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Book of Abstracts

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Keynote Lectures / 61**Applied and Fundamental Research at the High Flux Neutron Source FRM II/MLZ****Author:** Martin Meven¹¹ *RWTH Aachen***Corresponding Author:** martin.meven@frm2.tum.de

The Heinz-Maier-Leibnitz Zentrum (MLZ) is a leading centre for state-of-the-art research with neutrons and positrons offering a large variety of high-performant neutron scattering instruments to perform studies on many hot topics in physics, chemistry, biology, earth sciences, engineering or material sciences. The MLZ represents the cooperation between the Technische Universität München (TUM) and research centres of the Helmholtz Association, esp. Forschungszentrum Jülich (FZJ) and Helmholtz-Zentrum Geesthacht (HZG), to exploit the scientific use of the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) in Garching near Munich.

The presentation provides an overview of the neutron source itself and some of the available instruments and their applications.

Student Sessions / 60**Temperature dependent oxygen disorder in Pr(2-x)Sr(x) NiO(4+δ) by high-resolution single crystal neutron diffraction on HEIDI@MLZ****Author:** Sumit Ranjan Maity¹**Co-authors:** Werner PAULUS²; Winfried PETRY³¹ *Technical university of Munich*² *UNIVERSITE DE MONTPELLIER 2, France*³ *Technical University MÜNCHEN, Germany***Corresponding Author:** sumit050491@yahoo.com

Mixed-ionic electronic conductors (MIEC) offer significant advantages over conventional cathodes especially in the intermediate temperature range for solid oxide fuel cell applications. In this context, Ruddlesden-Popper type layered oxides have taken much attention. Among them Pr₂NiO(4+δ) is a promising candidate as it offers high electronic conductivity similar to those conventional cathode materials but in addition shows a very high oxygen diffusion coefficient even at room temperature. Behind these remarkable physical properties the oxygen atoms and their disorder between interstitial and apical sites play a key role in low-moderate temperature region, allowing phonon assisted diffusion in the moderate temperature region. In a similar way to high temperature superconductors, Sr doping or hole doping may increase the electronic conductivity but significantly lowers the delocalization of oxygen atoms. Nevertheless, it offers to make a direct comparison of oxygen diffusion mechanism with the undoped sample. For these reasons, our present work focuses to analyze apical oxygen disorder in Pr(1.5)Sr(0.5)NiO(4+δ) by single crystal neutron diffraction on HEIDI@MLZ as a function of temperature. Neutrons are point scatterer and thus a perfect tool to explore disordered structures.

We will discuss the displacement amplitudes of the apical oxygen atoms as a function of Sr-doping and temperature, analyzed by classical Fourier techniques and by Maximum Entropy algorithm, in order to conclude and separate possible static and dynamic contributions

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Next Generation III-V Nanowire-based Heterostructure Solar Cells and Photodetectors Integrated on Silicon

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III-V based nanowire (NW) heterostructures are one of the most promising candidates for future opto-electronic devices like light emitters and detectors, particularly when integrated onto the well-developed Silicon (Si) platform. Using nano-imprint lithography (NIL) to prepattern Si (111) wafer, NW arrays with very high growth yield (>90%) can be achieved over large-scale areas. Developing a state of the art UV-imprint process we could significantly enhance the flexibility of the NIL setup using a novel home-designed table top device. By producing replicas of NIL stamps with various patterns, full control over the inter-NW spacing could be achieved, one crucial prerequisite to further increase the efficiency of NW-based solar cells fabricated from InGaAs-InAlAs NW heterostructures. Using these optimized prepatterned substrates, NW growth is performed in a completely catalyst-free growth regime via molecular beam epitaxy, allowing detailed insight into morphology (scanning electron microscopy, SEM), luminescence properties (micro-luminescence, μ -PL) and absorption cross-section (Fourier transform infrared spectroscopy, FTIR) for different interwire spacings. This opens numerous opportunities to advance NW-based heterostructures, such as integrated nanophotonic sources on Si and NW-based photovoltaics.

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Power Die Embedding in a Power Electronics Converter

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This project, born from a partnership between Mitsubishi Electric R&D Centre Europe (MERCE) and the Ampère Laboratory in Lyon (France), consists in the enhancement of the design of conventional heat sinks, ubiquitous elements used in power electronics systems as heat dissipating units. The final goal of this project is to design, fabricate and validate a novel packaging solution that reduces the thermal resistance between the power chips (die) and the heat sink while keeping it safe to handle.

Most cases of study focus on the design of metallic heat sinks due to their easiness of shaping. Pi

Agreements have been made towards the design of novel heat sinks using a specific class of insulati

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High temperature chemical reactivity of potential SOFC materials in dry and wet gas atmospheres investigated by thermal analysis and in situ neutron powder diffraction

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Solid oxide fuel cells (SOFC) working around 900 °C have drawn a growing interest in the field of energy. Their operating temperature allows the use of complex combustible gases at the anode (natural gas, biomass gas). To prevent carbon deposition, contamination by sulfur and aging of the composite in the presence of water, one of the major challenges remains the replacement of the standard cermet anode material, Ni/YSZ (YSZ: yttria stabilized zirconia) with a mixed ionic and electronic conductor (MIEC).

In this view, manganite Ruddlesden-Popper (RP) phases; $n = 1$ (La,Sr)₂MnO_{4-δ} and $n = 2$ (La,Sr)₃Mn₂O_{7-δ} are promising SOFC anode materials [1,2] due to their good thermal stability in a reducing atmosphere and the mixed valence of Mn essential for electronic conductivity. The latter systems have not been studied for SOFC applications so far.

In this project, two RP $n = 2$ compositions, LaSr₂Mn₂O₇ and La_{1.2}Sr_{1.8}Mn₂O₇, are prepared by two synthesis methods. High temperature in situ X-ray diffraction (XRD) and neutron diffraction (D20/ILL, Grenoble) combined to thermogravimetric analysis (TGA) have been carried out under H₂ and air flow to characterize the behavior in operating SOFC conditions. The powder samples have been sintered by spark plasma sintering (SPS) for conductivity measurements. In addition thermal stability in wet atmosphere has been investigated.

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Developing High Entropy Alloys for High Temperature Applications

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High Entropy Alloys (HEAs) are defined as alloys consisting of five or more elements with concentration between 5 to 35 at%. Contrary to conventional alloys in which the main component provides a primary property and the alloying elements allocate secondary ones, HEAs involve usually 5 elements forming simple solid solutions rather than complex microstructures because of significant role of high configurational entropy: therefore, the number of phases in them is much less than that of phases allowed by the Gibbs phase rule. Interest in HEAs has been sparked by their high potential of improving mechanical properties due to four core effects: high-entropy, sluggish diffusion, severe lattice distortion and local anisotropy affecting thermodynamics, kinetics, structure and properties, respectively. Their phase and microstructural stability make HEAs convenient for both high temperature (HT) and cryogenic applications. HT performances of HEAs depend on facturing method, alloy composition, heat treatment, increasing contribution of mixing entropy at the elevated temperatures and unusual deformation mechanisms under HT conditions. Methods have been developed for prediction of phase formation in HEAs based on properties of the elements as well as computational techniques. This thesis project is based on the selection of metals according to a modern use of Hume-Rothery rules and to free energy calculation for solid solutions. Groups of transition elements

have been chosen for alloy synthesis, e. g. CrCoFrNiW and CrTaTiVZr in equimolar ratio, structural (diffraction techniques) and microstructural (microscopies) characterization and mechanical property (hardness, scratch test) studies. Materials are envisaged for HT application.

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Interplay between structural complexity and magnetism in non-stoichiometric Pr₂NiO(4+d) single crystals.

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Non-stoichiometric Pr₂NiO(4+d) has emerged as a model system for its application as oxygen conductor in solid oxide fuel cells due to ambient oxygen conductivity, thermal stability at higher temperatures, large oxygen solubility range and a large fully-reversible oxygen uptake window. It is also thought that introduction of interstitial oxygen activates specific low-energy phonon modes that mediate oxygen transport at low temperatures.

Associated with oxygen intercalation in stoichiometric Pr₂NiO₄ is the emergence of structural complexity in the form of a well-defined and long-range ordered oxygen superstructure. Because of the convenience with which oxygen doping can be controlled in it, Pr₂NiO(4+d) presents a system where we have the possibility to tailor the oxygen content and with that establish control over the resulting superstructure formation. The well-ordered superstructure indicates a correlation among the interstitial oxygen atoms which necessitates a deeper understanding of the role of electron density, Ni valence states and influence of the superstructure on the electronic properties of the compounds. We have made investigations on three different non-stoichiometric phases: Pr₂NiO_{4.12}, Pr₂NiO_{4.25} and Pr_{1.5}Sr_{0.5}NiO₄, which is isoelectronic to Pr₂NiO_{4.25}.

In this talk we discuss the interplay of structural complexity and its influence on valence states and magnetism in Pr₂NiO(4+d), which can give a new insight into emergence of novel and interesting properties via hole-doping in the Ruddlesden-Popper phases. We also present the preliminary results of neutron scattering, neutron spectroscopy and macroscopic magnetic measurements made on the different non-stoichiometric phases of Pr₂NiO(4+d).

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”The electronic structure of luminescent centers in doped phosphors”

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Barium magnesium aluminates doped with europium and manganese (BaMgAl₁₀O₁₇ (BAM): Eu+2 (1%) and Mn+2 (1%)) is widely used as phosphors material in optics and electronics applications, e.g.

PDPs (Plasma Display Panels), lamps, and LEDs (Light Emitting Diodes). Despite their widespread use the exact reason for the varying luminescent efficiency is not known and neither is the exact position of the Eu and Mn ions in the BAM structure. In order to address these questions we applied X-ray spectroscopy as an element selective probe to study the local coordination and electronic structure. The experimental data are compared to theoretical calculations based on the finite difference method (FDM) using FDMNES code.

Mn²⁺ may occupy octahedral or tetrahedral sites by replacing Mg/Al in the BAM structure while Eu²⁺ enters the mirror layer replacing a Ba ion. The X-ray absorption spectroscopic (XAS) data show a clear signature of Mn²⁺ in tetrahedral sites. However, XAS cannot rule out Mn in an octahedral environment and we therefore applied X-ray emission spectroscopy (XES) as a complementary tool to probe the occupied electronic orbitals. The rich XES spectrum is expected to show whether Mn also occupies octahedral sites.

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The combined effect of recycled aggregate implementation and cement overdosage on the durability properties of high performance concrete

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Since awareness of sustainable development, the construction industry has been searching for a way to reuse their wastes. The use of recycled aggregates (RA) in concrete is an interesting alternative. RA are composed of natural aggregates (NA) surrounded by an old mortar, which makes them more porous, lighter and more water absorbing compare to NA. The substitution rate of NA by RA plays a major role in the properties of concrete. Of course the quality of these aggregates will determine the strength of the concrete. The use in concrete of these RA should decrease its mechanical performances. The goal of this internship is to see if it has the same effect on the durability properties. Chloride diffusion, water absorption and carbonation experiments have been carried out in order to assess the feasibility of such a project.

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Monte Carlo Simulation of Terahertz Quantum Cascade Lasers

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Despite having multitude of potential applications as unique observations of characteristic vibrational and rotational molecular lines, non-ionizing bio-medical imaging, etc. the terahertz frequency range of the electromagnetic spectrum remains comparatively underdeveloped with respect to the nearby microwaves and infrared regions, mainly due to the lack of compact and efficient emission sources. From one side, generation of coherent terahertz radiation involving extension of electronic components to higher frequencies is limited by its internal parasitic roll-offs, from the other, the attempt to extend use of photonic sources to longer wavelengths is constrained by absence of material systems emitting radiation in range of the interest. In this regard, an alternative in the face of recently developed quantum cascade lasers[1,2] seems prospectively attractive.

The quantum cascade laser is an example of a device where exploited properties, such as the photon

wavelength or population inversion of charge carriers, are not originated from an intrinsic physical attribute of the material, but designed by a judicious adjustment of structure geometry and an appropriate engineering of the wave functions. Thus, fabrication of that type devices demands reliable prior calculations taking into consideration phenomena of quantum nature involved in its operation. One of numerical approaches to solve the standing issue by means of Monte Carlo method will be discussed in the talk.

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Magneto-resistance in electron under-doped cuprate superconductor $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$

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High-temperature cuprate superconductors (HTSC) are materials that become superconducting at unusually high temperatures. The interplay between antiferromagnetic (AF) and superconductivity (SC) is one of the most fascinating phenomena in the HTSC. The parent compounds of all the high-Tc cuprates are AF Mott insulators. Upon doping the antiferromagnetism vanishes and superconductivity appears together with the metallic state. In the electron-doped cuprates $\text{Ln}_{2-x}\text{Ce}_x\text{CuO}_4$, where $\text{Ln}=\text{Nd, Pr, Sm, Eu}$, the AF order is more stable against doping than in hole-doped cuprates. So, the question now is whether the AF and SC states coexist and, if yes, then whether this is an intrinsic phase separation or a microscopic coexistence.

In the present work we are going to investigate whether superconductivity and AF coexist in the electron - underdoped $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ (NCCO) for a broad doping range ($0.10 \leq x \leq 0.145$). To the end we carry out detailed studied of out of plane MR Magneto-resistance of NCCO which provides insight into the coupling between the charge carriers and the background magnetism. The focus is laid on manifestation of spin-dependent transport characteristic of a magnetically ordered state.

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Research Trends in Materials Science at AMU

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Light !

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Tracking the photo-induced phase transition in breathing-crystals

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The concept of photo-induced phase transitions and of time-resolved experiments will be illustrated on the basis of photoswitchable copper-nitroxide molecular magnets.

Molecular compounds with photoswitchable magnetic properties have been intensively investigated over the last decades due to their prospective applications in nanoelectronics, sensing and magnetic data storage. As a more recent material that allows optical manipulation of its magnetization, copper-nitroxide-based compounds have emerged as a new class of spin-crossover systems.

Unlike in classical spin-crossover compounds, the change in magnetic properties is based on reversible magneto-structural rearrangements between weakly and strongly exchange-coupled states of spin triads nitroxide-copper(II)-nitroxide (WS/SS states).

The mechanism of photoswitching between the two states and the resulting cooperative phenomenon is far from understood and requires ultrafast, time-resolved measurement techniques. Initial results covering a time range from femto- to microseconds using pump-probe absorption spectroscopy will be presented.

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Substrate-effect on Structural and Orientational properties of ZnO Thin Film-systems Grown by Pulsed Laser Deposition

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Ever since the discovery of GaN-based blue LED systems, renewed interests have sprouted around ZnO for similar applications. The arrival of blue LED has in turn facilitated the commercial availability of white light LED. Then ZnO, a widebandgap and inexpensive semiconductor, has huge potential to catalyse a small energy-saving revolution in terms of making low-cost acquisition, highly efficient and long-lasting white LED systems possible. Another advantage of ZnO over GaN-systems is the ease with which the electrical properties can be altered by varying growth parameters (e.g. oxygen partial pressure). Another advantage of ZnO is its high exciton binding energy (60 meV vs GaN 25 meV) which can enable stable blue/UV-lasers at even elevated temperatures.

Two major barriers are standing in the way: p-doping to make the necessary pn-junction possible (not touched) and secondly improving the crystalline quality of the grown ZnO thin films for better electrical properties.

Structural x-ray diffraction characterization of Pulsed Laser Deposited ZnO thin films on sapphire (0001), MgO (001) and YSZ (001) has been carried out with supportive X-ray reflective measurements and atomic force microscopy. Pole figures obtained from x-ray diffraction give an insight on the variation of misalignment angle (deviation from the ZnO c-orientation texture) on the different substrates. Furthermore, structural phase stability dependence on the cubic or hexagonal nature of substrate and level of cubic Mg doping are investigated.

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CDW - MH phase transition in [Pd(cptn)₂Br]Br₂ studied by 3D-PDF

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The occurrence of a Mott-Hubbard (MH) to Charge-Density-Wave (CDW) phase transition in the quasi-one-dimensional Bromo-bridged Pd compound [Pd(cptn)₂Br]Br₂ (cptn = (1R,2R)-trans-1,2-Cyclopentadiamine) was investigated by means of single crystal X-ray diffraction employing the novel 3D- Δ PDF method. Raman and STM measurements indicate that the phase transition occurs slightly above 100K and that should be accompanied by a dimerization of Pd-Br pairs along the 1D chain in order to stabilize the CDW state. The existence of such state is demonstrated by the measured variation of Spin susceptibility with temperature. However, no change of the Orthorombic structure over the relevant temperatures is observed. Clear evidence of the presence of diffuse scattering streaks above 100K allows for modelling of 1D disorder with the program Yell [1], which yields the expected dimerization in a layered fashion along with precise values of the present in- and out-of-plane correlations. The presence of unexpected Bragg peaks that could be assigned to a Monoclinic structure was also investigated and points to a phase separation phenomena.

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Synthesis and study of piezoelectric materials in α -quartz family

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Piezoelectric materials which can be used at very high temperature without degradation are sought for the control system in severe environmental conditions. However, the use of a piezoelectric material at elevated temperature presents many challenges such as possible phase transition, chemical degradation or structural defect propagation which can cancel or drastically decrease the piezoelectric properties. α -quartz, which is quite common piezoelectric material, cannot be used at temperatures higher than 573°C because of phase transition $\alpha \rightarrow \beta$ -quartz occurs. Among the piezoelectric materials, there are potentially powerful piezoelectric materials with α -quartz structure such as: 1) α -GeO₂, which has a very wide range of operating temperature (until 1115°C) because its strong structural distortion prevents the transition to β -quartz-type phase. 2) BaZnO₂ –some theoretical calculations showed that such a crystal with α -quartz structure possesses outstanding piezoelectric properties.

So, the main objectives of the work are: development of the experimental conditions to control the seeded crystal growth of α -GeO₂ with high crystalline quality by the high temperature flux method; study of the thermal, piezoelectric and dielectric properties of the crystals at different temperatures (up to 700°C); synthesis of pure powder of complex oxide BaZnO₂ and following crystal growth by flux-growth method.

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Investigating the magnetic structure of Ruthenium based 2H-perovskites.

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We are currently investigating the magnetic behaviour of Sr₃XRuO₆ (X=Li, Na) [1], these compounds belong to the family of the hexagonal perovskite oxides A₃A'B₃O₆ [2]. Principal members of this family are Ca₃Co₂O₆ [2,3], Sr₃NiIrO₆[4]; the most closely related member to the ones presented here is Ca₃LiOsO₆ [5]. These compounds are structurally characterized by infinite 1D chains of octahedra and trigonal prisms containing a transition metal oxide running along the c-axis in the hexagonal setting. Due to this configuration, they were first thought to behave as 1D magnetic systems in the low temperature phase. In reality the inter-chain magnetic exchange interactions are strong and play a fundamental role in stabilizing the complex magnetic ordering found in these compounds. I will present the results from recent resonant magnetic scattering experiments clearly indicating that both the samples order antiferromagnetically with a propagation vector (0,0,0), FDMNES code and magnetic scattering simulations in the dipolar approximation have been used to model the data. Further investigations will be necessary to fully confirm the magnetic structure.

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Mechanical design and instrumentation of a tribology device

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This work is part of the constant search of improvement for float glass manufacturing process (glazing for buildings or automobile). Nowadays, we have 2% of loss in the glass production due to flaws during the production. To solve that problem, we have to better understand the conditions in which we create defects. The float glass process requires the contact of hot glass with a colder metal support. This contact can have an impact on the quality of the produced glass through defects, whose generation is dependent from contact conditions (temperature, stress, surface condition, nature of the metal support...).

To improve the understanding of flaws generation, we decided to actively participate in the mechanical design and instrumentation of a tribology device to perform factory tests. These tests will identify key parameters for the optimization of process control.

Starting from an existing machine, we will design a device to play multiple contact conditions. It will be used in real production conditions, with high temperature constraints (the glass is at 630°C).

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Synthesis & Kinetics of Nanostructured Calcium Silicate Hydrates (C-S-H) with high Ca/Si ratio for applications in eco-friendly cement & concrete

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Cement is one of the most widely used materials and its production is responsible for 5 - 8 % of yearly man-made global CO₂ emissions. Calcium Silicate Hydrate (C-S-H) is the main product of the hydration of Portland cement and it's the key for the strength in cement based materials. A better understanding of the kinetics and growth mechanism will throw us some light in arriving at a new alternative material for substitution in cementitious material on a more scientific basis. Owing to the fact that the composition of real cementitious materials is complex with several different mineral phases, we have adopted a synthetic approach to precipitate C-S-H and gain more insight to its kinetics and growth mechanism. The contour of my master project starts with synthesising C-S-H via precipitation route at Ca/Si ratio varying from 1.0 to 1.75, based on the thermodynamics modelling predictions by Gibbs Energy Minimization Software (GEMS) and followed by Kinetic studies on C-S-H precipitation. The synthetic conditions adopted are focused to arrive as close as possible to real system C-S-H, in accordance to thermodynamic equilibrium conditions predicted by GEMS. The synthesised samples has been characterised by TGA, XRD, ICP-OES, FTIR, BET, TEM. The characterized sample helps in evaluating the prime conditions for arriving at C-S-H closest to the real system. The second part of the project deals with Kinetic studies aimed at elucidating the steps involved and evolution of the previously synthesised samples. It helps in understating the growth mechanism in formation of the precipitated C-S-H, in terms of morphology etc. Furthermore the kinetic data helps in development of population balance model for better prediction of the product formation for given starting conditions.

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Charge Density Wave Order in Doped Praseodymium Nickelate studied by Resonant Soft X-ray Scattering

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The solid oxide fuel cells (SOFCs) have attracted considerable attention due to their high energy conversion efficiency and lower production of pollutants. However, high temperature is needed creating issues related with compatibility, thermal expansion and stability.

Therefore, oxide materials with high oxygen ion conductivity are of particular interest especially in their applications as oxygen membranes and electrolytes in SOFCs. In particular, perovskite type oxides, A(2)BO(4) (Ruddlesen-Popper phase have shown interesting ionic and electronic transport properties and the possibility to tune the properties by doping (oxygen intercalation at room temperature).

The compounds in the K(2)NiF(4) family are the lanthanide oxides with the general formula of Ln(2)MO(4) (where Ln = La, Pr, Nd and M = Cu, Ni, Co). Their properties vary drastically on doping, which can be huge, modifying (anisotropic) oxygen mobility, the charge ordering and the valence of the transition metal, by changing the oxygen stoichiometry and the temperature.

Indeed, in K(2)NiF(4) family, structural changes are a function of charge transfer.

The chosen material to be investigated is Pr(2)NiO(4+delta), because at low temperature, besides the antiferromagnetism, long-range ordered superstructures can arise, generating an electronic correlation that only oxygen intercalation can induce. These superstructures are known as magnetic and charge-stripe phases, static or dynamic, i.e. local AFM regions with anti-phase boundaries.

Such phases are visible as incommensurate peaks by analysing the material with high-brilliance X-ray sources, like synchrotron. However, their interpretation is challenging and their origin can be often confused, due to their low intensity but also due to imperfections of the material, such as NiO

segregation or Pr(6)O(11) hydrolization.

For this reason, large single crystals of $\text{Pr}_2\text{NiO}_{4+\delta}$ will be prepared in order to achieve clear satellite peaks related to commensurate/incommensurate reflections.

Such very defined diagrams provided the motivation for this work.

This work will focus on the energy of the incommensurate peaks in order to identify from which physical phenomenon they are originated. Therefore, an energetic distribution of peaks will be performed, by exploiting Resonant Soft X-Ray Scattering (RSXS), an energy-dispersive analysis technique. The possible explanations are related to the charge or orbital ordering arising from Ni or O ions, whose transition energies are separated only by few eV.

The aim of this work is to give a better understanding of the structural and electronic properties of Ruddlesden-Popper phase perovskite oxide $\text{Pr}_2\text{NiO}_{4+\delta}$ with several δ values, as well as the lattice dynamics and the valence distribution of nickel ions.

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Platinum Ruthenium Core-shell Nanoparticles for H₂ oxidation kinetics in alkaline media

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As people concern about environment and clean energy production, hydrogen-based fuel cell attracts more and more attention of scientists. However, the rate of the hydrogen oxidation reaction (HOR) in the alkaline media is usually slow which limits the development of this promising energy source. Recently, a new type of catalyst—Pt_{0.1}Ru_{0.9} was found to give a high activity for the HOR, which is the maximum activity people achieve now (about 5 times more than Pt).

One hypothesis for the high catalytic efficiency of Pt_{0.1}Ru_{0.9} materials is the “Binding Energy” theory. It could be explained that when Pt and Ru form the alloy, the interaction between the two metal atoms will cause the different electrochemical behavior from the pure material. While another hypothesis for the high activity is the “Bifunctional Effect” theory. Ru could capture OH in the alkaline media, which can simultaneously provide active sites for the dissociative adsorption of H₂ and adsorption of reactive OH on the top of Ru-Pt atoms.

To explore more about the new, successful material, a Pt@Ru core-shell structure is designed to demonstrate the causes of the high activity. Compared the novel Pt materials, Ru could largely decrease the cost of novel Pt production if the electrochemical characteristic of Pt is not influenced by the Ru core. More importantly, avoiding the attachment of Ru from OH⁻, we can easily figure out either “Binding Energy” theory or “Bifunctional Effect” theory is more convincing with the H₂ oxidation reaction result in alkaline media.

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Hybrid Assemblies Based on Plasmonic Semiconductors

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Research on nanomaterials is becoming more and more popular each day as they find applications in many fields ranging from catalysis to drug delivery. Nanomaterials based on noble metals are

of special interest, due to the fact that they can hold the so-called localized surface plasmon resonances upon interaction with light.¹ Plasmonic nanomaterials however, are not limited to noble metal nanoparticles. Semiconductor nanoparticles with p-type doping also show similar plasmonic properties and a major advantage of plasmonic semiconductors over their metal counterparts is the possibility they offer to tune their optical and electronic properties by varying the free carrier concentration.² In the last few years our group has investigated the plasmonic properties of vacancy-doped copper chalcogenide nanocrystals; showing that their localized surface plasmons in the near infrared (NIR) spectral region originate from the collective oscillation of holes, and that it is possible to turn “on” and “off” their plasmonic properties by chemical means.³ Combining plasmonic semiconductors with other functional nanomaterials can serve as a starting point to investigate so far unexplored phenomena at the nanoscale.

The goal of this work is to develop a hybrid nanomaterial made of plasmonic copper chalcogenide supraparticles (namely Cu_{2-x}Se) enclosing magnetic cores to merge the plasmonic and magnetic properties of the individual components into a nanosized single system. Magnetic nanoparticles are widely employed for catalyst recovery and water purification due to their versatility as they enable one to control the system externally and are easily separable. By combining the intrinsic properties of magnetic nanoparticles with the optoelectronic properties of Cu_{2-x}Se it will be possible to investigate the interaction between a plasmonic semiconductor and a magnetic nanoparticle core, with the aided advantage provided by the possibility of “switching on” and “off” the plasmonic properties of the semiconductor building-block.

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Experimental setup of HHG-ARPES and first test measurement on Au (111)

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Angular resolved photoemission spectroscopy (ARPES) is known to be a powerful method to characterize the electronic band structure dispersion of crystalline solids. With the recent availability of laboratory scaled laser drive High Harmonic Generation sources (HHG) in the extreme ultraviolet, ARPES experiments can be performed with (sub-) femtosecond pulse and thus prove the way to measure ultrafast temporal electron dynamics in solids.

Thus, my thesis projects consists of three sub-projects.

1. Calibration of the ultrafast laser pulse. In our laboratory, a few-cycle driver laser amplifier is used to produce the ultrashort laser pulse (~4fs). The laser pulse needs to be calibrated by the special measurement systems including the CEP phase meter[1] regarding the pulse divergence to the carrier enveloped phase and FROG system (Frequency resolved optical gating)[2].
2. ARPES measurement by HHG. HHG is produced by non-linear process of the interaction between laser and gas target (Neon). The electron band structure of Au (111) is measured by the HHG-ARPES.

3. Using NIR-XUV system to analyze the photoemission electron under the ultrafast laser. In detail, NIR ultrafast laser pulse will perform as a probe and interact with the photoemission electron resulting in a change of the moment of the emission photos[3]. Finally, we can measure the electron dynamics on the Au surface on attosecond scale.

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Neutron scattering possibilities at SINQ

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The Swiss spallation neutron source, inaugurated in 1996 and situated at the Paul Scherrer Institut in Villigen is the center of the Swiss neutron research community. The source is operated continuously and its neutron flux is comparable to other national operated neutron scattering facilities as for instance LLB in Saclay, France or HZB in Berlin, Germany.

The SINQ hall is the home of 18 different instruments which cover the full spectrum of research with neutrons, from material science, over condensed matter physics to biology and chemistry.

In my contribution, I will present a geometric frustrated compound, Ho₂PdSi₃, as a scientific example for the application of neutron scattering to understand its complex magnetic properties. With data on this specific example I will try to elaborate the advantages (and disadvantages) of different techniques starting from powder diffraction and ending in single crystal spectroscopy.

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Revealing plasmonic-induced electron transfer with high resolution x-ray absorption spectroscopy in TiO₂/Au nanocomposites

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With the increasing demand for energy faced by modern society, the efficient exploitation of clean energy sources is fundamental. In this scenario TiO₂ represent a particularly interesting material: it is cheap and abundant and at most importantly it catalyzes for chemical reactions, from water

splitting to waste water treatment, when illuminated with UV light. Research is thus looking for ways to make TiO₂ more and more efficient under visible light, since UV represents only 4% of the solar spectrum. Coupling TiO₂ with metal nanoparticles is particularly promising: the collective excitation of conduction electrons, i.e. the localised surface plasmon resonance, resonates in the visible leading to huge absorption at specific wavelengths. Devices based on this coupling show good efficiencies under visible light illumination, demonstrating that energy is absorbed by plasmonic nanoparticles and then transferred to TiO₂ for photo-catalysis.

The process at the base of the efficient coupling of TiO₂ and plasmonic nanoparticles is still debated and device optimization would highly benefit from a deeper understanding of the mechanism working at the atomic level.

We present how we addressed this level of the problem using high resolution x-ray absorption spectroscopy: we probed the local electronic structure of Ti atoms in TiO₂/Au systems while exciting the collective excitation of Au nanoparticles with a 532 nm laser. Spectral differences observed are the signature of electrons injected into TiO₂ and trapped for long time near Ti atoms at the surface, favored by local distortions that is thus important for efficient catalyst production.

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Neutron imaging facilities and applications at the PSI spallation neutron source SINQ

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Neutron imaging, also known as neutron radiography, is a mainly non-diffractive application of highly collimated, large area, neutron beams for direct projection imaging with cold and thermal neutrons. Due to its direct (real space) imaging capabilities it is complementary to neutron scattering methods and is applied to a wide range of non-destructive testing problems arising in research and industry. This talk gives an overview of the facilities and methods used at PSI and presents results of selected neutron imaging investigations.