix

Nanostructured films composed of a polymer matrix and functional magnetic nanoparticles are promising materials due to their interesting physical properties in the areas of information storage and magnetic sensors. Hybrid films of the diblock copolymer polystyrene-block-poly (ethylene oxide) (PS-*b*-PEO) and surface-functionalized magnetic nanoparticles ($Fe_3O_4$ with hydrophobic coating) are prepared via spin coating. Both real-space and reciprocal-space techniques are employed to characterize the obtained hybrid films. The micro- and nanostructures of the magnetic films as a function of the nanoparticle concentration are probed using optical microscopy, scanning electron microscopy, atomic force microscopy, and grazing incidence small-angle X-ray scattering (GISAXS). The observed structures are explained in the framework of microphase separation and confinement. The electronic and magnetic structures of the hybrid films are studied through the technique of high energy resolution fluorescence detected (HERFD-XANES).

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**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **4** Type: **Student contribution**

# Printed fullerene-free thin films for photovoltaic applications

In the past decades, organic photovoltaics (OPVs) have attracted considerable attention owing to their remarkable characteristics, such as light weight, flexibility, easy processability, potential low-cost fabrication and high throughput. Fabrication techniques include spin-coating, doctor-blading, spray casting and roll-to-roll printing. Among these, the scalability of printing processes makes them attractive for industrial fabrication methods. Solution processed bulk heterojunction (BHJ) solar cells have been the most widely used method to build OPVs. In this type of solar cell, donor and acceptor are mixed and deposited together in one step to build up the active layer, which make them good candidates for printing techniques. In an ideal BHJ solar cell, the intermixing of donor and acceptor is a comb-like structure offering a high interfacial area. This is desired as the exciton diffusion length is about 10 nm. Hence, a donor-acceptor interface must be reached to separate the exciton before it recombines and so extract the charges, generating external current. Nevertheless, the morphology of the active layer is far from ideal and the efficiency lower than the theoretically possible, due to enlarged diffusion lengths which result in higher recombination rates. Fullerene materials have been so far the main choice of acceptor material combined with polymeric semiconductors as donors. In this work the fullerene-free blend poly(benzodithiophene-benzotriazole) (PBDBT):3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone)-5,5,11,11-tetrakis(4-hexylphenyl)-dithienol[2,3-d:2',3'-d]-s-indaceno[1,2-b:5,6-b']dithiophene (ITIC) is investigated. This mixture has shown outstanding power conversion efficiencies (PCE) in spin-coated devices [1], and hence it is promising a material system for printing coating techniques. The work presented consist in the design and fabrication of a printing setup capable to deposit the active layer for photovoltaic applications following the design introduced by Pröller et al [2]. The design of this printer can simulate the conditions that might be encountered during industrial processing. Thus, the printer is capable to print under various atmospheric conditions and offers the possibility to perform in situ studies on the active layer´s inner morphology using advanced scattering techniques, like grazing incidence small angle X-ray scattering (GISAXS) and grazing incidence wide angle X-ray scattering (GIWAXS). Due to the fact that the final morphology depends on the film deposition´s conditions the parameters have to be studied. For this goal, two different strategies are carried out: evaluate the printing conditions itself (substrate temperature, solution flow rate and coating speed) and study the material properties (such as weight ratio of the polymers and concentration). The differences on the active's layer thickness and absorption spectra are then used to obtain the optimal parameters for printing this mixture. The information can be correlated with the usually obtained photoelectrical properties, giving full characteristics of the printed solar cells. Hence, understanding the formation process of the active layer and its morphology in comparison to data obtained using lab-scale deposition techniques is of high interest.

References:

[1] Wenchao Zhao et al., Adv. Mater. 28 (2016): 4734-4739
[2] Stephan Pröller et al., Adv. Energy Mater. 6 (2016):1501580

**Primary author:** DELGADO ANDRÉS, Rodrigo

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **5** Type: **Student contribution**

# Quantitative Phase Analysis of Industrial Vanadyl Phosphate Catalyst

Vanadyl phosphate catalyst has been used industrially for the last few decades for selective oxidation of n-butane to maleic anhydride. However, owing to containing different phases within the catalyst system, the exact nature of the relation between the phases and catalytic properties are still under dispute. The main crystalline phase is supposed to be V4+ of (VO)2 P2 O7 (VPP) together with amorphous and crystalline minor phases of V5+ or V4+ oxidation state. The initial test samples were collected from different furnace position during activation stage followed by test conducted on bench scale unit under reaction condition. XRD has been conducted on Bragg-Brentano mode and quantitative phase analysis has been carried out on Reitveld refinement software. The refinement result reveals the presence of a phase (V4+, VO(PO3)2) which is commonly not cited in the literature due to a different preparation route unlike the industrial synthesis process. Furthermore, from the refinement result it is found that there is a positive correlation between the catalytic activity and the amount of crystalline VPP phase present in the bulk. In order to get a full picture of the activity in relation to bulk properties other characterisation techniques need to be employed together with detailed knowledge of the surface properties.

**Primary author:** Ms SHARNA, Sharmin

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **6** Type: **Student contribution**

# Analysis and Reconstruction of X-ray and Neutron diffraction computed tomography data

The X-ray diffraction computed tomography (XRD-CT) –an experimental tool combining the powder diffraction in transmission mode with computed tomography, that can deliver spatially resolved structural information from the interior of the chemically non-homogeneous objects. Originally demonstrated as a laboratory technique, this method has been at most using high-energy synchrotron X-ray radiation. The use of high-energy synchrotron beams is needed for studies of millimeter-sized samples, but it is often limited by the contrast (elemental sensitivity) of X-rays and by the potentially-introduced radioactive damage.

The aim of this work is to adopt the technique of neutron diffraction computed tomography (ND-CT) similar to the well-established XRD-CT. Thermal neutrons with energies in meV range are supposed to have no such disadvantages as X-rays have, in particular, they are proven to be sensitive to isotope sample composition providing an enhanced contrast. With simple "phantom" sample, object displaying contrast sufficient for the method validation, it is shown that diffraction CT technique is able to provide one with spatially resolved physico-chemical information.

Two kinds of diffraction tomography experiment were performed with the developed "phantom" sample: one based on synchrotron radiation and for the first time ever proposed ND-CT experiment at the instrument STRESS-SPEC of FRM II. The sets of collected raw diffractograms were analyzed after integration procedure applying necessary corrections and reconstructed with filtered back-projection algorithm. The obtained tomograms clearly reveal components of the "phantom" sample, which demonstrates the feasibility of imaging approach in the reconstruction of not only X-ray but also neutron diffraction data.

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**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **7** Type: **Student contribution**

# Nanoscale Exsolution and Interface Structures in High-Temperature Shape Memory Alloys

Ti-Ta alloys possess an attractive high temperature shape memory properties with potential to be utilized for aerospace and MEMS applications. However, their applications are limited by the formation of complex omega phase during thermo-mechanical cycling, which hampers the martensitic transformation and shape memory effect.To overcome this problem, exsolution of omega phase through rapid heating has been suggested to be a solution. In this work, we investigate the formation and exsolution of omega phase using Transmission Electron Microscopy(TEM) supported with Synchrotron X-ray Powder Diffraction. Selected Area Diffraction(SAD) was performed to acquire structural information on matrix, martensites, and omega phase. Chemical analysis with ultimate spatial resolution was studied by using Atom Probe Tomography(APT).

**Primary author:** Mr LIAO, Kun-Yen

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **8** Type: **Student contribution**

# Structural and electronic correlations in $PSNO_x$

Structural and electronic ordering in co-doped nickelates compounds, such as $Pr_{2-x}Sr_xNiO_{4+\backslash delta}$, leads to a complex phase diagram and interesting physical properties. Interstitial oxygen ordering has been shown to be the fundamental for the high oxygen ion mobility, making of this material a model for SOFCs electrodes. On top of that, charge and spin ordering, in the form of stripes and checker-boards, yields to the exotic physics that is shared with high-$T_c$ superconductors. One of the frontiers that still need more investigation in these type of materials is the possible correlation between oxygen and electronic ordering, together with their related dynamics, which are taken into consideration in this study. High-quality single crystals, with different oxygen and Sr-content, were grown and preliminary characterized via STOE at the ICGM of Montpellier and successively measured through single crystal diffraction at ESRF (ID28 side-station) and neutron scattering at FRM II (PUMA), to have an insight on this possible structural-electronic correlation. Preliminary findings from this Master thesis project will be presented and commented, showing the progress achieved up to the present moment.

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**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **9** Type: **Student contribution**

# Abstract:creation and quantum optical characterization of colour centres in artificial diamond

In quantum technologies perspective, the long term-goal is a quantum web where quantum computers, simulators and sensors are interconnected via quantum network distributing information and quantum resources. For what concerns quantum cryptography in quantum communication, a withstanding issue is represented by the need of efficient single photon sources characterized by high stability, long durability in time and being on demand. Single photon sources are not currently completed developed and different physical system act as a single photon emitter. Diamond is one of the preferred choices for its crystalline structure, which can host different impurities, its wide energy range, which cover the visible spectrum, and the low phonons density at room temperature. Moreover, ions irradiation was developed in these years as an efficient technique to defects of different species in the material and thus optimizing their quantum optical properties.
In collaboration with the ion-micro beam facility of the INFN National Laboratories of Legnaro, different implantation campaign would be planned at different energies species and fluencies to explore the ideal condition for the creation of colour centres characterized by desirable emission properties. Subsequently, the colours centres will be characterized by confocal microscopy, by means of which it is possible to study the photoluminescent emission at the single photon level. In this configuration, the centres will be assessed in their quantum optical properties via Hanbury-Brown and Twiss interferometry.
Different colour centres are taken under analyses, starting from the easiest nitrogen-centres vacancies to more complex tin and nanodiamonds. In order to characterize single photon sources, different measurements are taken of g^((2)) and spectra to recognise the particular element that is being studied. Moreover, an analysis of data is performed to extrapolate the time life and bunching time of the metastable state. Eventually an analysis in power are carried out in order to study how the parameters of the colour centre would change according to different power with which it is excited.

**Primary author:** SARDI, Fiammetta

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **10** Type: **Student contribution**

# Modulated synthesis of MOF MIL-88A: a preliminary study for its biomedical application

Metal organic frameworks (MOFs) are porous materials possessing a modular structure of inorganic secondary building units (metal ions or clusters) connected by organic linkers. MOFs have a wide range of applications, thanks to their large surface area, easily tunable composition and pore size variability: catalysis, gas separation, optically active materials, biomedicine [1]. One of the potential uses of MOFs is as nanoscale carriers for drug delivery and imaging [2]. A promising family of MOFs in this field is MIL-88, an iron carboxylate framework, whose pore size and swelling characteristics [3] depend on the carboxylate linker used and can be adapted to host the desired bioactive molecule.

We focused on the synthesis and characterization of MIL-88A, an iron fumarate framework obtained through non-toxic, microwave –assisted hydrothermal synthesis, which ensures the achievement of particles with sizes in the range of 100 nm. Small acid molecules are reported to be competitors of the fumaric acid linker in the formation of MIL-88A [4], so they can be used as inhibitors to control the nanoparticle growth. In order to master the modulation of the structural characteristics of MIL-88A we carried out a series of syntheses involving different acids in gradual concentrations. In fact, formic acid in increasing concentration leads to a decrease in DLS diameter. Also acetic acid and benzoic acid seem to have the same effect, but the obtained particles are very prone to agglomeration. On all the samples XRD and FTIR were performed to characterize the crystalline phase and the organic linkers. Some selected samples are going to be analysed with TEM.

Future steps of the research include the use of bioactive molecules as modulators, the characterization of the obtained structures and a study in vitro of their applicability as targeted delivery drug carriers, in collaboration with the biology department of the Southern Federal University.

References

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[2] P. Horcajada, T. Chalati, C. Serre et al. (2009). Porous metal–organic-framework nanoscale carriers as a potential platform for drug delivery and imaging. Natural Materials, 9, 172-178.

[3] G. Férey, C. Serre (2009). Large breathing effects in three-dimensional porous hybrid matter: facts, analyses, rules and consequences. Chem. Soc. Rev., 38, 1380-1399.

[4] T. Chalati, P.Horcajada, R. Gref et al. (2011). Optimization of the synthesis of MOF nanoparticles made of flexible porous iron fumarate MIL-88A. J. Mater. Chem, 21, 2220-2227.

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**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **11** Type: **Student contribution**

# Spray cast organic solar cells

Besides having a research focus on preparation methods, deposition techniques play an important role in producing solar cells as well. In particular, next generation solar cells are typically based on a wet chemical approach and therefore enable completely new pathways of device manufacturing. Compared to laboratory-based routines such as spin coating, large-scale coating processes such as spray coating and printing are of particular interest due to their potential for having an adaptability to industrial processes. In particular, spray coating is a very cost-effective method that provides the possibility for a rapid and large-scale film deposition on complex-shaped surfaces. However, spray coating as a rapid solution-based preparation route usually features complex evolutions of the film structure and morphology. For a better understanding of the complex behavior of the involved kinetic processes, in situ morphology investigations are highly desirable but as well imply a great experimental challenge. The necessary characterization requires a continuous detection of the inner film morphology without interrupting the spray coating process or destroying the deposited films. Moreover, the in situ measurements need to be compatible with the experimental environment of spray coating under ambient conditions. Grazing-incidence wide-angle x-ray scattering (GIWAXS) measurements perfectly match the requirements of an in situ morphology characterization. This advanced scattering technique allows probing the inner film morphology in the nano- and mesoscale while sampling over macroscopic sample areas, which yields very high experimental statistics. In this project tailored polymer nanostructures based on spray coating were prepared. The GIWAXS experiment enabled to follow the structure evolution and to probe the morphology with a high statistical relevance.Moreover, active layers of different mixtures of conjugated polymers forming organic bulk hetero-junctions were prepared to investigate the influence of different mixtures on the film‘s morphology and photophysical properties.

**Primary authors:** Ms CHAKRABORTY, Debamitra (Mamaself Master Student); Mr GROTT, Sebastian (MSc); Prof. MÜLLER-BUSCHBAUM, Peter (Professor)

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **12** Type: **Student contribution**

# Synthesis, structure, valence state and physical properties in Fe-containing perovskite matrix for energy materials

Due to the demands on energy, the search and improvement of energy materials have become one of the most popular topics around the world. Among them, the development of oxygen ion conductor is receiving increasing attention due to its importance in solid oxide fuel cells (SOFCs), batteries, electrodes, sensors, and catalysis. SOFCs, for example, has several advantages over other types of fuel cells, including high power generation efficiency and high impurities resistance in the fuel. However, the operation of SOFC requires high temperature, which often leads to compound degradation and indirectly limits the choice of acceptable materials [1].
In this regard, brownmillerite type structure has been reported as a promising candidate material showing oxygen mobility at ambient temperature. A system such as Sr2ScGaO5 has been fully investigated through structural analysis, lattice dynamics etc[2]., in order to understand the fundamentals of oxygen mobility mechanism.
Inspired by the previous work, this project aims to replace Ga with Fe and explores the effect of iron valence state which no one has reported. Our major interest is driven by the ability of iron to adopt various oxidation states Fe2+(FeII), Fe3+(FeIII), Fe4+(FeIV), with fixed, closed-shell Sc3+substitution. The doping concentration remains constant as x = 0.5 in SrScxFe1-xO3-δ (SFSO); while the oxygen non-stoichiometry is between 2.5≤ 3-δ ≤2.75 by topotactic redox process. The valence state is expected to compensate for oxygen and changes the structure, electrical properties as well as magnetic properties. Preliminary analysis by X-ray diffraction (XRD), Thermogravimetry Analysis (TGA) with Mass Spectroscopy (MS), and Superconducting Quantum Interference Device (SQUID) is performed at the Institut Charles Gerhardt Montpellier (ICGM). Oxygen content and local structure are obtained by high-resolution two-axis neutron powder diffractometer (D2B) at the Institut Laue Langevin (ILL, Grenoble, France). High-resolution X-ray spectroscopy at the ESRF is also performed to obtain the local electronic structure because of its sensitivity of iron valence states.

**Primary authors:** Ms YANG, Chia-Jung; Prof. CERETTI, Monica; Prof. PAULUS, Werner; Dr GLATZEL, Jan Pieter

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **13** Type: **Student contribution**

# Gold nanoparticles embedded into porous matrices: structural and electronic properties

Noble metal nanoparticles (NPs) play an important role in modern catalysis. Embedded into metal organic frameworks MOFs, they are part of the new branch of hybrid materials having been studied with the scope of applications in the fields of heterogeneous catalysis and hydrogen storage. The scope here is to achieve a highly loaded porous material with cavity-size matching NPs and well defined spatial and homogeneous size dispersion. The preparation methods include solvothermal and microwave synthesis of Metal-Organic framework [1]. The focus is on zeolitic imidazole frameworks ZIFs, which have a structure similar to that of zeolites, specifically ZIF-8 embedded with gold NPs. The latter obtained via solvothermal synthesis of gold NPs using a modified Turkevich method[2]. The hybrid material is obtained via core shell synthesis. The materials obtained have been characterized with UV-Vis and IR spectroscopies .
The work presented here employs a number of different synthesis method in order to find the most efficient, green and with the maximum loading of the pores in gold. Furthermore, we aim to characterize the material at the core shell boundary, to understand the interactions binding the ZIF with the NP. As well as the potential applications of the obtained hybrid material in the field of catalysis.

References

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[3] L.Chen,Y.Peng,H.Wang, Z.Gua ,C.Duan (2014) Synthesis of Au@ZIF-8 single- or multi-core–shell structures for photocatalysisChem. Commun.50, 8651,2014.

**Primary authors:** LELOUCHE, sorraya; Prof. BUDNYK, Andriy (Smart Materials)

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **14** Type: **Student contribution**

# Self-assembly of polymeric bottle brushes in aqueous solutions

Molecular brushes, characteristic for their unique architecture, consist of a polymeric backbone with densely grafted side chains. When a molecular brush contains both hydrophobic and hydrophilic segments, its special self-assembly behavior in water makes it a potential drug carrier in the human body. Poly(2-oxazoline)-based molecular brushes are especially well-suited to this purpose due to their high biocompatibility.
In the present work, morphological study on poly(2-isopropenyl-2-oxazoline)-g-poly(2-ethyl-2-oxazoline) dilute aqueous solution has been accomplished with respect to particle size and inner structure dependence on temperature ranging from 25℃ to 50℃. With its hydrophobic backbone and hydrophilic side chains, experimental results from dynamic light scattering show two different sizes for the molecular brush, approximately 5 nm and ranging from 120 nm to 220 nm. As a further step, small-angle neutron scattering experiment was performed, leading to a disk-like brush, partially packed, with an effective radius of approximately 14 nm.

**Primary author:** SHEHU, Kaltrina

Contribution ID: **15** Type: **Student contribution**

# Investigation of high-temperature multiferroic perovskites

The increasing miniaturazation of electronic components is constantly pushing the material scientists and ingeneers to seek for new materials which could accomplish more than one task at a time. Multiferroics, and their versatility, are of great interest for the new generation of data storage devices. The O-defficient double perovskite YBaCuFeO5 hosting magnetoelectric properties is a serious candidate to be part of our future numeric environment. Although its electric polarization seems to be rather weak, it displays magnetic spirals that happened to be relatively easy to tune by modifying the synthesis conditions. This talk will give a exhaustive description of the studied material and introduce the current investigations aiming at a further control of the magnetism in YBaCuFeO5.

**Primary author:** Mr PORÉE, Victor (Paul Scherrer Institut)

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **16** Type: **Student contribution**

# Antibacterial nanofiber with smart release of drug

Nanofiber brings larger surface to fibre, indicating more contact area. When drug is blended in the nanofiber, nanofiber has the possibility to release the loaded drug on demand. Therefore, the properties of the nanofiber, the carrier, are of great significance. Polymers with Tg around 25 ℃ are chosen as the carrier, so that drug can be released at body temperature during sporting. Since body odour is from the digest of sweat by bacteria, antibacterial drug released at around 37 ℃ is effective to prevent body odour. To find a suitable nanofiber with effective drug loading, which can be released at higher skin temperature during sweating, is my adventure of smart nanofiber.

**Primary author:** PAN, Fei (Empa & LMU)

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **17** Type: **Student contribution**

# Corrosion inhibition of water-steam cycles in power plants by film forming amines

Good treatment program for steam cycle boiler feed water is crucial to the smooth operation of steam generators. Faulty treatment can cause damage to the plant, with attendant high costs. Conventional treatment programs have three components: oxygen scavengers, alkalising amines, and phosphate. In a treatment program based on film-forming amines (FFAs), the functions of both oxygen scavenger and phosphate are replaced by the FFAs. FFAs form a thin compact hydrophobic film on the metallic surfaces, preventing oxygen from coming into contact with the metal, and therefore preventing corrosion . FFAs have been successfully used in real applications for decades. Good results have sometimes been achieved even in cases where conventional treatment programs failed to provide satisfying results.

The operational regime of steam generators may demand short- or long-term shutdown, during which protective measure have to be taken to avoid damage of the equipment due to corrosion. Dry lay-up is recommended for long-term shutdown periods, but this type of procedure demand a significant effort and a plant design which is not always available or acceptable for the operator. Due to their specific mode of action, FFA provide an excellent potential for lay-up of steam generators .

Test specimens from carbon steel were used to simulate the real conditions of a long-term shutdown. Dividing the process into three steps: surface preparation, film-formation and exposure. The main objective of this investigation is to determine the duration of action of the protective film against corrosion, during stand-by periods in a power plant under typical conditions.

**Primary authors:** HATER, Wolfgang (Kurita Europe GmbH); ALVAREZ CASTRO, Ericka

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **18** Type: **Student contribution**

# Na+ diffusion in Na-ion battery materials investigated by neutron diffraction

Batteries are playing prominent role in energy storage technology, both for portable devices and large-scale stationary storage. Presently, most battery technologies are based on diffusion of light Li-ions between the host materials at the anode and the cathode. Given the scarcity and the increasing price of lithium, cheaper and more abundant sodium, that has close chemistry but bigger in size, is emerging as alternative at least for use in large-scale high-energy batteries that are needed to achieve sustainable energy development.

The main goal of this work is to investigate the Na+ diffusion in layered oxide NaxCoO2. This material is the Na-analogue of LixCoO2, one of the most popular cathode materials in mobile and laptop batteries. The results of the work are supposed to shed light upon ionic diffusion in Na cobaltites, help to understand the relationship between Na-vacancy order and Na dynamics in NaxCoO2. Furthermore, fundamental principles of ion-diffusion could further open the way to design tailored energy materials with improved functional performance.

Keywords: Sodium-Ion Batteries, Cathode materials, Na+ diffusion, Neutron diffraction

The project is being realized at PSI under the supervision of Dr. Marisa Medarde (Group Physical Properties of Materials) and Dr. Claire Villevieille (Battery Materials Group). The detailed work plan is listed below:

- Synthesis of the layered oxide NaxCoO2 with x = 0.72 and 0.66;
- Investigation of the Na+ diffusion using neutron diffraction. The experiments are performed at the neutron diffractometer HRPT (SINQ);
- Data analysis: to determine the changes in the structure and the diffusion paths of Na+ ions for each composition as a function of temperature the set of programs FullProf Suite is used;
- Electrochemical assessment of cobaltites'performance and it comparison with NaFeO2 and NaFe1/2Co1/2O2 is going to be carried out with the collaboration of University of Montpellier.

**Primary author:** Ms KORIUKINA, Tatiana

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **19** Type: **Student contribution**

# Molecular brushes investigated by scattering methods

Molecular brushes consist of a polymeric backbone with densely grafted side chains. In case a molecular brush contains both hydrophobic and hydrophilic segments, it takes on an elongated shape, which makes it a potential drug carrier in the human body . Poly(2-oxazoline)-based molecular brushes are especially well-suited to this purpose due to their high biocompatibility .
In the present work, a bottle brush copolymer with a hydrophobic poly(2-isopropenyl-2-oxazoline) backbone and hydrophilic side chains of poly(2-ethyl-2-oxazoline); P(iPOx)-g-P(EtOx), is investigated with respect to its size and inner structure in aqueous solution in dependence on temperature. Experimental results from dynamic light scattering show two different kinds of particles, namely 5 nm and 120-220 nm. We attribute the smaller value to the single molecular brush, and the larger one to aggregates or byproduct from the synthesis. The solution becomes turbid at 48℃, which is assumed to be due to the aggregate formation because the thermoresponsive P(EtOx) sidechains collapse and become hydrophobic. As a further step, temperature-resolved small-angle neutron scattering experiment were performed, revealing that the molecular brush does not have the shape of an elongated particle, as expected, but rather forms prolate ellipsoids with equatorial and polar radii of 7 nm and 2.5 nm, respectively. Thus, more advanced modeling is needed to fully describe the inner structure.

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**Primary author:** SHEHU, Kaltrina

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **20** Type: **Student contribution**

# Electronic Characterization of Functional Oxides using advanced photoemission spectroscopy techniques

The properties of the La2/3Sr1/3MnO3/SrTiO3 (LSMO) interface have been subject of interest since the discovery of the possibility of use this composite as a magnetic tunnel junction (MTJ) due to its half-metallic character in its ferromagnetic phase, which leads to high tunnel Magnetoresistance (TMR) effect. By other side, interesting studies on polar metals in thin films of perovskite nickelates (ANiO3) have been done in order to understand their properties, such as anisotropic thermoelectrical responses and magnetoelectric multiferroicity. Specifically, for NdNiO3 (NNO), metal insulator transition (MIT) has been observed awaken the interest of studding its electronic structure as a function of temperature.
In this project, advanced photoemission spectroscopy techniques are used to characterize the electronic structure of LSMO and NNO oxides. Angled-Resolved Photoemission Spectroscopy (ARPES) is used to obtain the electronic band diagram of NNO thin films. Parallel to this experiment, the study of the band alignment and chemical states as a function of applied bias and barrier type in LSMO oxides is performed by the HArd X-ray PhotoElectron Spectroscopy (HAXPES) technique. These experiments reflect the power of the photoemission spectroscopy as a method for understand the electronic structure of solids.

**Primary author:** RUANO MERCHÁN, Catalina

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **21** Type: **Student contribution**

# Exploring oxygen ion conductor ceramics: synthesis, structure and ion conductivity

Potential ionic oxygen conductors with unit formula Sr2TiO4 and Fe-, V-, Nb- and Mo-doped Sr2TiO4 were synthesized through solid state reaction technique. The effect of doping at Ti-site of Sr2TiO4 with Fe3+, Nb4+, V5+ and Mo5+ on oxygen ionic and mixed ionic-electronic conductivity have been investigated. The crystalline structures of these specimens were studied with X-ray diffraction (XRD) for phase determination and the cell parameters were calculated. Surface morphology and composition were studied by SEM-EDS technique. The mixed ionic-electronic conductivity of all prepared compositions of Sr2TiO4 and Fe-, V-, Nb- and Mo-doped Sr2TiO4 were measured by complex impedance spectroscopy (CSI) as a for different dopant concentrations function of frequency and temperature in the ranges of 0.1Hz 1MHz and 25-600 ˚C respectively.

**Primary author:** Mr ELMASRI, Moustafa (Master Student)

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **22** Type: **Student contribution**

# Investigation of Li de/insertion in Multi cation substituted Mn-Spinels

The rapid development in the automobile and energy sectors has led to the demand of improved lithium ion batteries. Since the electrochemical performance of a battery is limited by its cathode, therefore, cathode materials with high rate capability, specific capacity and long cycling life are required. Ni-doped Mn spinel (LNMO) materials are promising candidates due to their high intercalation/deintercalation potential, environmental friendliness, low cost and good thermal stability. However, their electrochemical properties are dependent on the crystal structure. It has been previously reported that the disordered LNMO shows better electrochemical performance than the ordered structure. Moreover, doping modifications efficiently enhance the structural stability and rate capability.

In the present work, the synthesis of multi-cation substituted Mn-spinel is aimed to obtain the disordered Fd-3m phase with better electrochemical properties. Sol-gel method is adopted to synthesize LiNi0.3-xCu0.1+xFe0.2Mn1.4O4 (x= 0, 0.1). The effect of different dopant concentrations and annealing temperatures on the structure and electrochemical performance are investigated by different techniques. The structural and morphological investigations are carried out by ex situ X-ray powder diffraction, NMR, and scanning electron microscopy. Along with electrochemical measurements, in-situ XAS is performed to determine active redox couples. The elemental composition and thermal behavior are also studied.

**Primary author:** SHARMA, Priyanka

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **23** Type: **Student contribution**

# Ionosilica nanofibrous membranes for anion exchange

**Abstract on the « ionosilica nanofibrous membranes for anion exchange/decontamination of water » presentation**

This presentation will present the advancement on the synthesis and the properties of these ionosilica membranes.

It will first be focused on the synthesis of the ionic liquid precursors and their physico-chemical interest that will be later used in solutions for electrospinning.

Then, we will have an overview of the electrospinning technique and the work we have made with the ionic liquid solutions in order to obtain homogeneous mats of fibers.

Depending on the results obtained in the ongoing work, electronic and/or sorption properties of the membranes will also be presented.

**Primary author:** LENNE, Quentin

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **24** Type: **Student contribution**

# Simultaneous measurement of relaxation times and proton density fat fraction in bone marrow using Magnetic Resonance Spectroscopy

Clinical application of magnetic resonance (MR) technique has been developed for several tens of years since late 1970. Currently, MR plays an important and irreplaceable role in disease diagnose and trace of therapy response. Compare to MR imaging, MR spectroscopy gives additional information of quantification of different resonance signals due to chemical shift. This contrast of chemical shift allows us to non-invasive analyze organ composition. Despite there are advantages of MR spectroscopy, this technique is not widely used in clinical application due to requirement of professional knowledge in data processing and excessive scanning time. The aim of this work is to build up processing pipeline of MRS data, simultaneous characterize both relaxation time T1 and T2, and quantify bone marrow composition.

**Primary author:** CHEN, Ian

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **25** Type: **Student contribution**

# Abstract Brian QUERE

Nonlinear recombination processes in perovskite materials for solar cells

**Primary author:** QUERE, Brian

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **26** Type: **Student contribution**

# Immobilisation of Gold nanoparticles by selected antiHCC antibodies - preliminary studies

The noble metal nanoparticles have been intensively studied for a long time. The photonic properties of gold or silver particles are appealing for materials applications. For example gold nanoparticles offer a wide spectrum of applications in biomedicine. When it is used for biomedicine, there is a crucial issue which is their cytotoxicity. It depends on various factors, including morphology. Because nanoparticles have an effect on cell membrane integrity, due to their different geometries as well as physical and chemical interactions with cell membranes.
We focused on the development modification of gold nanoparticles (GNP) using selective antibodies. Gold the immobilization process of GNP (size range 10-40 nm) is carried out through the click-chemistry method. The immobilized GNP systems characterized by using microscopic methods (AFM, TEM) and by interaction with the target protein - HCC.

**Primary author:** ICHIBA, Kaito

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **27** Type: **Student contribution**

# XAS and EXAFS of dioxygen binding to binuclear copper complexes.

Tyrosinase is an essential enzyme in many organisms, including humans. Its ability to oxidize molecules by utilizing molecular oxygen is commonly applied in nature for the synthesis of melanin, a pigment which has many protective properties. Being highly efficient and selective, the reaction could also have interesting industrial applications. However, the exact geometric structure of the binuclear copper site in the active center during oxygen binding, and therefore the mechanism of the reaction, is not fully understood yet, as experimental and theoretical structure determinations have not been conclusive. In the course of this work, X-ray absorption measurements (XAS) have been conducted with model complexes for tyrosinase to try and understand the structure of the intermediate and the reaction mechanism. As the active site of the enzyme is the binuclear copper complex, the fine structure of the copper K-edge (EXAFS) can selectively be analyzed to derive the interatomic distances during oxygen binding. The data obtained and processed to this point will be presented and discussed in the oral presentation.

**Primary author:** BAUR, Philipp (Stanford University)

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **28** Type: **Student contribution**

# Ultrafast photo-switching in dielectric materials with spin cross over

It has been admitted that classical phase transition in materials can be driven by external parameters such as changes in temperature and pressure. More recently light has been used to drive phase transitions faster (because of the use of short light pulses) and especially differently since femtosecond pulses could couple to electronic degrees of freedom before the system can move.

The main goal of the master thesis work is to study the ultrafast switching of spin transition materials. These compounds are prototypes of bistable molecular systems with two electronic states called High Spin (HS) and Low Spin (LS). This change of electronic states is accompanied by structural changes mainly around the central metal ion. We were particularly interested in two classes of Fe-based molecular systems: FeII (LS $\longrightarrow$ S = 0, HS $\longrightarrow$ S = 2) and Fe III (LS $\longrightarrow$ S = 1/2, HS $\longrightarrow$ S = 5/2).

**Primary author:** DAVID, amaury

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **29** Type: **Student contribution**

# Characterization & Assessment of Residual Stress Fields in Laser Welded Ti6Al4V Components for Satellite Application

See Attached

**Primary author:** Mr RINALDI, Daniel

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **30** Type: **Student contribution**

# structural transormations of photoswitchable complexes captured by quantitative XANES

structural transormations of photoswitchable complexes captured by quantitative XANES
by LIU Xuanran
1. Introduction to XANES
2. Finite difference method
a) Finite Difference Method (FDM) and Green formalism
b) multi-electronic extension using the "Time-Dependent DFT"
c) Convolution with the FDMNES
3. Result of calcutaions for ground states of Febpy, Fedcpp and Fe-terpy: by using the coordinates of the molecule, we calculate the XANES by FDMNES and compared it to the experimental spectrums.
4. Simulation of the excited state by deformation of the molecule: we deform the molecule manually to simulate the reaction of the molecule when excited by the X-ray laser. And compared it to the experimental spectrum.
5. using of machine learning
a) Approximation of XANES as a function of structural parameters
b) Extra free method
c) Quadratic refression
d) Direct prediction of structure parameters from experimental XANES
e) Extra free methods
f) Convolutional neural networks

**Primary author:** LIU, xuanran

**Session Classification:** Student session

**Track Classification:** Student contribution

Contribution ID: **31** Type: **not specified**

# Departure

*Friday, 25 May 2018 13:00 (6 hours)*

timetable ship back to Prien:
7:30/ *8:15* | 9:50 | 10:35 | 11:00/ *11:05* / *11:35* / *12:15* / *13:15* / *13:45* / *14:00* | 14:15 | 14:45 | 15:15 |16:00/ *16:30* / *17:00* / *17:40* | 18:30 | 19:00* | * = nicht nach Gstadt

timetable train back to Munich Hbf:
10:06 /10:24/11:06/12:06/12:44/13:06/14:06/14:44/15:06

Contribution ID: **32** Type: **not specified**

# Early afternoon session (III)

Contribution ID: **34** Type: **not specified**

# SUNSET EVENT CHIEMSEE

*Wednesday, 23 May 2018 20:15 (1 hour)*

Contribution ID: **36** Type: **not specified**

# ARRIVAL/ ROOM ALLOCATION

*Tuesday, 22 May 2018 12:00 (6 hours)*

Contribution ID: **37** Type: **not specified**

# Consortiums Meeting

*Thursday, 24 May 2018 16:50 (1 hour)*

Contribution ID: **38** Type: **Main Lecture**

# Even the scattered photon does not forget

*Thursday, 24 May 2018 20:15 (1 hour)*

**Presenter:** Dr GLATZEL, Pieter (ESRF)

Contribution ID: **39** Type: **Main Lecture**

# PRESENTATIONS FEEDBACK AND CONCLUSIONS

*Friday, 25 May 2018 10:40 (1 hour)*

Contribution ID: **40** Type: **Student contribution**

# Fe-Base Alloy design for Additive Manufacturing

Additive Manufacturing is a new and continuously growing market, for that reason much work is being done by many companies and research institutions to optimize this promising production process still without exploiting.
Additive manufacturing offers many advantages that traditional production methods can't rather due to geometrical or process restrictions rather for economical reasons. Additive Manufacturing is defined as "the process by which digital 3D design data is used to build up a component in layers by depositing material"(International Committee F42 for Additive Manufacturing Technologies, ASTM).
The advantages of this technology is that the raw material is directly transformed into the finished piece, forgetting the intermeddle processes, and is not restricted by the conventional manufacturing constraints. So the market possibilities are as broad as you can imagine.
The functional principle is scoping an application, then developing a material for this app requirements, a 3D CAD model is done and some simulations for optimizing the material and the 3D printing process are done and then the materials processing and layering is studied, selecting the parameters for the printing window to obtain the final piece. This is an iterative process that helps us to affine and optimizing the process and parameters.
There are many additive manufacturing technologies depending on the materials they can process, the cost, accuracy, speed of scanning, layer thickness and the technique applied to create the layers and to join them.
ArcelorMittal is interesting in all kind of materials and technologies, but due to its strategic position in the market, there is a preferred interest in metal alloy design, especially, Fe-based alloy. In this field the most used technology for 3D printing purposes is SLM (Selective Laser Melting). However, a lack of suitable materials for this application is a fact, and this is because the extreme conditions the material is submitted during the atomization process and during the melting-printing process. Here it is where all the actual work is focusing to try to understand the thermodynamics and the external factors which can affect too. Moreover the little list of the metal alloys used nowadays in 3D printing were not develop for this purpose, so improving these alloys is a must regarding two ways: 1) Improving the final physical and mechanical properties of the material and 2) improve the processability of the material using the Additive Manufacturing Facilities.

**Primary author:** SÁNCHEZ PONCELA, Manuel (ArcelorMittal)

**Presenter:** SÁNCHEZ PONCELA, Manuel (ArcelorMittal)