Spin-Orbital-Lattice correlations induced phenomena in emerging materials

July 3-4, 2023

Sala Lauree, Department of Physics

Sapienza University of Rome

BOOK OF ABSTRACTS

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PROGRAM

Sapienza-Japan meeting on

Spin-Orbital-Lattice correlations induced phenomena in emerging materials

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Monday 3 July, 2023

S1 (Chairperson: N.L. SAINI)

08:30-09:00	**Registration** – *Sala Laurea*
09:00-09:10	**Opening** – *Sala Lauree*
09:10-09:45	**Takuro Katsufuji, Waseda University Tokyo** *Metal.insulator transition and large negative magnetoresistance in* $Ba_{3-x}Cu_xNb_5O_{15}$
09:45-10:10	**Valerio Scagnoli, ETH-PSI Zurich** *Coupling between electronic band structure and magnetic ordering in* $NaOsO_3$*: insights from magnetization dynamics experiments*
10:10-10:30	**Yuki Sakai, KISTEC Kanagawa** *A-site and B-site charge ordering in perovskite-type* $PbCoO_3$

10:30-11:00 Coffee Break

S2 (Chairperson: T. KATSUFUJI)

11:00-11:35	**Takashi Mizokawa, Waseda University Tokyo** *Domain-dependent surface states with peculiar spin texture in* $IrTe_2$
11:35-12:05	**Marco Grilli, Sapienza Roma** *Inhomogeneity and filamentary superconductivity in oxide and transition metal dichalcogenides heterostructures*
12:05-12:30	**Antonio Polimeni, Sapienza Roma** *Strained-induced exciton hybridisation in transition metal dichalcogenide monolayers unveiled by high magnetic field photoluminescence*

12:30-14:00 Lunch

S3 (Chairperson: T. MIZOKAWA)

14:00-14:35	**Hiroshi Eisaki, AIST Tsukuba** *Competing order in the 1144-type iron-based superconductors*
14:35-15:00	**Nicola Poccia, IFW Dresden** *Advances in the twistronics of high temperature superconductors*
15:00-15:15	**Luca Tomarchio, Sapienza Roma** *The Electrodynamics Properties of Superconducting $Nd_{0.8}Sr_{0.2}NiO_2$ Nickelate*
15:15-15:30	**Giovanni Tomassucci, Sapienza Roma** *Temperature dependent local inhomogeneity and local magnetic moment of $Li_{1-x}Fe_xOHFeSe$ superconductor*

15:30-16:00 Coffee Break

S4 (Chairperson: M. GRILLI)

16:00-16:25	**Lilia Boeri, Sapienza Roma** *Search for ambient superconductivity in the Lu-N-H system*
16:25-16:50	**Riccardo Mazzarello, Sapienza Roma** *Phase change materials for data storage and neuromorphic computing*
16:50-17:15	**José Lorenzana, ISC-CNR Roma** *Rashba driven superconductivity in incipient ferroelectrics*
17:15-17:40	**Lorenzo Celiberti, Wien University Wien** *Janh-Teller polaron in the spin-orbit multipolar magnetic oxide Ba_2NaOsO_6*
17:40-18:00	**Mattia Udina, Sapienza Roma** *Terahertz driven ionic Kerr effect and dynamical multiferroicity in $SrTiO_3$*

Tuesday 4 July, 2023

S5 (Chairperson: H. EISAKI)

08:30-09:05	**Masaki Azuma, Tokyo Institute of Technology Tokyo** *Magnetization reversal by electric field in Co substituted $BiFeO_3$*
09:05-09:30	**Eugenio Del Re, Sapienza Roma** *Spontaneous formation of polarization chiral lattices and supercrystals in near-transition ferroelectric potassium-lithium-tantalate-niobate*
09:30-09:55	**Boby Joseph, Elettra Sincrotrone Trieste** *Pressure enhanced superconductivity in cage-type quasi-skutterudite compounds*
09:55-10:20	**Hena Das, Tokyo Institute of Technology Tokyo** *Competing magnetic phases and spin-reorientation transitions in ortho-and hexa-ferrites*

10:30-11:00 Coffee Break

S6 (Chairperson: M. AZUMA)

11:00-11:25	**Eugenio Paris, SwissFEL – PSI Villigen** *Probing ultrafast dynamics in correlated materials with time-resolved resonant inelastic x-ray scattering*
11:25-11:50	**Gaetano Campi, IC-CNR Roma** *Quantum materials as seen by high resolution X ray synchrotron techniques*
11:50-12:10	**Federico Stramaglia, SLS-PSI Villigen** *Probing the interfacial band structure of BaTiO3/La0.8Sr0.2MnO3 multiferroic heterostructures with ARPES*
12:10-12:30	**Takumi Nishikubo, KISTEC Kanagawa** *Systematic charge distribution changes in Bi, Pb-3d transition metal perovskite oxides*
12:30	**Closing**

Metal-insulator transition and large negative magnetoresistance in $Ba_{3-x}Eu_xNb_5O_{15}$

Takuro Katsufuji, Kenta Iwamoto, Wataru Sekino, Ryosuke Takei, Satomi Ito, and Haruki Takei[1]

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$Ba_3Nb_5O_{15}$ has a tetragonal tungsten bronze structure with 0.2 electrons per Nb in the 4*d* orbital, which is responsible for its metallic conduction. It is known that it becomes insulating by substituting Sr for Ba [1-3], though the nominal number of electrons per Nb remains the same. We grew single crystals of the series of compounds in which Ba is substituted by various rare earths *R*. We found that *R* = Eu becomes divalent and its substitution for Ba results in the metal-insulator transition, similarly to the Sr substitution. We also found that $Ba_{3-x}Eu_xNb_5O_{15}$ exhibits a large negative magnetoresistance, probably caused by the coupling between the conduction electrons in Nb 4*d* orbitals and the 4*f* spins in the Eu ions, and its magnitude $\rho(0)/\rho(H)$ is enhanced and amounts to $\sim 5 \times 10^3$ near the metal-insulator phase boundary [4]. We also measured the Hall coefficient, Seebeck coefficient, and optical conductivity of these compounds, and found a substantial decrease in the number of conduction electrons as approaching the metal-insulator phase boundary, which may be responsible for the enhancement of negative magnetoresistance.

[1] T. Yasuda *et al.*, Phys. Rev. B **102**, 205133 (2020).

[2] Y. Kondoh *et al.*, Phys. Rev. B **104**, 125128 (2021).

[3] R. Nakamura *et al.*, J. Phys. Soc. Jpn. **91**, 064711 (2022).

[4] K. Iwamoto *et al.*, J. Phys. Soc. Jpn. **91**, 033702 (2022).

Coupling between electronic band structure and magnetic ordering in $NaOsO_3$: insights from magnetization dynamics experiments

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The strong connection between the electronic band structure and magnetic ordering of $NaOsO_3$ has garnered considerable interest recently [1-3]. $NaOsO_3$ undergoes an insulator to metal transition at the unusually high temperature of 411 K and presents also low temperature anomalies in the resistivity that has sparkled interest both on the nature of the phase transition and of the evolution of the band gap with temperature. We have used muon spin rotation spectroscopy and time-resolved x-ray diffraction at free electron laser to get more insight on the role of the magnetic fluctuations and magnetization dynamics in the vicinity of the phase transition. Our x-ray measurements demonstrate that the antiferromagnetic long-range order in question melts within sub-100 fs, significantly faster than the lattice dynamics observed in the intensity of selected Bragg structural reflections, which decrease over several ps [4]. Furthermore, we conducted muon spin relaxation measurements around T_A = 30 K, as this temperature range was implicated in the emergence of an anomaly in the electrical resistivity, potentially linked to a gradual decrease in the Os magnetic moment caused by spin fluctuations [2]. Our findings indicate that there is no significant alteration in the frequency of spin fluctuations at T_A, as observed within muon probing time scale [5].

[1] S. Calder *et al.*, Phys. Rev. Lett., **108**, 257209 (2012)

[2] B. Kim *et al.*, Phys. Rev. B, **94**, 241113 (2016)

[3] J. G. Vale *et al.*, Phys. Rev. Lett., **120**, 227203 (2018)

[4] F. Giorgianni *et al.*, Phys. Rev. B., **105**, 155147 (2022)

[5] N. Gurung *et al.*, J. Phys.: Condens. Matter, **33**, 335802 (2021)

A-site and B-site charge ordering in perovskite-type $PbCoO_3$

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Charge degree of freedom in transition metals gives rise to various fascinating properties such as charge ordering associated with metal–insulator transition, high-temperature superconductivity, colossal magnetoresistance and high thermopower. Metal ions with half-integer valence tend to split into two integer valence ions and these get spatially ordered as typically observed in $La_{0.5}Ca_{0.5}Mn^{3.5+}O_3$.[1] To realize a half-integer valence state and charge ordering in the B site of a perovskite ABO_3, it is generally necessary to mix two or more elements with different valences in the A site. Perovskite $PbCoO_3$ synthesized at 12 GPa was found to have an unusual average charge distribution of $Pb^{3.5+}Co^{2.5+}O_3$ with half-integer valences in both of A and B sites in spite of the simple chemical composition of Pb, Co, and O. Comprehensive studies using electron diffraction, synchrotron X-ray diffraction (SXRD), neutron powder diffraction (NPD), Hard X-ray photoemission spectroscopy, soft X-ray absorption spectroscopy and measurements of magnetic and electrical properties provide evidence of lead ion and cobalt ion charge ordering leading to $Pb^{2+}Pb^{4+}{}_3Co^{2+}{}_2Co^{3+}{}_2O_{12}$ quadruple perovskite structure.[2] Moreover, a series of *in situ* high-pressure measurements including electrical transport, NPD, SXRD, emission, and absorption spectroscopies revealed the pressure-induced sequential spin state transition and intermetallic charge transfer in $PbCoO_3$.[3] Here we show that half-integer valence states in both the A and B sites can be stabilized by tuning the energy levels of Pb 6*s* and transition metal 3*d* orbitals.

[1] P. G. Radaelli et al., *Phys. Rev. B*, **55**, 3015–3023 (1997).

[2] Y. Sakai et al., *J. Am. Chem. Soc.*, **139**, 4574-4581 (2017).

[3] Z. Liu, Y. Sakai et al., *J. Am. Chem. Soc.*, **142**, 5731-5741 (2020).

Domain-dependent surface states with peculiar spin texture in $IrTe_2$

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Angle-resolved photoemission spectromicroscopy with submicron resolution (nano-ARPES) is a powerful technique to study electronic structure of microcrystals and microdomains. $IrTe_2$ is a unique layered transition-metal dichalcogenide which exhibits a first order phase transition with stripe-type charge-orbital order at about 280 K [1,2] associated with the orbitally induced Peierls mechanism [3]. In a recent nano-ARPES study on $IrTe_2$ surface, we observed two types of domains with striped texture at 250 K and three types of domains with trijunction texture at 47 K [4]. The evolution of domain texture at the surface is related to the periodicity change of the charge-orbital order in the bulk. Each domain harbors quasi one-dimensional surface bands forming fragmented Fermi surfaces (Fermi arcs). The direction of the Fermi arcs is perpendicular to that of the stripe-type charge-orbital order. The Fermi arcs exhibit peculiar spin polarization which can be probed by spin-resolved ARPES. The spin texture of the domain-dependent surface states indicates that the Ir 5d and Te 5p spin-orbit interaction plays an important role in the charge-orbital order of $IrTe_2$.

The present work has been performed in collaboration with A. Barinov, V. Kandyba, A. Giampietri, R. Matsumoto, Y. Okamoto, K. Takubo, K. Miyamoto, T. Okuda, S. Pyon, H. Ishii, K. Kudo, M. Nohara, and N. L. Saini.

[1] S. Pyon, K. Kudo, and M. Nohara, *J. Phys. Soc. Jpn.* **81**, 053701 (2012).

[2] J. J. Yang, Y. J. Choi, Y. S. Oh, A. Hogan, Y. Horibe, K. Kim, B. I. Min, and S.-W. Cheong, *Phys. Rev. Lett.* **108**, 116402 (2012).

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[4] T. Mizokawa, A. Barinov, V. Kandyba, A. Giampietri, R. Matsumoto, Y. Okamoto, K. Takubo, K. Miyamoto, T. Okuda, S. Pyon, H. Ishii, K. Kudo, M. Nohara, N. L. Saini, *Adv. Quantum Technol.* **5**, 2200029 (2022).

Inhomogeneity and filamentary superconductivity in oxide and transition metal dichalcogenides heterostructures

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Keywords : twodimensional superconductors, transition metal dichalcogenides, electronic phase separation

Recent progress in the fabrication of 2D highly ordered thin films and in increasing their electron density both by chemical doping or gating has opened a new field with a wealth of interesting physical effects. These range from superconductivity in monolayers, sizable spin-orbit coupling, competition with spatially ordered phases like CDW. We analyze transport properties in terms of a phenomenological model of an exactly solvable random impedance network, representing an inhomogeneous system where superconducting regions are embedded in a normal metal matrix. We find that $LaAlO_3/SrTiO_3$ heterostructures, TMD systems like $TiSe_2$, MoS_2, or ZrNCl are electronically inhomogeneous [1-3], with filamentary superconducting condensate whose macroscopic coherence still needs to be fully investigated and understood. We show how the dissipative (reactive) response of the system non-trivially depends on both the macroscopic and microscopic characteristics of the metallic (superconducting) fraction. We compare our calculations with resonant-microwave transport measurements performed on $LaAlO_3/SrTiO_3$ heterostructures over an extended range of temperatures and carrier densities finding that the filamentary character of superconductivity accounts for unusual peculiar features of the experimental data.

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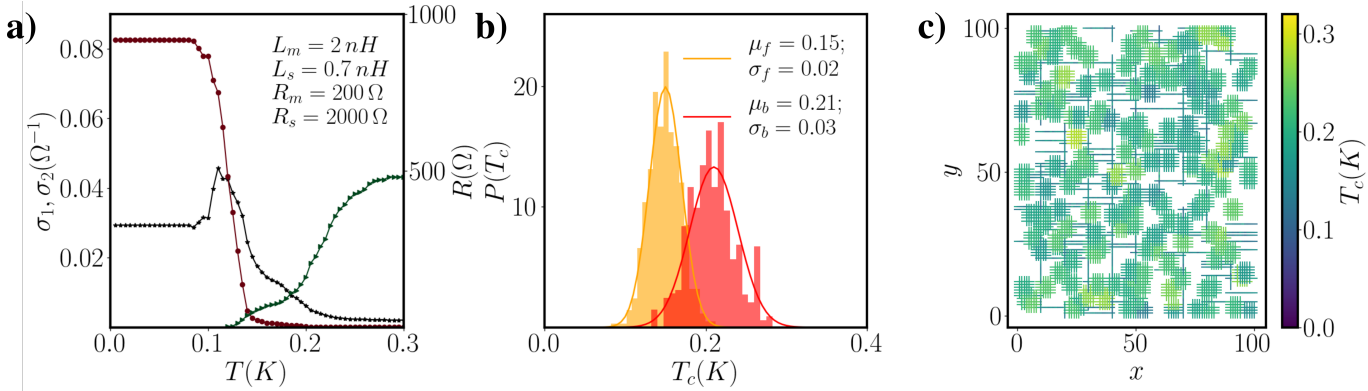

Figure: Temperature dependence of complex conductivity and DC resistivity (a) calculated with the Random Impedance Network model (b,c) to describe the overdoped regime of $LaAlO_3/SrTiO_3$

Strained-induced exciton hybridisation in transition metal dichalcogenide monolayers unveiled by high magnetic field photoluminescence

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Within the variegated family of two-dimensional crystals, semiconducting transition-metal dichalcogenides (TMDs) show alluring optoelectronic and spin properties in the monolayer (ML) limit, featuring a direct bandgap which results in an efficient visible/near-infrared light emission, and a strong spin-orbit coupling. Furthermore, these materials display exceptional flexibility and robustness and can be subjected to remarkable strains.

Here, we explore new strategies to tune the peculiar properties of 2D TMDs by engendering localised strains in TMD MLs exploiting on low-energy hydrogen-ion irradiation of bulk flakes. This process leads to the formation of ML-thick, highly pressurised micro-/nano-sized domes filled with molecular hydrogen [1].

The domes are durable and incredibly robust, and, due to their single-layer nature, TMD domes behave as efficient light emitters [2,3]. The high strain fields they host cause dramatic changes in the TMD opto-electronic properties, and photoluminescence (PL) steady-state and time-resolved studies enabled the characterisation of the strain-induced band-structure modifications and revealed intriguing phenomena, such as a strain-induced direct-to-indirect bandgap crossover [2]. Magneto-optical measurements allowed us to study the effect of strain on the magnetic moment of the excitons in TMD MLs, and to pinpoint hybridisation phenomena between direct and indirect excitons [4].

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Competing order in the 1144-type iron-based superconductors

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In Iron-based high- transition temperature (high-T_c) superconductors, various ordered phases exist in the vicinity of the superconducting phase. In typical materials, such as $BaFe_2As_2$ – based (122) and LaFeAsO -based (1111) systems, competing order shows up when their structures changes from tetragonal to orthorhombic, which stabilize stripe spin-density wave (SSDW) magnetic order. However, in $CaKFe_4As_4$, so-called 1144 type system, substitution of Fe for other transition metals *TM* (= Co, Ni) stabilizes the hedgehog-type antiferromagnetism (H-AFM) while maintaining the tetragonal crystal structure [1]. Since different ordered phases appear in this 1144 system, despite having similar crystal structures and constituent elements, a comparative study is important for elucidating the relationship between the superconductivity and the competing ordered phase.

In this study, we synthesized $Ca_{1-x}La_xKFe_4As_4$, in which out-of-plane Ca is substituted with La, and studied their physical properties. Here La substitution is expected to dope electrons as *TM* substitution without introducing disorder into Fe planes.

We have found that T_c decreases monotonically with La substitution. This behavior is quite different from that of 122-type $Ba_{1-x}K_xFe_2As_2$. Neutron diffraction results indicate that the magnetic order is also H-AFM type. The magnetic transition temperature T_N was found to be higher with La substitution compared with *TM* substitution. The possible origin for stabilizing H-AFM will be discussed.

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[2] A. Kreyssig et al., Phys. Rev. B 97, 224521 (2018) .

Advances in the twistronics of high temperature superconductors

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Van der Waals heterostructures formed by mechanically stacking layers of 2-Dimensional (2D) materials possess unique properties and new functionalities, not seen in standard materials, that make them an irreplaceable platform for emergent electronics. One of the stumbling stone that hinders the progress in utilizing van der Waals' attractive features in technology, is the fact that many of them, especially the novel topological quantum states and related phenomena are restricted to low temperatures. This poses the challenge of creating van der Waals heterostructures harboring novel topological quantum matter physics at elevated temperatures. This challenge is met by employing high temperature superconductors-based 2D crystals which offer the most advantageous route to increase the temperature range in which the topological states and phenomena associated with van der Waals devices can be used. Realizing this daunting task requires understanding the microscopic mechanisms underlying their properties as well as the developing technologies for their engineering and manipulation. This talk addresses the use of Bi-2212 optimally doped crystals (Tc = 90 K), their chemical complexity is analyzed by studying the role of the oxygen dopants and incommensurate lattice modulation which is a key element for understanding the electrical properties of cuprates. Utilizing solvent- and polymer-free nanofabrication at cryogenic temperatures makes it possible to create Josephson junctions based on high temperature superconductors. This seminar describes the fundamental properties of such twisted junctions and discusses the possibility of introducing twisted high temperature superconductors in electrodynamical quantum circuits.

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The Electrodynamics Properties of Superconducting $Nd_{0.8}Sr_{0.2}NiO_2$ Nickelate

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The intensive search for alternative non-cuprate high-transition-temperature (T_c) superconductors has taken a positive turn recently with the discovery of superconductivity in infinite-layer nickelates. This discovery is expected to be the basis for disentangling the puzzle behind the physics of high T_c in oxides. In the unsolved quest for the physical conditions necessary for inducing superconductivity, we report on a broad-band optical study of a $Nd_{0.8}Sr_{0.2}NiO_2$ film measured using optical and Terahertz spectroscopy, at temperatures above and below the critical temperature $T_c \sim 13$ K. The normal-state electrodynamics of $Nd_{0.8}Sr_{0.2}NiO_2$, can be described by a scattering time at room-T (τ=1.3 × 10^{-14} s) and a plasma frequency (ω_p =5500 cm^{-1}) in combination with an absorption band in the Mid-Infrared (MIR), characteristics of transition metal oxides, located around $\omega_0 \sim 2500$ cm^{-1} and with an amplitude ω_{MIR} of about 8000 cm^{-1}. The degree of electronic correlation can be estimated using the ratio $\omega^2_p/(\omega^2_p + \omega^2_{MIR})$. In the present system, this value is about 0.32 indicating a strong electron correlation in the NiO_2 plane with a similar strength as cuprates. From 300 K to 20 K, we observe a spectral weight transfer between the Drude and MIR band, together with a strong increase in the Drude scattering time, in agreement with DC resistivity measurements. Below T_c, a superconducting energy gap $2\Delta \sim 3.3$ meV can be extracted from the Terahertz reflectivity using the Mattis-Bardeen model.

Temperature dependent local inhomogeneity and local magnetic moment of $(Li_{1-x}Fe_x)OHFeSe$ superconductor

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We have combined extended X-ray absorption fine structure (EXAFS) and X-ray emission spectroscopy (XES) to investigate the local structure and the local iron magnetic moments of $(Li_{1-x}Fe_x)OHFeSe$ (x∼0.2) superconductors. The local structure, studied by Fe K-edge EXAFS measurements, is found to be inhomogeneous that is characterized by different Fe–Se bond lengths. The inhomogeneous phase exhibits a peculiar temperature dependence with lattice anomalies in the local structural parameters at the critical temperature T_c (36 K) and at the spin density wave (SDW) transition temperature T_N (130 K). Fe Kβ XES shows iron to be in a low spin state with the local Fe magnetic moment evolving anomalously as a function of temperature. Apart from a quantitative measurement of the local structure of $(Li_{1-x}Fe_x)OHFeSe$, providing direct evidence of nanoscale inhomogeneity, the results provide further evidence of the vital role that the coupled electronic, lattice and magnetic degrees of freedom play in the iron-based superconductors.

[1] G. Tomassucci et al., Physical Chemistry Chemical Physics, **25**(9), 6684-6692 (2023).

Search for ambient superconductivity in the Lu-N-H system

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Recently, Dasenbrock et al. reported room-temperature superconductivity at near-ambient pressure in N-doped lutetium hydride [1], stimulating a heated debate on the reproducibility of their results.[2] In the absence of conclusive experimental information on the nature and composition of the superconducting phase, first-principles crystal structure prediction represents an invaluable tool to explore the phase diagram and identify candidate phases that could explain the observed superconductivity. [3]

In this work we performed a comprehensive, detailed study of the phase diagram of the Lu-N-H system, sampling over 200,000 different structures to search for superconducting phases. Out of the more than 150 structures predicted to be metastable within ~ 50 meV from the convex hull we identify 52 viable candidates for conventional superconductivity, for which we computed their superconducting properties from Density Functional Perturbation Theory. Although for some of these structures we do predict a finite superconducting T_c, none is even remotely compatible with room-temperature superconductivity reported by Dasenbrock-Gammon et al. [4] Our results are in agreement with other studies that employ different methods for crystal structure prediction, which also conclude that room or even high-temperature superconductivity within the conventional electron-phonon scenario is extremely unlikely in the Lu-N-H system. [5]

[1] N. Dasenbrock-Gammon et al., Nature **615** , 244 (2023).
[2] *see for example:* X. Ming et al., Nature 2023, and N. P. Salke et al., cond-mat/2306.06301.
[3] J.A. Flores-Livas et al., Physics Reports **856**, 1-78 (2020).
[4] P.P. Ferreira et al., cond-mat/2304.04447.
[5] M. Liu et al, cond-mat/2303.06554; K.P. Hilleke et al., cond-mat/2303.15622; M. Gubler et al., cond-mat/2306.07746.

Phase change materials for data storage and neuromorphic computing

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Phase-change materials (PCMs) are an important family of alloys employed in non-volatile memories and neuromorphic devices. These devices exploit the ability of PCMs to undergo rapid and reversible transitions between crystalline and amorphous states showing resistivity contrast. In this talk, I will provide an introduction to PCMs and then discuss phase-change heterostructures, which consist of alternately stacked ultrathin layers of PCMs and transition-metal dichalcogenides (TMDs). These heterostructures are promising candidates for high-performance neuro-inspired computing, in that the TMD layers act as confinement materials and diffusion and thermal barriers, thus reducing energy consumption, long-range atomic migration and drift of the amorphous state of PCMs.

Rashba driven superconductivity in incipient ferroelectrics

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SrTiO3 (STO) and KTaO3 (KTO) are known for their proximity to a ferroelectric phase. STO shows bulk superconductivity with a characteristic domelike behavior resembling systems close to a quantum critical point. Several mechanisms have been proposed to link these phenomena, but the abundance of undetermined parameters prevents a definite assessment. We use ab-initio computations supplemented with microscopic modeling to test different coupling models between conduction electrons and the ferroelectric soft transverse mode. In the case of STO, we find that a Rashba-type one-phonon spin-orbit-assisted coupling can explain the magnitude of the critical temperature and the dome-like behavior (Fig. 1). The dome is attributed to a momentum-dependent quenching of the angular momentum due to a competition between spin-orbit and hopping energies. The optimum density for having maximum Tc results in good agreement with experiments without free parameters. These results make the generalized Rashba dynamic coupling to the ferroelectric soft mode a compelling pairing mechanism to understand bulk superconductivity in doped SrTiO3. We will also discuss a two-phonon mechanism and its applicability to these and other materials.

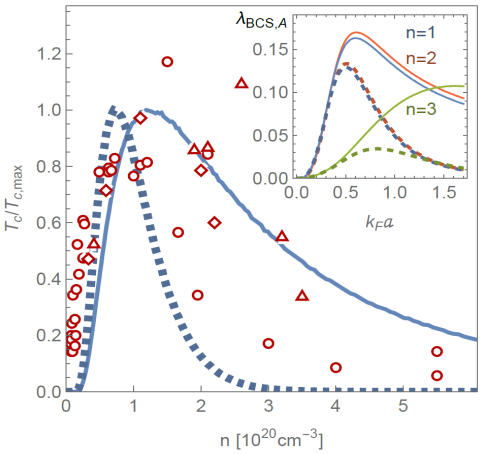

Figure 1. Tc dome (normalized to its maximum value) vs. carrier density. The full (dashed) line neglects (includes) the hardening of the TO mode with density. Inset: band resolved λ_{BCS} using the ab initio results. Open symbols are bulk Tc experimental data from C. S. Koonce et al, PRB 1967 (circles), C. Collignon et al. PRB 2017 (triangles) and Thiemann et al. PRL 2018 (diamonds) using Tc,max = 0.35K.

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Janh-Teller polaron in the spin-orbit multipolar magnetic oxide Ba_2NaOsO_6

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Complex oxides hosting 5d electrons present a variety of exotic phases arising from spin-orbital (SO) interactions and electronic correlation (EC) [1]. In the Mott insulator Ba_2NaOsO_6, a canted antiferromagnet with multipolar interactions [2], strong EC together with Jahn-Teller (JT) lattice activity pave the way for bridging polarons and SO coupling, distinct quantum effects that play a critical role in charge transport and spin-orbitronics [3, 4]. Polarons are quasiparticles originating from strong electron-phonon interaction and are ubiquitous in polarizable materials, especially in 3d transition metal oxides [3]. Despite the more spatially delocalized nature of 5d electrons, we demonstrate the formation of *Jahn-Teller spin-orbital polarons* in electron doped $Ba_2Na_{1-x}Ca_xOsO_6$ by combining ab-initio calculations with nuclear magnetic resonance and muon spin rotation measurements. The polaronic charge trapping process converts the Os $5d^1$ spin-orbital $J_{eff} = 3/2$ levels, characteristic of pristine BNOO, into a $5d^2$ $J_{eff} = 2$ manifold, leading to the coexistence of different J-effective states in a single-phase material. Moreover, we suggest that polaron formation creates robust in-gap states that prevent the transition to a metal phase even at ultrahigh doping, thus preserving the Mott gap across the entire doping range from d^1 BNOO to d^2 Ba_2CaOsO_6.

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Terahertz driven ionic Kerr effect and dynamical multiferroicity in $SrTiO_3$

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The Kerr effect measures the birefringence induced in an otherwise isotropic material by a DC or AC applied electric field. Its ultrafast implementation with AC optical pulses has been widely used to investigate the nonlinear optical properties of many different systems. More recently, its THz counterpart has shown the ability to induce a largely enhanced response due to the resonant excitation of Raman-like processes involving lattice vibrations[1] or broken-symmetry electronic and magnetic collective modes[2,3]. In a recent work[4], we have provided experimental evidence that in insulating $SrTiO_3$ also infrared-active lattice vibrations can give rise to a sizeable terahertz Kerr effect, named ionic Kerr effect, thanks to a non-linear excitation of multiple phonon modes[5]. Such a signal can be disentangled from the off-resonant electronic excitations responsible for the conventional electronic Kerr effect by moving out the light-phonon resonance condition with temperature. Its identification is made possible thanks to a quantitative theoretical modelling[6] linking the measured birefringence signal to the microscopic processes responsible for the time and polarization dependence of both the ionic and electronic contribution. When circularly polarized pulses are applied, an additional contribution besides the Kerr effect has been observed[7]. We have shown that this component can be related with a quasi-static macroscopic magnetization induced by the circular motion of the ions, in agreement with the theory of dynamical multiferroicity[8].

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Magnetization reversal by electric field in Co substituted $BiFeO_3$

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Electric field manipulation of magnetization is intensively investigated because of potential application in low-power-consumption non-volatile magnetic memory devises. Ferroelectric $BiFeO_3$ has a cycloidal space-modulated spin structure with a periodicity of 62 nm superimposed on the G-type antiferromagnetic structure which prohibits the appearance of net ferromagnetic magnetization due to spin canting. We have observed a spin structure transition from low-temperature cycloidal one to high-temperature collinear one with at ~200 K using Mössbauer spectroscopy in rhombohedral $BiFe_{0.1}Co_{0.9}O_3$ thin films fabricated by PLD on $SrTiO_3$ (STO) (111) substrate [1, 2]. Spontaneous magnetization of 0.03 u_B/f.u. confined in a magnetic easy plane perpendicular to the electric polarization is generated by Dzyaloshinskii-Moriya interaction. Films fabricated on $GdScO_3$ (110) substrate has out-of-plane component of magnetization which can be observed by magnetic force microscopy (MFM). It is demonstrated that the out-of-plane magnetization can be reversed by electric polarization reversal using piezoresponse force microscopy (PFM) at room temperature [3, 4] while the magnetization reversal is absent when the polarization reversal is in-plane [5].

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Spontaneous formation of polarization chiral lattices and supercrystals in near-transition ferroelectric potassium-lithium-tantalate-niobate*

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In this talk I will review our recent experimental and theoretical exploration of spontaneous 3D ferroelectric vortex structures in near-transition potassium-lithium-tantalate-niobate. Results include linear and nonlinear optical analysis, broadband spectroscopy, and structural studies, these compared to phase-field numerical simulations. The picture opens up an interesting setting where high-dimensional symmetry breaking transitions support new mesoscopic crystal states with unexpected behavior, such as giant optical refraction and constraint-free second-harmonic-generation

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Pressure enhanced superconductivity in cage-type quasi-skutterudite compounds

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Recently, we have been involved in systematic HP studies of both $R_5Rh_6Sn_{18}$ (R= Sc, Y) and $R_3Rh_5Sn_{13}$ (R = Sr, Ca, La) quasi-skutterudite systems [1,2]. In most of the investigated systems, there is a continuous increase in Tc with pressure. For example, the $Sc_5Rh_6Sn_{18}$ system show a continuous increase in Tc from 4.99 K at ambient pressure to 5.24 K at 2.5 GPa [1] and $Sr_3Rh_5Sn_{13}$ show a continuous increase in Tc from 4.85 K at ambient pressure to 6.43 K at 3.2 GPa [2]. Rattling atom (R) in the quasi-skutterudite lattice is found to lead to Raman-modes whose pressure-dependence can contribute to the understanding of electron-phonon coupling in these systems. Our HP Raman investigation combined with x-ray diffraction studies indicated a smooth evolution of lattice under pressure in the 0-10 GPa range in most of the above systems. Combining several members from each of the two families permit us to combine both physical and chemical pressure effects to provide a more universal PT phase diagram.

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Competing magnetic phases and spin-reorientation transitions in ortho- and hexa- ferrites

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When multiple magnetic sublattices are formed in a single-phase structure, mutual magnetic interactions between these sublattices lead to unique magnetic and related phenomena, such as spin-reorientation (SR) transitions, ferrimagnetism, magnetoelectricity and topological orders. The formation of these magnetic sublattices can be attributed to many factors, such as certain chemical compositions or the formation of unique charge-ordered (CO) states. In this presentation, I will discuss magnetic properties of two ferrite systems, $PbFeO_3$ [1] and $LuFeO_3$ [2-3], where the multiple magnetic sublattices originate from unique CO states and hence bear significant consequences. In $PbFeO_3$ ortho-ferrite, we have observed SR transition at high temperature (~ 418 K). We showed that a non-trivial Pb^{2+}/Pb^{4+} CO state creates two magnetic Fe1 and Fe2 sublattices with mutually competing magnetic anisotropies and hence trigger the SR transition. In $LuFeO_3$ based hexa-ferrites, certain non-polar phonon distortion ($\boldsymbol{Q_{K_3}}$) not only induces ferroelectric (FE) and ferromagnetic (FM) orders, but also a strong coupling between them and topological orders [2]. Recently, we have proposed an idea to realize non-collinear Fe^{2+}/Fe^{3+} CO ferrimagnetic orders near room temperature having a considerably high magnetization $\mathbf{M} \sim 1.1 - 1.3\ \mu_B$/Fe their strong coupling with FE ($\mathbf{P} \sim 6 - 15\ \mu C/cm^2$) order driven by the antisymmetric Dzyaloshinskii-Moriya (DM) exchange interaction between the localized spins in the electron doped $LuFeO_3$ [3]. I shall deliberate upon that and discuss in detail the microscopic mechanisms to achieve electric field induced spin-reorientation transitions and magnetic switching phenomena.

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Probing ultrafast dynamics in correlated materials with time-resolved resonant inelastic x-ray scattering

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In the realm of strongly correlated materials with entangled degrees of freedom, accessing the ultrafast dynamics involving different energy scales in a single experiment, with momentum resolution, promises excellent scientific insight. With the recent advent of free-electron lasers (FEL), time-resolved resonant inelastic x-ray scattering (tr-RIXS) has emerged as a unique technique capable of unraveling such information. However, its complete realization has been hindered thus far by the limitations of available time and/or energy resolution. In this talk, I will present early results in this field and introduce Furka, the soft-x-ray experimental station for condensed matter of the SwissFEL. Its primary goal is to provide state-of-the-art tr-RIXS experiments in combination with a widely tunable pump laser radiation. Having successfully completed the installation phase, Furka is set to launch its user program in 2024.

Quantum materials as seen by high resolution X ray synchrotron techniques

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Dynamical structural disorder at different length scale plays an important role in the functionality of complex materials [1]. Here different topological templates and weak interactions between building units produce phase separation in different ultrastructure configurations with correlated disorder [2-4]. Achieving optimal material performance requires a quantitative knowledge of this functional correlated disorder, as well as its evolution under external stimuli. In this contest we propose new experimental approaches based on high resolution probes, jointly to advanced modelling and statistical tools for big data analysis [4,5]. Examples of complex functional materials can be found in different fields ranging from biology to quantum science where unique and anomalous properties such as high-temperature superconductivity can emerge, due to the interplay of dopants, charge and spin ordering at nanoscale, in atomic layers or in low-dimensional materials [6-8].

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Probing the interfacial band structure of $BaTiO_3/La_{0.8}Sr_{0.2}MnO_3$ multiferroic heterostructures with ARPES

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We have studied the interfacial band structure of $BaTiO_3$/ $La_{0.8}Sr_{0.2}MnO_3$ multiferroic heterostructures for two different ferroelectric polarizations of the $BaTiO_3$ film, with the goal to link the orbital occupancy with the variation in the magnetic properties in the $La_{0.8}Sr_{0.2}MnO_3$ layer. The ferroelectric polarization of the $BaTiO_3$ is determined by controlling the termination of the $SrTiO_3$ substrate and the heterostructures are characterized with transport and SQUID measurements, confirming the hole accumulation and depletion state of the $La_{0.8}Sr_{0.2}MnO_3$. We take advantage of soft x-ray angle resolved photoemission spectroscopy to probe the buried interfacial $La_{0.8}Sr_{0.2}MnO_3$ band structure; specifically, the $e_{g(z2-r2)}$ derived electron band and $e_{g(x2-y2)}$ hole bands are probed as we switch the ferroelectric polarization of the $BaTiO_3$ layer, changing the interfacial $La_{0.8}Sr_{0.2}MnO_3$ charge state from depletion to accumulation state.

Systematic charge distribution changes in Bi, Pb-3d transition metal perovskite oxides

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Bi and Pb have a unique $6s^0$ and $6s^2$ electron configuration that creates charge degrees of freedom. Due to the lack of this $6s^1$ electron configuration, a property called valence skipper, Bi takes 3+ and 5+ and Pb takes 2+ and 4+. In particular, for perovskite compounds containing Bi or Pb at the A site, the valence state changes according to the depth of the d-orbitals of the transition metal ions corresponding to the order in the periodic table of the elements due to the close relationship between the 6s level of Pb or Bi and the 3d level of the 3d transition metal ions. For example, for $BiMO_3$, M= Cr, Mn, Fe, Co, the state is $Bi^{3+}M^{3+}O_3$, while $BiNiO_3$ has a specific valence state of $Bi^{3+}_{0.5}Bi^{5+}_{0.5}Ni^{2+}O_3$. $PbMO_3$ has $Pb^{2+}_{0.5}Pb^{4+}_{0.5}MO_3$ for M= Ti and V, $Pb^{2+}_{0.5}Pb^{4+}_{0.5}M^{3+}O_3$ for M= Cr and Fe, $PbCoO_3$ has $Pb^{2+}_{0.25}Pb^{4+}_{0.75}Co^{2+}_{0.5}Co^{3+}_{0.5}O_3$, $PbNiO_3$ has $Pb^{4+}Ni^{2+}O_3$. In $BiNiO_3$ and $PbMO_3$ (M = Cr, Fe and Co), Bi and Pb become charge disproportionated in the $6s^0$ and $6s^2$ states, and temperature- and pressure-induced elimination of charge disproportionation and charge transfer phase transitions occur. The valence of the transition metal M is changed in this process, which leads to unique properties such as metal-insulator transition and negative thermal expansion. In this study, we evaluated the electronic states of these materials by HAXPES, and the crystal structure distortions caused by these electronic states were investigated by crystal structure analysis using synchrotron radiation X-ray diffraction and local structure analysis using atomic pair distribution function (PDF) obtained from synchrotron radiation X-ray total scattering patterns.

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2-Sunday	3-Monday	4-Tuesday	5- Wednesday
	08:30-10:30 **Registration** **(S1-N L SAINI)** **09:00 Opening** 09:10-09:45 T. Katsufuji 09:45-10:10 V. Scagnoli 10:10-10:30 Y. Sakai	**08:30-10:30** **(S5-H. EISAKI)** 08:30-09:05 M. Azuma 09:05-09:30 E. Del Re 09:30-09:55 B. Joseph 09:55-10:20 H. Das -Remote	**D** **E** **P** **A** **R** **T**
	10:30 -11.00 Coffee Break	**10:30 -11.00 Coffee Break**	
	11:00-12:30 **(S2-T. KATSUFUJI)** 11:00-11:35 T. Mizokawa 11:35-12:05 M. Grilli 12:05-12:30 A. Polimeni	**11:00-12:30** **(S6- M. AZUMA)** 11:00-11:25 E. Paris 11:25-11:50 G. Campi 11:50-12:10 F. Stramaglia 12:10-12:30 T. Nishikubo	
	12:30-Lunch Break	**12:30 - Closing**	
	14:00-15:40 **(S3- T. MIZOKAWA)** 14:00-14:35 H. Eisaki 14:35-15:00 N. Poccia 15:00-15:15 L. Tomarchio 15:15-15:30 G. Tomassucci		
	15:30-Coffee Break		
A **R** **R** **I** **V** **E**	**16:00-18:00** **(S4- M. GRILLI)** 16:00-16:25 L. Boeri 16:25-16:50 R. Mazzarello 16:50-17:15 J. Lorenzana 17:15-17:40 L. Celiberti 17:40-18:00 M. Udina		