ESRF - EBS Workshop Series

STREAMLINE

ESRF-EBS
Extremely Brilliant Source

Workshop on Quantum Materials

ESRF - Grenoble - France
5 - 6 - 7 October 2022

Venue	**ESRF**
Organisers	**Björn Wehinger, ESRF, Grenoble** **Nicholas Brookes, ESRF, Grenoble**
Assistants	**Claudine Roméro, ESRF, Grenoble** **Eleanor Ryan, ESRF, Grenoble**
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Scope

Quantum many body effects that alter the macroscopic behaviour of materials give rise to exciting new phenomena to be exploited in future quantum technology. This workshop focuses on novel experimental capabilities for the discovery of exotic phases and characterisation of their fundamental excitations. We aim on bringing together the most recent advances in quantum many body physics and materials science, thereby showing how exceptional materials properties can be obtained by controlling electronic and magnetic properties by materials design and by application of external stimuli such as temperature, magnetic field and pressure.

The program comprises state-of-the-art talks on the frontier of the field followed by a detailed discourse on the most advanced experimental techniques at the ESRF. In this context, a special focus is dedicated to the new high-pressure beamline ID27 with its outstanding capabilities for experiments at extreme pressures and temperatures combined with state-of-the art sample environments. We will furthermore discuss future challenges beyond current capabilities to define possible efforts in experimental developments.

STREAMLINE

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EBS workshop on Quantum Materials

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ESRF, Grenoble, France

ESRF auditorium

ESRF The European Synchrotron

P R O G R A M M E

Wednesday 5th October 2022

08:15 - 09:15	**Registration in the ESRF Central Building entrance hall and welcome coffee**	
09:15 - 09:30	**Welcome and introduction by N. Brookes**	
09:30 - 10:30	**Session 1** ***Chair: N. Brookes***	
09:30 - 10:05	The Use of Synchrotron Radiation to reveal Some Quantum Properties in Hydrogen under Pressure: Past, Present and Future	**P. Loubeyre,** *CEA Bruyères-le-Chatel, France*
10:05 - 10:30	Magnetic Imaging at High Pressure inside Diamond Anvil Cells using Ensembles of Nitrogen-Vacancy Centers	**L. Toraille,** *CEA Bruyères-le-Chatel, France*
10:30 - 11:00	**Coffee break**	
11:00 - 12:30	**Session 2** ***Chair: P. Loubeyre***	
11:00 - 11:35	Quantum materials in and beyond equilibrium	**C. Rüegg,** *PSI Villigen, Switzerland*
11:35 - 12:00	Quantum Simulation of Spin-charge Separation by Inelastic Scattering Experiments	**B. Wehinger,** *ESRF Grenoble, France*
12:00 - 12:25	Bose-Einstein Condensate of Dirac Magnons	**J. Schaltegger,** *Yale University New Haven, USA*
12:30 - 14:00	**Lunch at the EPN campus restaurant**	
14:00 - 15:25	**Session 3** ***Chair: P. Bruno***	
14:00 - 14:35	Do Quantum Worms order into a Crystal? Quantum Spin Ice in a [100] Magnetic Field	**O. Sikora,** *Cracow University of Technology, Poland*
14:35 - 15:00	Investigation of New S_{eff} = ½ Pyrochlore Antiferromagnets: Structural and Magnetic Properties of $NaCdM_2F_7$ (M = Cu^{2+}, Co^{2+})	**A. Kancko,** *Charles University Prague, Czech Republic*
15:00 - 15:25	*Ab Initio* Study of Random Hexagonal Close-Packed Phase in Platinum - Workshop on Quantum Materials	**L. Burakovsky,** *Los Alamos National Laboratory, USA*
15:30 - 16:00	**Coffee break**	
16:00 - 17:00	**Session 4** ***Chair: O. Sikora***	
16:00 - 16:35	Narrow Bands and Dissipation in Quantum Materials	**F.M. Grosche,** *Cavendish Laboratory Cambridge, UK*
16:35 - 17:00	Singularity and Magnetism Engineering – the role of structure-property relationships in controlling quantum materials	**A.W. Rost,** *Laboratory University of St Andrews, UK*
17:30 - 19:00	**Poster session with drinks followed by dinner at the EPN campus restaurant**	

Thursday 6th October 2022

09:00 - 10:25	**Session 5** ***Chair: G. Garbarino***	
09:00 - 09:35	Materials Science and Crystallography: from the Gigapascal to the Terapascal	**D. Laniel,** *University of Edinburgh, UK*
09:35 - 10:00	Imaging Dilute Antiferromagnetic Spin Textures in a Single Shot Geometry using Resonant Coherent X-ray Diffraction	**R. Basak,** *University of California San Diego, USA*
10:00 - 10:25	5*f* Electron Occupancy and Hybridization in the UTe_2 Superconductor from XANES and XMCD Studies	**F. Wilhelm,** *ESRF Grenoble, France*
10:30 - 11:00	**Coffee break**	
11:00 - 12:15	**Session 6** ***Chair: N. Brookes***	
11:00 - 11:25	Proximity Induced Novel Cu-CDW and Cu-magnons in Epitaxial $YBa_2Cu_3O_7$/ $Nd_{1-x}(Ca_{1-y}Sr_y)_xMnO_3$ Interface	**S. Sarkar,** *University of Fribourg, Switzerland*
11:25 - 11:50	Undamped Spin Waves in the Intermetallic Antiferromagnet $CeCo_2P_2$	**G. Poelchen,** *ESRF Grenoble, France*
11:50 - 12:15	Extreme Conditions Studies at the EBS-ESRF	**G. Garbarino,** *ESRF Grenoble, France*
12:30 - 14:00	**Lunch at the EPN campus restaurant**	
14:00 - 15:30	**Beamline Visits (ID12, ID27, ID28, ID32)**	
15:30 - 16:00	**Coffee break**	
16:00 - 17:30	**Session 7** ***Chairs: N. Brookes and M. Mezouar***	
16:00 - 16:45	Summary on Novel Experimental Capabilities	**M. Mezouar, A. Rogalev and T. Schulli**, *ESRF Grenoble, France*
16:45 - 17:30	Discussion on Future Experiments and Development of Novel Capabilities	
20:00 - 22:30	**Workshop dinner at the Restaurant Pèr'Gras, La Tronche**	

Friday 7th October 2022

09:00 - 10:25	**Session 8** ***Chair: B. Wehinger***	
09:00 - 09:35	Interacting Electrons in Layered Materials - shall we go to Extremes?!	**J. Geck,** *TU Dresden, Germany*
09:35 - 10:00	Uncovering the *S* = ½ Kagome Ferromagnet within a Family of Metal-organic Frameworks	**S. Ivko,** *University of Birmingham, UK*
10:00 - 10:25	Resolving Emergent Structure States in 2D Systems by High-energy X-ray Diffraction	**V. Petkov,** *Central Michigan University, USA*

10:30 - 11:00	**Coffee break**	
11:00 - 12:15	**Session 9** ***Chair: C. Sahle***	
11:00 - 11:25	Uniaxial Pressure Tuning of Charge-stripe Order in La-based Cuprates	**Q. Wang,** *Universität Zurich, Switzerland*
11:25 - 11:50	Charge and Spin Excitations in Infinite-layer Superconducting Nickelates	**L. Martinelli,** *Politecnico di Milano, Italy*
11:50 - 12:15	**Closing remarks by J. Geck**	
12:15 - 14:00	**Lunch at the EPN campus restaurant**	

Speakers' Abstracts

Magnetic Imaging at High Pressure inside Diamond Anvil Cells using Ensembles of Nitrogen-Vacancy Centers

L. Toraille[1,2], A. Hilberer[2], M.-P. Adam[2], M. Schmidt[2], F. Occelli[1], P. Loubeyre[1], J.-F. Roch[2]

[1]CEA, DAM, DIF, F-91297 Arpajon, France, [2]Université Paris-Saclay, CNRS, ENS Paris-Saclay, CentraleSupélec, LuMIn, 91405, Orsay, France

The diamond anvil cell (DAC) is the tool that allows scientists to create pressures comparable to those existing in the Earth core, above the megabar. These conditions lead to new states of matter with specific magnetic and superconducting properties. However, the minute size of the sample and the constraints associated to the DAC make the implementation of magnetic diagnostics highly challenging. We will report the realization of an optical magnetometry technique that can detect the sample magnetic behavior through the diamond anvil, based on Nitrogen-Vacancy (NV) centers located at the surface of the anvil.

The NV center is a quantum object with a spin-dependent photoluminescence. By combining a microwave excitation and an optical excitation/readout (see Figure 1), we can access the relative positions of its energy levels, which give us a direct information on its environment. We focus on the reconstruction of the full vector magnetic field inside the diamond anvil cell, which we managed to do at pressures as high as 80 GPa so far. Furthermore, the relative simplicity of the setup enables its transportation and use on a synchrotron beamline.

As a proof-of-principle, we detected the α-ε phase transition of iron with pressure through the monitoring of its magnetization, while simultaneously following the crystalline phase transition via X-ray diffraction [1]. We will also report experiments performed on MgB_2 that demonstrate the detection of a superconducting state through the observation of the Meissner effect [2].

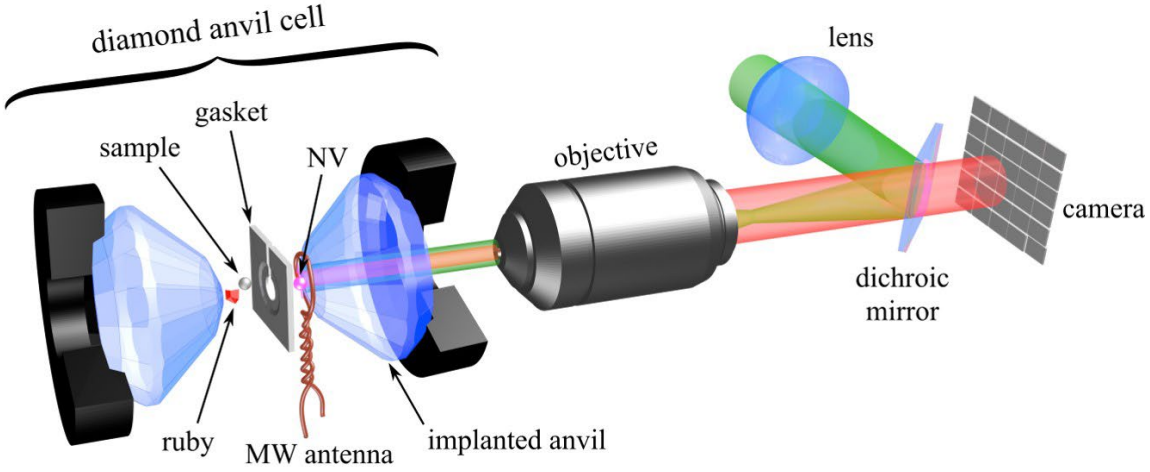

Figure 1: NV magnetometry setup for wide-field imaging at high pressure.

References

[1] - L. Toraille *et al.*, *New J. Phys.* **22** 103063 (2020).
[2] - L. Toraille *et al.*, *Science*, **366**, 1359 (2019).

Quantum Materials in and Beyond Equilibrium

C. Rüegg

Paul Scherrer Institute, Department of Quantum Matter Physics, University of Geneva, Department of Physics, ETH Zurich, Institute of Physics, EPF Lausanne, Switzerland

Spins form well-defined lattices in many insulating magnets. They serve as model systems to study many-body quantum states such as interacting quantum dimers, Luttinger liquids, or magnon Bose-Einstein condensates. Neutrons and photons are unique tools for high-precision studies of such states in and beyond equilibrium and under multi-extreme conditions in temperature, pressure and magnetic field. An overview of current frontiers in the field will be presented with special focus on exciting new opportunities that free electron lasers like SwissFEL offer to study out-of-equilibrium many-body quantum phenomena.

Quantum Simulation of Spin-charge Separation by Inelastic Scattering Experiments

B. Wehinger[1,2], N. Kestin[2], F. Lisandrini[3], P. Bouillot[2], S. Ward[4], D. Biner[5], K.W. Krämer[5], R. Bewley[6], B. Normand[4], C. Collath[3], T. Giamarchi[2], Ch. Rüegg[2,4]

[1]European Synchrotron Radiation Facility, Grenoble, France, [2]University of Geneva, Switzerland, [3]University of Bonn, Germany, [4]Paul Scherrer Institute, Villigen, Switzerland, [5]University of Berne, Switzerland
[6]ISIS Facility, Rutherford Appleton Laboratory, Chilton, UK

In a quantum many-body system, the spin and charge components of the electron can both separate and fractionalize, but probing such exotic phenomena accurately in real materials is complicated by their high charge energy scales. I will present how spin-charge separation can be measured in full, momentum-resolved detail by neutron spectroscopy on an insulating quantum spin ladder. Furthermore, I will discuss advances on quantitative analysis of diffuse scattering and show how elastic and magnetoelastic properties can be determined with high precision.

Bose-Einstein Condensate of Dirac Magnons

J. Schaltegger[1], P. Sukhachov[2], A.V. Balatsky[1,3]

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A Dirac-like quasiparticle spectrum is generated for localized magnetic moments on a 2D honeycomb lattice. The bosonic nature of these excitations and pumping allow for an accumulation of Dirac bosons and open up the possibility of Bose-Einstein condensation at the Dirac point.

We explore the formation and collective modes of Bose-Einstein condensate of Dirac magnons (Dirac BEC) [1]. We derive a phenomenological multi-component model of pumped bosons together with bosons residing at Dirac nodes and study the dynamics of the condensates. The condensate coherence and its multi-component nature are manifested in the Rabi oscillations whose period is determined by the gap in the spin-wave spectrum. This Haldane-like gap also allows one to control the properties and stability of the collective modes.

We further explore the vortex solutions in Dirac BEC [2]. We find that three distinct classes of vortices are possible, classified by their far-field behaviour. The Dirac structure is responsible for different phase windings on different components of the spinor, hence creating a multi-core vortex. We establish a phase diagram of the three vortex classes as a function of the model's parameter space.

A Dirac magnon BEC remains yet to be experimentally realized. We hope that our findings will stimulate the corresponding experimental search.

References

[1] - P.O. Sukhachov, S. Banerjee, and A.V. Balatsky, Bose-Einstein condensate of Dirac magnons: Pumping and collective modes. Phys. Rev. Research **3**, 013002 (2021).
[2] - J. Schaltegger, A.V. Balatsky, Vortex Excitations of Dirac Bose-Einstein Condensates. arXiv:2202.07594 (2022).

Do Quantum worms order into a Crystal? Quantum Spin Ice in a Magnetic Field

O. Sikora[1], K. Penc[2], F. Pollmann[3], Y.-J. Kao[4], N. Shannon[5]

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Quantum spin ice is a frustrated system supporting the existence of a quantum liquid, still providing questions about possible ordered and liquid phases. We consider a model with short-range exchange interactions in [100] magnetic field and study properties of states with strings of flipped spins – or "worms" – inserted into the maximally-polarized spin-ice configuration.

A single worm states can be understood by a mapping onto an S = 1/2 XXZ chain with gapped (confined) and gapless (extended) phase. We investigate multiple-worm states using both perturbation theory and Monte Carlo methods previously applied to quantum spin ice in zero field [1].

We find the ordered ground state at half polarization, previously demonstrated for the classical model, and identify a new ordered ground state at polarization two-thirds, stabilized by quantum fluctuations.

References

[1] - N. Shannon, O. Sikora, F. Pollmann, K. Penc and P. Fulde, Phys. Rev. Lett. **108**, 067204 (2012).

Investigation of New S_{eff} = ½ Pyrochlore Antiferromagnets: Structural and Magnetic Properties of $NaCdM_2F_7$ ($M = Cu^{2+}$, Co^{2+})

A. Kancko[1], G. Giester[2], R.H. Colman[1]

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The $A_2B_2X_7$ pyrochlores (X = O, F), materials containing A- & B-site sublattices of corner-sharing tetrahedra, offer a rich playground in the frustrated magnetism community due to the plethora of exotic magnetic ground-states (eg. spin-ice, spin-glass and spin-liquid states). In particular, the utilization of low-spin (S_{eff} = ½) magnetic ions on the pyrochlore lattice is of interest due to their large quantum fluctuations at low temperature, which serve to destabilize magnetic order and can potentially result in a disordered highly-correlated quantum spin-liquid state, which remains dynamic down to T = 0 K.

The previously studied pyrochlore materials mainly comprised of rare-earth oxides, but more recently a class of 3d transition metal fluorides has garnered the attention of the condensed matter community. The greater extent of the 3*d* orbitals, compared to the rare-earth 4*f* orbitals, leads to stronger magnetic interaction strengths via fluoride ligands of $\theta_{CW} \sim$ -100 K in all studied members of the family, although no magnetic transitions are observed down to < 4 K, where a spin-glass freezing occurs. [1,2] The spin-glass state is attributed to magnetic bond disorder arising from fully random, mixed occupancy of the non-magnetic pyrochlore A-site. Theoretical models support this interpretation.

The true Hamiltonian of the Co^{2+} pyrochlores is somewhat contentious: inelastic neutron scattering measurements indicate short range correlations with an XY anisotropy [3] and strongly anisotropic g-tensor [4], supported also by PDF analysis of magnetic correlations [5]; despite this, both low-field and high-field magnetisation data for $NaCaCo_2F_7$ measured along various crystallographic axes show no signs of anisotropy; and ESR measurements indicate a much smaller experimental g-factor of 2, compared to that expected from the INS results. [6] More materials and studies are needed to gain better understanding of these systems, and high-field magnetisation measurements are an important tool for confirming the magnetic interaction Hamiltonian. No Cu^{2+}-based pyrochlores have yet been studied due to the strong Jahn-Teller effect present in Cu^{2+} octahedral complexes.

I will present the structural and magnetic properties of two new members of the family, $NaCdCu_2F_7$ (S = ½) and $NaCdCo_2F_7$ (S_{eff} = ½). I will compare with the previously investigated members. Notably the A-site Na/Cd ion size discrepancy is greater than the previously studied Na/Sr and Na/Ca analogues, leading to greater magnetic bond disorder and as well as an enhanced spin-glass freezing temperature in $NaCdCo_2F_7$, however further measurements, including in high-fields, are desperately needed to fully understand this material. No magnetic transition is observed in $NaCdCu_2F_7$ down to the lowest measured temperature of 1.8 K, making in a new promising quantum spin liquid candidate.

References

[1] - J. W. Krizan and R. J. Cava, $NaCaCo_2F_7$: A Single-Crystal High-Temperature Pyrochlore Antiferromagnet, Phys. Rev. B **89**, 214401 (2014).

[2] - J. W. Krizan and R. J. Cava. $NaSrCo_2F_7$, a Co^{2+} Pyrochlore Antiferromagnet, J.Phys. Condens. Matter **27**, 296002 (2015).

[3] - K. A. Ross et al. Static and Dynamic XY -like Short-Range Order in a Frustrated Magnet with Exchange Disorder, Phys. Rev. B **93**, 014433 (2016).

[4] - K. A. Ross et al. Single-Ion Properties of the S_{eff} = XY Antiferromagnetic Pyrochlores $NaACo_2F_7$ (A = Ca^{2+}, Sr^{2+}), Phys. Rev. B **95**, 144414 (2017).

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Ab Initio Study of Random Hexagonal Close-Packed Phase in Platinum - Workshop on Quantum Materials

L. Burakovsky[1], D.L. Preston[1], D. Errandonea[2]

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Random hexagonal close-packed (rhcp) phase is a solid structure that has recently been widely discussed in the literature. It is realized when structures with different stacking sequences (AB . . . for hcp, ABC . . . for fcc, ABAC . . . for dhcp, ABCACB . . . for thcp, ABCBCACAB . . . for 9R, etc.) generally called hexagonal polytypes are energetically very close. Hence, the energy cost of forming a stacking fault between two such structures is virtually zero. Consequently, the actual layer stacking could be non-periodic and, in principle, random, thus forming rhcp. Rhcp was first introduced for hard-sphere colloids [1], and later on has been proposed for several elemental solids, e.g., Fe, Ir, Pt, Ag, and Au. For Pt, rhcp was first proposed in our previous Z-methodology-based theoretical study [2]. Here we use the technique of three-phase *ab initio* quantum molecular dynamics simulations to demonstrate the appearance of rhcp for Pt, and to determine the phase boundary that separates rhcp from the ambient face-centered cubic (fcc) phase of Pt on its phase diagram. These simulations consist in evolving a system containing layers of two different hexagonal polytypes separated by liquid regions until the system reaches its final equilibrium state. The example of such a three-phase simulation is shown in Figure 1: an initial system containing layers of fcc and 9R evolves towards the final rhcp state. It then appears that the results of the most recent experimental study on the melting curve of Pt [3] map out the melting curve that virtually coincides with the fcc-rhcp phase boundary that we present here, see Figure 2. The reasons for misinterpreting the fcc-rhcp solid-solid transition as melting will be briefly discussed.

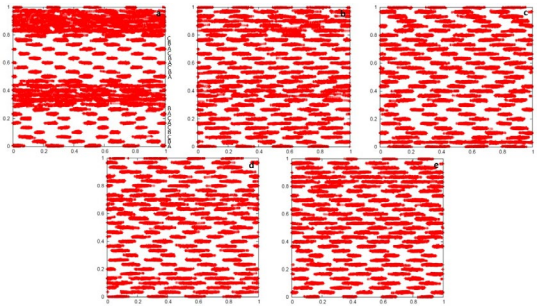

Figure 1: Example of a three-phase *ab initio* quantum molecular dynamics simulation.

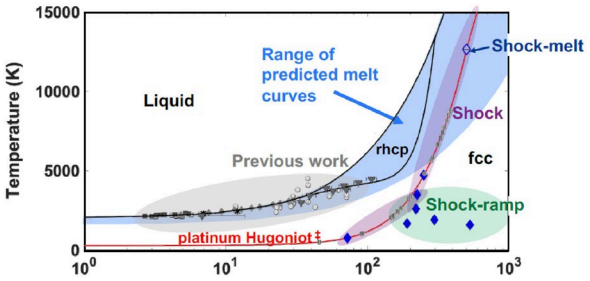

Figure 2: The phase diagram of Pt according to [4].

References

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[2] - L. Burakovsky, S.P. Chen, D.L. Preston and D.G. Sheppard, J. Phys. Conf. Ser. **500**, 162001 (2014).
[3] - Z.M. Geballe *et al.*, Phys. Rev. Mater. **5**, 033803 (2021).
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Narrow Bands and Dissipation in Quantum Materials

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Whereas fine-tuning to a quantum critical point leads to long-lived excitations in tightly defined regions of parameter space, narrow bands may more generally be caused by built-in mechanisms:

(a) If a continuous structural phase transition is suppressed to low temperatures (e.g. [1]), low-energy vibrational excitations can arise that boost superconductivity and cause a linearly temperature dependent electrical resistivity. In aperiodic high-pressure host-guest structures, such as that found in high-pressure bismuth [2], a low-energy sliding phonon mode is built in. Related findings in high pressure antimony and in Nowotny chimney-ladder phases suggest that strongly damped low-frequency vibrations are essential for thermodynamic and transport properties.

(b) On-site electronic interactions such as the Coulomb interaction near the threshold of Mott localisation, and Kondo coupling in *d*- and *f*- electron systems, in some cases augmented by Hund's coupling, can cause strong electronic mass renormalisation. Quantum oscillation measurements resolve the electronic Fermi surface and carrier mass in the pressure-metallised Mott insulator NiS_2 [3] and in the Fe-based superconductor YFe_2Ge_2 [4], enabling detailed comparison with theoretical scenarios.

The interplay between local mechanisms and fine-tuning to a quantum critical point is explored in the Kondo lattice system $CeSb_2$, which superconducts over a narrow pressure range at magnetic fields that exceed the Pauli limit by nearly an order of magnitude.

References

[1] - S.K. Goh *et al.,* Phys. Rev. Lett. **114,** 097002 (2015).
[2] - P. Brown *et al.,* Science Advances **4,** eaao4793 (2018).
[3] - K. Semeniuk *et al.*, arXiv:2202.04024 (2022).
[4] - J. Baglo *et al.*, Physical Review Letters **129**, 046402 (2022).

Singularity and Magnetism Engineering – the role of structure-property relationships in controlling quantum materials

A. W. Rost[1], A. S. Gibbs[2,3]

[1]School of Physics and Astronomy, University of St Andrews, UK, [2] School of Chemistry, University of St Andrews, UK, [3]ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, UK

Among the key tuning parameters for the properties of quantum materials are structural degrees of freedom which can be accessed by a variety of techniques such as effective 'chemical pressure' by elemental substitution, uniaxial strain or hydrostatic physical pressure. Such approaches have been widely and successfully used to tune superconductivity, reach quantum critical points or access putative spin liquid phases.

In order to develop a microscopic understanding of how the individual 'tuning-axis' is modifying the crystal structure and thereby the electronic structure, high quality and complementary physical and structural experiments are key. This allows the development of strategies for efficiently combining e.g. different dopants or physical tuning axes to reach unique singular points in Hamiltonian space.

The necessary experimental studies for building up a map through Hamiltonian space are extremely challenging to do, for example, on small single crystals of doped compounds or in restrictive geometries (e.g. strain, pressure). This holds for both physical property measurements and structural property determinations.

I will briefly discuss two recent examples which we are studying in our groups. The first focuses on 'singularity engineering' - understanding the impact of different structural distortion modes on the properties of the Van Hove singularity (singularity in density of states) which controls physical phenomena in members of the Ruddlesden-Popper series $Sr_{n+1}Ru_nO_{3n+1}$ such as the superconductor Sr_2RuO_4 and the quantum phase transition in $Sr_3Ru_2O_7$. One of the goals here is identifying a pathway to reach the singular point in the phase diagram of multicritical Lifshitz transitions recently identified by theoretical work.

The second example focuses on α-Li_2IrO_3 whose magnetic phase diagram has been widely discussed in terms of quantum spin liquid physics driven by spin-orbit coupling effects. Here we will show how compositional tuning can destabilise the low temperature magnetism, potentially broadening the temperature regime over which spin liquid physics can be observed.

In both cases structural tuning is achieved in a way that allows for synthesis of only small single crystals and sample masses. This poses challenges for both the determination of the structural (local and average) and excitation spectrum changes as well as the accurate measurement of thermodynamic and transport properties. In this context I will present some instrumentation recently developed by us for this purpose as well as highlight opportunities for transformative input through synchrotron experiments, specifically in relation to new capabilities at the ESRF through e.g. ID27.

Materials Science and Crystallography: from the Gigapascal to the Terapascal

D. Laniel

Centre for Science at Extreme Conditions and School of Physics and Astronomy, University of Edinburgh, EH9 3FD Edinburgh, UK

The thermodynamic parameter pressure is a powerful tool to tune compositional energy landscapes and favour the formation of exotic, and otherwise inaccessible, materials. Despite its clear potential for the synthesis of novel materials, the pressure parameter is significantly underexploited with only ~3% of known solids [1] having been produced at pressures higher than one atmosphere. Part of the difficulties related to the common usage of high pressure for materials' synthesis is the limited available *in-situ* characterization methods, which often leads to poor knowledge of the solids' composition and crystal structure-both at the very root of their properties. In recent years, however, the development of a novel crystallographic approach that allows the *in-situ* crystal structure determination of high-pressure samples, concomitantly with the rapid improvement of synchrotron X-ray diffraction beamlines, ushered high-pressure methods to the forefront of materials science.

This talk will first focus on presenting the game-changing crystallographic methodology that greatly facilitates obtaining reliable structural solutions at extreme pressure-temperature conditions, followed by a series of striking materials that it enabled to discover. These materials include the Re_7N_3 compound, formed and characterized at close to one terapascal [2]; high-energy density nitrogen-based compounds composed of previously unobserved polymeric or cyclic nitrogen species [3,4,5]; complex sulfur hydrides [6]; as well as a series of long-sought-after carbon nitrides (see Figure 1), rivaling diamond's hardness. Moreover, it will be demonstrated that these exotic materials can be recovered to ambient conditions, in some cases even despite being produced well above 100 GPa. These results demonstrate the incredible promises of high-pressure materials science and pave the way to technological prospects.

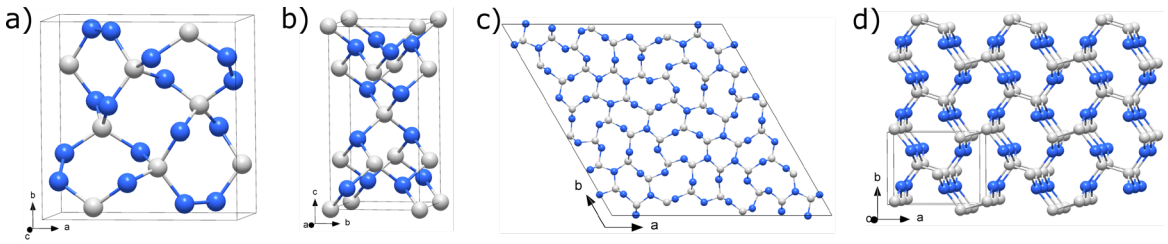

Figure 1: Crystal structure of the a) CN, b) α-C_3N_4, c) β-C_3N_4, and d) CN_2. All are composed of a 3D framework of the corner-sharing $C(CN_3)$ or CN_4 tetrahedra. All four are recoverable to ambient conditions. The blue and white spheres represent, respectively, nitrogen and carbon atoms.

References

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[2] - L. Dubrovinsky *et al.*, Nature **605**, 274-278 (2022).
[3] - D. Laniel *et al.*, Nat. Comm. **10**, 4515 (2019).
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Imaging Dilute Antiferromagnetic Spin Textures in a Single Shot Geometry using Resonant Coherent X-ray Diffraction

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We show[1] that single shot Resonant Coherent X-ray Diffraction (RCXD) can be used to quantify the sizes and separations of nascent domains in a paramagnetic to anti-ferromagnetic(AFM) first-order phase transition. The experimental verification is carried out on a PrNiO3 thin film hosting an AFM order of q=(¼, ¼, ¼) at temperatures below 120K. At the onset of the AFM transition, the first nucleated ordered domains are dilute in the beam footprint, thus resulting in relatively simple interference patterns (Fig), which can be inverted manually through a combination of visual inspection, system knowledge, and trial and error. As an outlook to our findings, we first show how topological textures of antiferromagnetic order parameter field can be studied using this method. RCXD from such topological textures, for example, AFM skyrmions, leave a non-trivial signature in the single shot RCXD patterns. Furthermore, we discuss how the single shot aspect can be utilized to study the time evolution of the dilute distribution of AFM textures. The success of our analysis suggests that a resonant Bragg coherent diffractive imaging approach with iterative phase retrieval algorithms may be effective in studying both these and even more complex antiferromagnetic spin textures. Finally, since we are expanding on the resonant aspect of X-ray scattering, one can utilize the experimental method to investigate the formation and evolution of dilute domains of other electronic orders - ubiquitous in quantum materials.

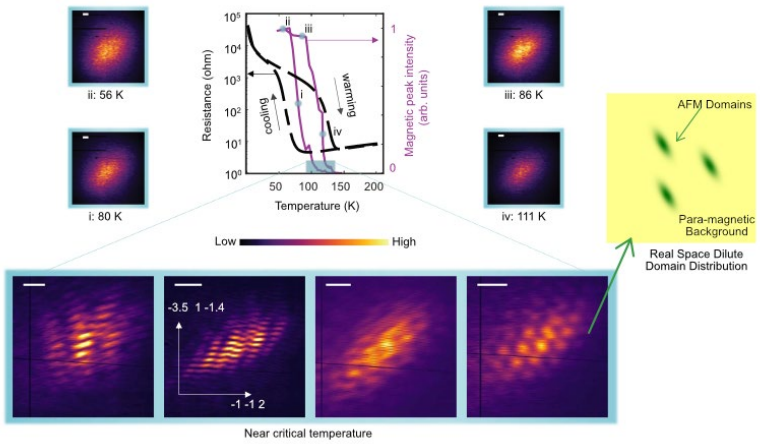

Figure 1: RCXD patterns observed as we cycle through the phase transition with novel coherent diffraction patterns appearing at the onset of the phase transition where domain distribution is dilute.

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5*f* Electron Occupancy and Hybridization in the UTe_2 Superconductor from XANES and XMCD Studies

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UTe_2 which is a newly discovered unconventional superconductor [1,2] has been investigated by x-ray absorption (XANES) and magnetic circular dichroism (XMCD) at the U- $M_{4,5}$ edges at 2.7 K at the ESRF ID12 beamline. The value of the branching ratio of the U- $M_{4,5}$ white lines confirms that the U ions are in an intermediate valence state between three (U^{3+}) and four (U^{4+}). The analysis of the XMCD data at the U-$M_{4,5}$ edges allows to conclude that the 5*f* electron count is about 2.8, *i.e.*, close to U^{3+}. Our finding agrees with other measurements (soft x-ray ARPES, core level photo- electron spectroscopy [3,4]) as well as with some band structure calculations [5,6]. This is an important conclusion. It invalids theoretical models promoting a dominant contribution of the $5f^2$ electronic configuration [7]. Furthermore, the reduction of the uranium orbital to spin magnetic moment ratio, compared to the free ion U^{3+} value, is a fingerprint of the 5*f* electron delocalization (hybridization). Another important breakthrough is the peculiar pressure dependence of the 5*f* electron count. We observe a decrease (increase) of about 0.2 e- of the 5*f* count (valence) at the transition at $P_c \approx 1.45$ GPa towards a magnetically ordered state [8]. This tiny change of the valence is accompanied by a modification of the electronic structure, a decrease of the magnetic anisotropy and the disappearance of the superconductivity. The decrease of the valence above 3 GPa could be due to a further change of the electronic structure associated to a structural transition. To conclude, it appears that the interplay between magnetism and valence instabilities is a key factor to understand the superconductivity in UTe_2. Our conclusions open the roads to further experiments under high pressure (XMCD, resistivity, x-ray or neutron diffraction) and theoretical models.

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Proximity Induced Novel Cu-CDW and Cu-magnons in Epitaxial $YBa_2Cu_3O_7$/ $Nd_{1-x}(Ca_{1-y}Sr_y)_xMnO_3$ Interface

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Resonant soft X-ray scattering (RIXS/REXS) study of epitaxial $YBa_2Cu_3O_7/Nd_{1-x}(Ca_{1-y}Sr_y)_xMnO_3$ heterostructures (NYN) show that the Copper charge density wave (Cu-CDW) order of the near optimally doped $YBa_2Cu_3O_7$ layers can be strongly modified via the hole doping and tolerance factor of $Nd_{1-x}(Ca_{1-y}Sr_y)_xMnO_3$, i.e. by changing x and y and external magnetic field.

For x=0.35, we observe a quasi-2D d_{x2-y2} type Cu-CDW order at $Q_{\parallel}\approx0.3$ r.l.u., that gets strongly enhanced as the tolerance factor of the manganite layers[1] is decreased and its CE-type antiferromagnetic and charge/orbital ordered (COO) is reinforced[2]. Using REXS at Bessy II, HZB, Germany, we showed that this Cu-CDW order can be abruptly enhanced up to ~170% by an application of external magnetic field above 6T at low temperatures[2]. Magneto-electric transport measurements have been used in conjunction with spectroscopy to explain said observations[2]. High resolution RIXS study at DLS, Oxford, UK on this superlattice indicates a unique two-magnon behavior of the cuprate layer[3]. The RIXS spectra can only be fitted by considering at least two different magnons, two phonons, a bimagnon as well as a set of crystal-field excitations. Contrary to the previous measurements in bulk cuprates, these two observed magnons rarely disperse in Q and exhibit a crossover in the Q-space in terms of relative weight. RIXS polarimetry confirms the presence of spin-flip scattering at the position of both these magnon-features. We shall try to explain these features as two-component spectrum originating from the bulk-like part of the cuprate and the proximity-induced interface part.

Upon increasing the hole doping of the manganite layers to x=0.5, we observe a new kind of Cu-CDW order, which has a much smaller wave vector of $Q_{\parallel}\approx0.1$ r.l.u., a larger correlation length of about 40nm, and a different orbital character, i.e. d_{z2} rather than d_{x2-y2}, than the one commonly found in the bulk cuprates[4]. RIXS polarimetry study at ID32 beamline at ESRF indicated no spin-flip scattering at the elastic channel of the spectra. The origin of this Cu-order has been explained in terms of the proximity effect of neighboring manganite layers with CE-type charge orbital order (Mn-COO).

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Undamped Spin Waves in the Intermetallic Antiferromagnet $CeCo_2P_2$

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Collective spin excitations in magnetically ordered crystals, called magnons, are the basis for magnonic applications where a spin flow is utilized without the need of an electrical current. However, the required long lifetimes of the magnons are strongly reduced in the high-frequency range, especially in metallic compounds.

Here, we present our study of the intermetallic antiferromagnetic compound $CeCo_2P_2$, which exhibits long-living magnons in a large energy range. Based on our resonant inelastic X-ray scattering (RIXS) measurements, we can show that nearly undamped spin excitations exist up to the THz regime. This can be understood as a result of a reduced density of states around the Fermi level in $CeCo_2P_2$, which reduces low-energy spin-flip Stoner excitations, which are the main contributors to the damping of magnons in metals. By comparison to the isostructural $LaCo_2P_2$, we can see that the substitution of Ce to La restores the damped magnon regime common to metallic systems (see Figure 1).

In this regard, and in combination with its large ordering temperature of T_N = 440 K [1,2], $CeCo_2P_2$ can be an interesting material to study long-living magnons in the THz range up to room temperature. Especially the tuneability of the magnetic order by substitution with La [3] and its interesting surface properties including Kondo and magnetic sublattices [4] makes $CeCo_2P_2$ further a potentially promising candidate as starting point for exploring metallic magnonic devices.

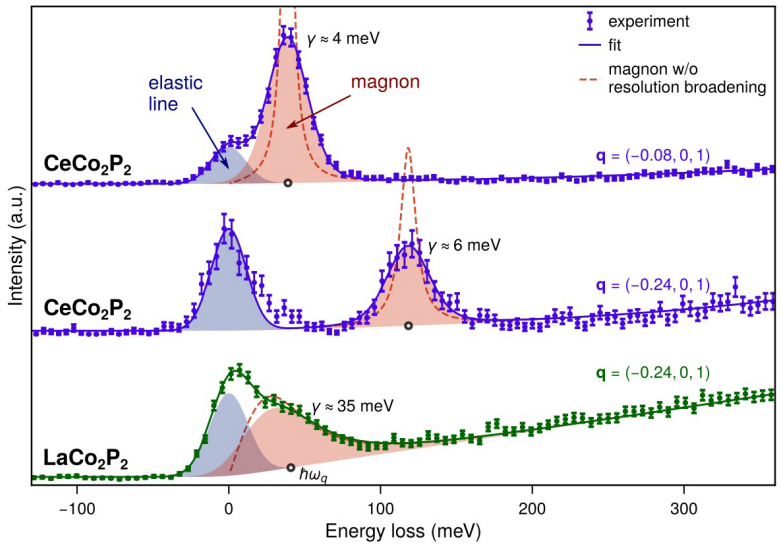

Figure 1: RIXS spectra of $CeCo_2P_2$ and $LaCo_2P_2$ taken at the Co L_3 absorption edge. The spectra can be described by an elastic peak at zero energy loss and a magnon peak at higher energy loss. While for $CeCo_2P_2$ the magnon peak width is dominated by the experimental resolution, for $LaCo_2P_2$ a strong damping can be observed.

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Extreme Conditions Studies at the EBS-ESRF

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The new EBS-ESRF light source allows a great improvement of our fundamental understanding of materials under high compression due to the unprecedented characteristics of the generated X ray beams. In this presentation, we will expose some condensed matter studies devoted to quantum materials developed under extreme conditions at the EBS-ESRF. We will also present the portfolio of available techniques on different beamlines and the user and in-house support by the high pressure laboratory.

Interacting Electrons in Layered Materials - shall we go to Extremes?!

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Time and again the field of interacting electrons has driven important innovations in modern solid-state physics, with new collective ground states playing a key role. Regarding the latter, interacting electrons in layered quantum materials have proven to provide and extremely fertile ground for new discoveries. Famous and intensively studied examples include unconventional superconductivity, charge density waves, Kitaev-quantum spin liquids and other topological states of matter.

In this talk I will discuss two cases in point, namely $IrTe_2$ and $RuCl_3$, which both exhibit an unusual interplay between the electrons and the lattice. Our X-ray diffraction study of $IrTe_2$ provides unprecedented structural information as a function of applied pressure up to 42 GPa. We find a pronounced stabilization of localized molecular orbitals with increasing pressure and discover an unusual mechanism of local bond formation in this itinerant material. The latter is expected to result in strong electron-phonon interactions.

For the Kitaev-material $RuCl_3$, we report the discovery of an intriguing pressure-driven phase transformation. By analyzing both the Bragg scattering as well as the diffuse scattering of high-quality single crystals, we analyze the evolution of the structure during this transformation and reveal a collective reorganization of the layer stacking throughout the crystal. Importantly, this transformation also effects the structure of the $RuCl_3$-honoeycomb layers, which acquire a higher symmetry as compared to ambient conditions. Hydrostatic pressure therefore allows to tune $RuCl_3$ towards the ideal Kitaev-limit.

These two examples illustrate that hydrostatic pressure enables to stabilize and study new collective ground states in quantum materials. Notwithstanding, for many quantum materials the high-pressure ($p > 50$GPa) and low temperature ($T \sim 1$K) region remains unexplored - So, yes, we should go to extremes!

Uncovering the $S = ½$ Kagome Ferromagnet within a Family of Metal-organic Frameworks

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Kagome networks of $S = ½$ magnetic moments are important models in the pursuit of novel quantum materials; lattices of antiferromagnetically coupled moments are hypothesised to host the long-sought quantum spin liquid state,[1] whereas ferromagnetic kagome lattices can display a diverse array of intriguing properties, including formation of topological magnon bands[2] and creation and control of the movement of skyrmions.[3] We have explored a family of Cu^{2+}-containing metal-organic frameworks (MOFs) bearing $S = ½$ kagome layers pillared by ditopic organic linkers with the general formula $Cu_3(CO_3)_2(x)_3 \cdot 2ClO_4$ (MOF-*x*), where *x* is 1,2-bis(4-pyridyl)ethane (*bpe*), 1,2-bis(4-pyridyl)ethylene (*bpy*), or 4,4'-azopyridine (*azpy*).[4] In these materials, Cu^{2+} ions are coordinated to tridentate tris-chelated carbonate ligands in the *ab* plane to form kagome layers that are pillared along the *c* axis by a ditopic organic linker, *x*. Conflicting reports on the magnetic ground state of these materials existed in the literature,[5,6] and thus it was unknown whether the underlying model is that of a $S = ½$ kagome ferromagnet or antiferromagnet. Elucidation of the nature of magnetic exchange in these complex materials requires a variety of complementary experimental techniques. In this work, through the combination of magnetometry, neutron powder diffraction and muon-spin spectroscopy measurements, we show that the magnetic ground state of this family of MOFs consists of $S = ½$ ferromagnetic kagome layers that are coupled antiferromagnetically via a ten-atom superexchange pathway along the organic pillars.

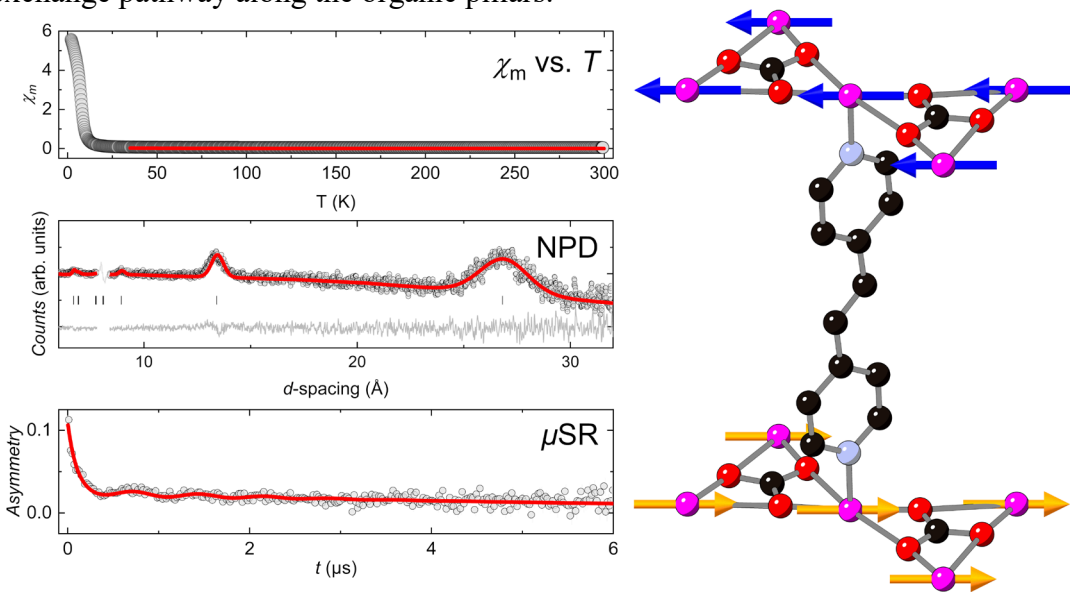

Figure 1: Through a combination of magnetometry, neutron powder diffraction and muon-spin spectroscopy measurements, we show that the ground state in this family of MOFs consists of ferromagnetic kagome layers that are coupled antiferromagnetically along their organic pillaring linkers.

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Resolving Emergent Structure States in 2D Systems by High-energy X-ray Diffraction

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Materials exhibiting reduced dimensionality and strongly interacting charge and lattice degrees of freedom can appear in various crystal structure states that harbor fascinating quantum phenomena. The complexity of the states, however, often makes it challenging to understand the nature of the phenomena, impeding their exploration for practical applications. Typical examples are the emergence of charge density waves (CDWs) and Wyel semimetal phases in transition metal dichalcogenides. We will show that the problem can be solved by using high-energy x-ray diffraction coupled to atomic pair distribution function analysis. Examples will include results of our recent studies on the genesis of CDWs in 2H-$TaSe_2$ [1] and 1T-TaS_2 [2], and local structure memory effects in the Wyel semimetal $MoTe_2$ [3].

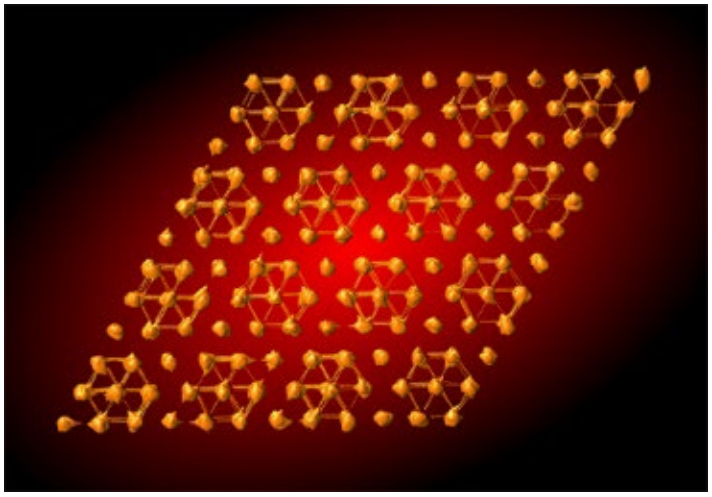

Figure 1: Fragment from the CDW in 2H-$TaSe_2$ as revealed by high-energy XRD [1].

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Uniaxial Pressure Tuning of Charge-stripe Order in La-based Cuprates

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Charge order has long been known to coexist with high-temperature superconductivity in copper-oxide materials. Its microscopic description, however, remains controversial. Using uniaxial pressure as an external stimulus, we successfully lift the domain degeneracy and reveal the unidirectional nature of charge order in $La_{1.88}Sr_{0.12}CuO_4$ [1]. Furthermore, a much weaker uniaxial pressure is found to pin the slanted stripe order to the crystal axis [2]. These results are discussed combining both a phenomenological Landau model and a strong-coupling real-space picture that reveal a rather weak transverse stripe stiffness. Such a weak spatial stiffness suggests transverse quantum fluctuations may play a critical role for stripe order to coexist with superconductivity in La-based cuprates [2].

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Charge and Spin Excitations in Infinite-layer Superconducting Nickelates

L. Martinelli[1], G. Krieger[2], S. Zeng[3], L. E. Chow[3], K. Kummer[4], R. Arpaia[5], M. Moretti Sala[1], N. B. Brookes[4], A. Ariando[3], N. Viart[2], M. Salluzzo[6], G. Ghiringhelli[1], and D. Preziosi[2]

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The discovery of superconductivity in infinite-layer nickelates RNiO2 (with R being a rare-earth) has generated much excitement in the physics community. Many experiments and calculations have been performed to shed light on their electronic structure, in order to establish similarities and differences with respect to (infinite-layer) cuprates, of which they mimic the structure.

Recently, we have carried out RIXS measurements on $NdNiO_2$ thin films with different doping levels, both with and without SrTiO3 capping layers. In the capped films we have established, in agreement with other experiments [1], the presence of dispersing magnetic excitations strongly similar to the ones found in cuprates. At the same time, in the capping-free films we have discovered the presence of charge order with a similar periodicity than in cuprates, although with a different doping and temperature dependence. Interestingly, the capping-free films (which still display superconductivity) show no sign of magnons and also display a stronger hybridization between Nd and Ni atoms, which effectively increases the three-dimensional character of the electronic structure. Our results represent an important step towards the understanding of nickelate superconductors, and show that strain is probably playing a crucial role. They have been recently published on Physical Review Letters [2].

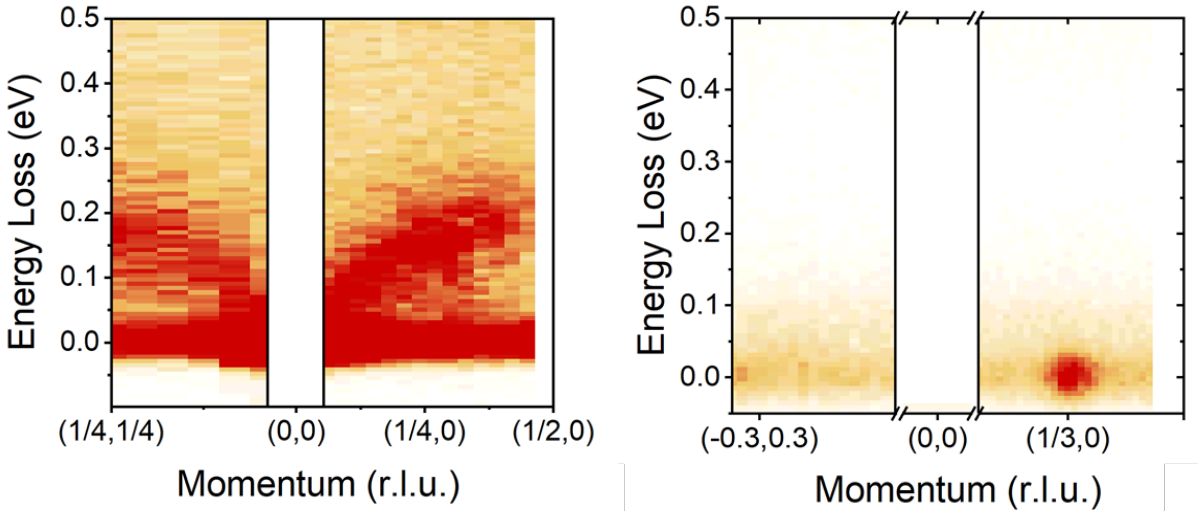

Figure 1: Left panel: momentum dependence of magnetic excitations measured in STO-capped $NdNiO_2$ films. Right panel: observation of a charge-order peak in capping-free $NdNiO_2$ at H=0.33 r.l.u.

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Poster Abstracts

EBS workshop on Quantum Materials

List of Posters

N. BASSOT	Non superconducting $(Ln_{1-x}A_x)NiO_{2+y}$ layered bulk nickelates (Ln = Nd, Pr ; A = Sr, Ca)
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T. DOLLING	Investigating Kagome-Containing Stacked Metal-Organic Frameworks: Bulk Magnetism and Exfoliation Approaching the Monolayer Limit
Q. HE	Infrared Ellipsometry Study of K-doped Pterphenyl Bulk
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Non Superconducting $(Ln_{1-x}A_x)NiO_{2+y}$ Layered Bulk Nickelates (Ln = Nd, Pr ; A = Sr, Ca)

N. Bassot, C. Domingos, A. Sulpice, Ch. Lepoittevin, P. Toulemonde

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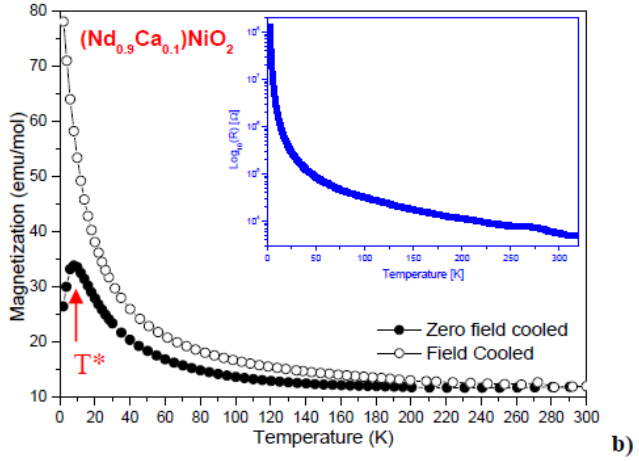
The discovery of superconductivity below $T_c \sim 15$ K in doped infinite layer $Nd_{1-x}Sr_xNiO_2$ nickelate thin films on $SrTiO_3$ substrates in 2019 has generated an enormous interest in the condensed matter community because of their great similarities with cuprates [1]. Then, superconductivity was also found with maximal T_c reaching 20 K, using other rare earth or alkaline earth doping elements, such as La,Sr (or Ca) [2,3] and Pr,Sr [4] based systems and on a different substrates $(LaAlO_3)_{0,3}(Sr_2AlTaO_6)_{0,7}$ [5,6].

In our laboratory, we have studied the analogous bulk materials of such systems. We have synthesized good quality polycrystalline samples of Sr doped $(Nd_{1-x}Sr_x)NiO_2$, $(Pr_{1-x}Sr_x)NiO_2$ up to x = 0.2 and Ca doped $(Nd_{1-x}Cax)NiO_2$ series up to x = 0.5. Physical measurements carried out on these systems revealed no superconductivity in any of these compounds so far, but a spin-glass like (below T*) and insulating behaviour at low temperature was observed (**Fig a**).

We also synthesized a new polycrystalline phase $NdNiO_{2+y}$, a partial reduced form of $NdNiO_3$. Although its powder X-ray diffraction (XRD) pattern looks very similar to the one reported by Moriga et al. [7], the crystal structure we found by Transmission Electron Microscopy (TEM) is totally different. The Selected Area Electron Diffraction (SAED) evidenced a modulated structure in a tetragonal subcell with the parameters a ≈ 3.8 Å and c ≈ 3.5 Å. Due to the commensurate nature of the modulation, the structure can be described in a monoclinic supercell with the parameters a ≈ 16.4 Å, b ≈ 7.8 Å, c ≈ 5.5 Å and β ≈ 105° (**Fig b**). A first structural model has been determined using 3D electron diffraction crystallography and has been refined from powder XRD data. The full determination of oxygen positions, as well as the physical properties studies are still under progress.



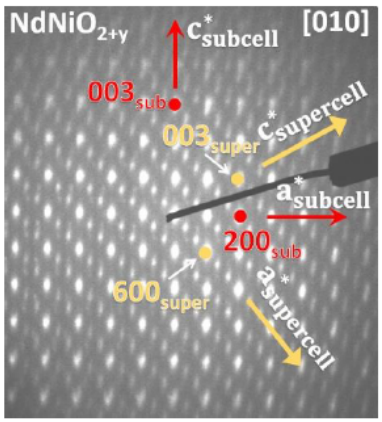


Figure a: Magnetization of $Nd_{0.9}Ca_{0.1}NiO_2$ pellet from 300 K down to 2.5 K in applied field of 100 Oe (with T* ~ 10 K). Inset: its electrical resistance in the 2.5 - 320 K range. **b:** TEM [010] SAED pattern of $NdNiO_{2+y}$.

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Structural Phase Diagram of the $Ba_{1-x}Eu_xTiO_3$ Solid Solution

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$BaTiO_3$ (BTO) is one of the most studied perovskite type oxide materials due to its physical properties like ferroelectricity (FE), piezoelectricity, high dielectric constant. It undergoes three phase transitions on lowering the temperature and the resulting structures belong to space groups $Pm\bar{3}m, P4mm, Amm2$ and $R3m$, respectively. FE ordering arises at the $Pm\bar{3}m \rightarrow P4mm$ transition. In combination with magnetoelectric $EuTiO_3$, BTO forms a complete solid solution $Ba_{1-x}Eu_xTiO_{3-\delta}$ (BETO) which combine properties of both its constituents [1].

In this work, $Ba_{1-x}Eu_xTiO_{3-\delta}$ (BETO; $0.05 < x_{Eu} < 0.30$) samples were synthetized and annealed at different temperatures (T_{ann} = 1273 K, 1473 K and 1673 K). Their structures were studied during two powder diffraction experiments at ID22@ESRF beamline in the range of 10 K ≤ T ≤ 450 K. [2].

This study aims: i) building the Ba-rich portion of the phase diagram for BETO; ii) revealing the effect of composition and annealing temperature on the phase transitions of BETO; iii) establishing the structure and electrical polarization of BETO samples at the local and average scale.

The average structure as a function of x_{Eu}, T and T_{ann} was determined using Rietveld refinements. While samples annealed at 1473 K and 1673 K display all the phase transitions of BTO, with smoothly decreasing transition temperatures on raising the Eu concentration, the FE ordering seems to be frustrated in all the samples fired at 1273 K and they remain cubic down to 10 K. The local structure of BETO samples was investigated at 10 K using Pair Distribution Function [PDF/$G(r)$]. $G(r)$ functions were analyzed using Real Space Rietveld Analysis. In order to minimize the parameters/data ratio, all the models describing the phases have been simplified. Starting from the cubic model, the coordinates of Ti and the ones of its oxygen octahedral cage were allowed to vary in opposite directions along the [100], [110] or [111] directions in the $P4mm, Amm2$ and $R3m$ phases, respectively. Other constraints to cell parameters and Debye - Waller factors were added.

The analysis revealed that at the local scale the structure of all the samples (included the ones annealed at 1273 K) is not cubic but it is well described using a rhombohedral model. Electric dipoles with similar magnitude exist at the local scales in all the samples. Dipole momenta are disordered in the 1273 K annealed (cubic) samples leading to null polarization on average. In the 1473 K and 1673 K annealed ones the polarization is higher at the local than at the average scale, suggesting that also in these last samples, even if more ordered than the previous ones, some disorder is still present.

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Investigating Kagome-Containing Stacked Metal-Organic Frameworks: Bulk Magnetism and Exfoliation Approaching the Monolayer Limit

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The applications of magnetic $S = ½$ kagome materials range from the long-sought quantum spin liquid, to low-energy data storage, spintronics, logic gates and quantum computing.[1,2] In recent work,[3] we uncovered the magnetic ground state of a family of $S = ½$ kagome-containing metal-organic frameworks (MOFs) with the general formula $Cu_3(CO_3)_2(x)_3 \cdot 2ClO_4$. In these materials, Cu^{2+} cations are chelated by carbonate anions forming kagome layers in the *ab* plane (Figure 1c) that are pillared along the *c* axis by ditopic organic linkers, *x*. Following the discovery of three-dimensional magnetic order in these MOFs, our attention has turned to two new MOFs with the formula $Cu_3(CO_3)_2(y)_6 \cdot 2ClO_4$ where *y* is 4-methylpyridine (*mp*) or 2,4'-bipyridine (*bipy*). Substituting the pillaring linkers used previously for these monodentate ligands effectively removes the interplane covalent linkage, which, it is expected, will disrupt the three-dimensional ordering observed in the pillared systems. Furthermore, the discrete layers in these structures (Fig. 1a,b) may also allow for the exfoliation of these MOFs into magnetic nanosheets, which have a plethora of potential applications including as ultrathin semiconductors and spin valves.[4,5] Work on understanding the bulk magnetism of these systems, as well as preliminary studies on their exfoliation will be presented herein.

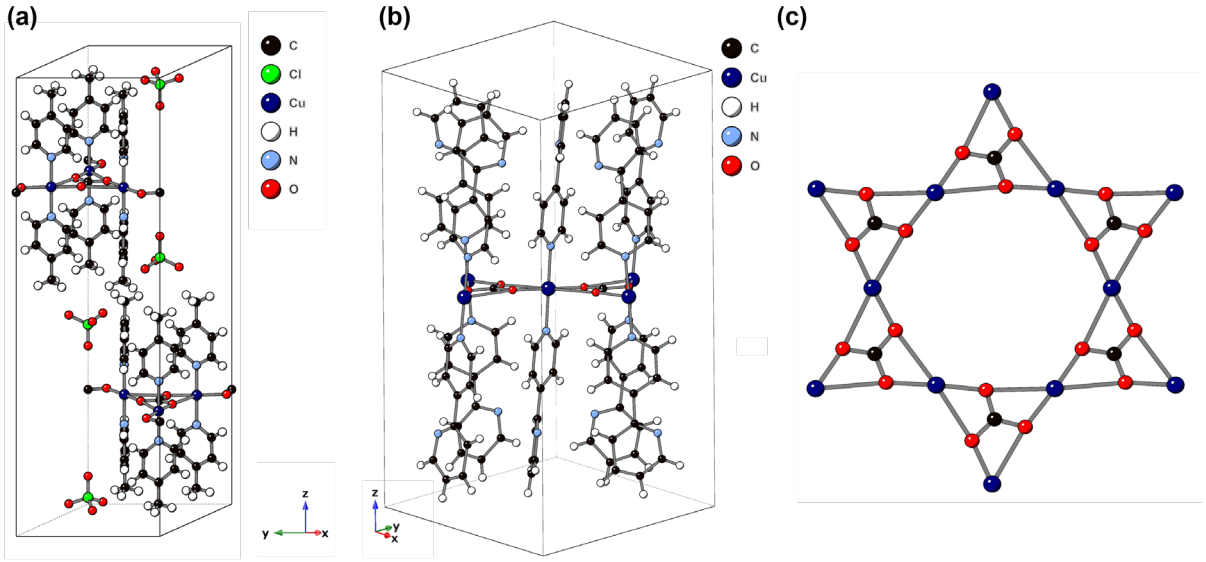

Figure 1: Structural models of MOF-*mp* and MOF-*bipy*. (a) The unit cell of MOF-*mp* solved in the $P6_3/m$ space group. (b) The unit cell of MOF-*bipy* solved in the $P\bar{3}$ space group (perchlorate anions omitted). (c) The breathing kagome lattice featuring a network of Cu^{2+} cations chelated by CO_3^{2-} anions (perchlorate anions omitted).

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Infrared Ellipsometry Study of K-doped Pterphenyl Bulk

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With infrared ellipsometry we studied the lattice and charge dynamics of polycrystalline samples of heavily K-doped and undoped p-terphenyl. For the doped samples with a nominal compositions of K3-p-terphenyl[1], we observed a pronounced enhancement of some low-energy phonon modes that is in fair agreement with the prediction of lattice dynamical calculations. Moreover, we observed a strong decrease of the eigenfrequency of the high-energy phonons involving C-H vibrations that are not predicted by the calculations. We interpret this latter anomalous phonon softening in terms of a weak polymerization of the K3-p-terphenyl ions. We also observed electronic excitations that give rise to a pronounced polaronic band and a weak Drude-like peak at the origin that is due to free carries with a plasma frequency. As a function of decreasing temperature, the width(scattering rate) and the plasma frequency of this Drude-peak exhibit a gradual reduction that sets in below a structure phase around 190K and evolves continuously toward lower temperature. No anomalous changes of the Drude-response have been observed in the low temperature regime that could be taken as evidence of a bulk-like superconducting transition. An inhomogeneous SC state with a very small volume fraction cannot be excluded based on our optical data.

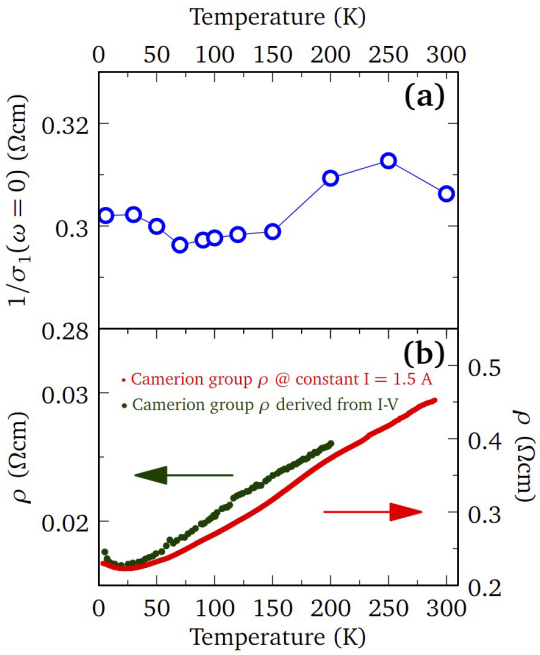

Figure 1:(a) Temperature dependence of the inverse dc–conductivity as obtained from our ellipsometry data, (b) Dc–resistivity measurements on a corresponding sample with the setup described in Ref. [2]

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Structures and Transport Properties of TiZr Alloys with Hydrogen under High Pressure

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Effects of pressure on the structure, electronic resistance, and the critical magnetic field values for superconductivity of pristine and hydrogenated TiZr alloys were investigated, and the results were compared with the ones measured under hydrogen environment. With increasing pressure using Ne as a pressure medium from ambient to 55 GPa, structures of pure TiZr alloys at equiatomic composition changed from an hcp to a bcc through an hcp-omega phase, while hydrogenated ones exhibit various intermediate phases, including bcc-H and tetragonal phases. Superconducting transition temperature, Tc, of pure TiZr alloys significantly increased from 2.7 K to 11.7 K with increasing pressure from 5.4 GPa, and 50 GPa, respectively. Interestingly, the superconducting transition temperature, Tc, values for hydrogenated samples increased from 3.4 K to 9.4 K at 6 GPa and 32 GPa, respectively, but decreased to 8 K with increasing pressure further to 55 GPa. Applying the external magnetic field suppressed Tc value. Our combined results with the structure and transport measurements demonstrated that applying pressure increases the Tc while hydrogen atoms contribute to decreasing the values. The combined results of structure and superconducting transition temperature under high pressure and hydrogen environment will be presented.

Electronic Properties of Sr_2IrO_4 - $YBa_2Cu_3O_{7-\delta}$ Thin Film Heterostructures

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We report the pulsed laser deposition (PLD) of multilayers of the cuprate high-T_C superconductor $YBa_2Cu_3O_{7-\delta}$ (YBCO) and the iridate Sr_2IrO_4 (SIO) which exhibits a strong spin-orbit coupling (SOC) [1]. The latter has a crystal structure similar to La_2CuO_4 [2] alongside peculiar magnetic properties [3] and is an ideal candidate to explore the influence of both strong SOC and magnetism on the superconductivity of the neighboring YBCO layers.

The magneto-transport characteristics of the heterostructures are investigated. They reveal a strong and comparatively long-ranged proximity effect. This gives rise to a suppression of the superconducting response of the YBCO layers up to a thickness of about 14 nm. Samples with thinner layers show a complex insulating behavior at low temperatures. Slowly increasing the YBCO thickness leads to an extremely broad superconducting transition until superconductivity is fully restored at ≈ 20 nm of YBCO. Moreover, we find a strong and unusual magnetic field dependence.

These results point towards a complex interplay between the strong SOC in SIO and superconductivity in YBCO and call for further studies of the microscopic electronic and magnetic properties of these layers.

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Melting Curve of Black Phosphorus and Associated Colossal Volume Jump

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Phosphorus exhibits a very rich polymorphism under ambient but also under high P and T conditions. Among them, black phosphorus (bP) occupies a very special place as the most stable allotrope in a wide P,T region of its phase diagram. Due to the exceptional anisotropic properties of solid bP[1] and the existence of a first-order liquid-liquid transition[2], this element has been extensively studied. However, several important questions remain open regarding its liquid state and melting line. In particular, it is expected that significant changes occur on the melting curve in the vicinity of the liquid-liquid-solid triple point. However, there are still large discrepancies in the literature regarding its shape and position. In order to redetermine the controversial melting curve of bP, as well as the density change across this transition, we performed combined *in situ* X-ray diffraction and density measurements.

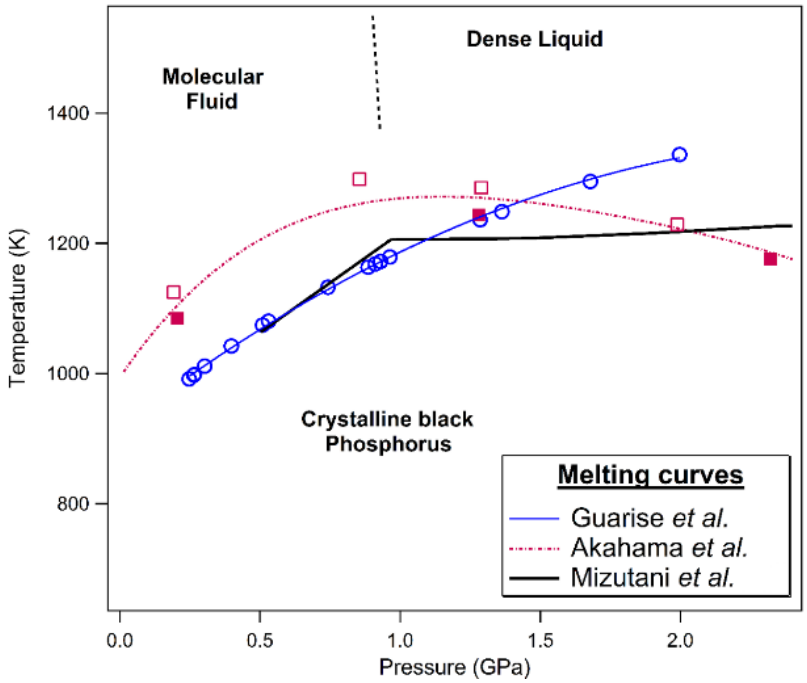

Figure 1: Phase diagram of phosphorus showing the various melting curves from the literature[3,4,5].

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Structural Evolution of Polyiodides at High Pressure

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Polyiodides represent one of a few classes of compounds that can form extensive inorganic homoatomic polymeric networks. The great variety of polyiodide structures arise from the ability of iodine to catenate through donor-acceptor interactions. We have explored their potential to form even more extended bonding at high pressure, and examined their properties.

CsI_3 is an archetypical example of asymmetric triiodide. It undergoes a similar sequence of phase transitions, *Pnma-P*-3*c*1-*Pm*-3*n,* to many other alkali metal trihalides (e.g. KBr_3, $NaCl_3$, KCl_3) at high pressure. We studied this system *via* single-crystal X-ray diffraction and theoretical analysis. Our experiments show that a reversible phase transition above 1.24 GPa transforms the layered system into a 3D orthogonal assembly of linear iodine chains. Phonon calculations revealed that the trigonal phase is dynamically unstable at ambient conditions and becomes stable only with the support of compression. Although such chains in CsI_3 were predicted to be metallic at high pressure, the conductivity experiments showed their semiconducting nature. Such results corroborate with our calculations which predict a bangap closure from 1.68 to 0.51 eV upon compression to 10 GPa.

Electrical conductivity in an organic polyiodide was studied to validate the hypothesis of formation of continuous electronic bands within iodine chains upon compression. A suitable system: tetraethylammonium diiodine triiodide, containing I_3^- and I_2 units in a close proximity (~3.42 Å) at ambient conditions was chosen for X-ray diffraction, electrical resistivity and Raman studies. We found that compression above 10 GPa of the orthogonal $I_3^- \cdots I_2$ contacts, below 3.32 Å, leads to a drop in electrical resistivity by 9 orders of magnitude. Raman spectra show progressive quenching of I_2 stretching vibrations (~180 cm^{-1}) and formation of higher polyiodide bands is observed. Bonding analysis showed that more covalent I-I bonds are formed

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Anti-site Disorder Driven Enhanced Intrinsic Anomalous Hall Conductivity in Spin Gapless Semiconducting Mn_2CoAl Heusler Compound

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Spin gapless semiconductors, a novel state of material, have attracted immense interest in the field of spintronics because of finite gap in one spin channel and no gap in another. This state has been experimentally investigated in Mn_2CoAl Heusler compound for the first time. The transport measurement reflects that this compound has larger anomalous Hall conductivity (AHC) compared to the theoretically reported value. The detailed structural analysis reveals that the system crystallizes with anti-site disorder between Mn and Al atoms. The scaling analysis of anomalous Hall data shows that the AHC is primarily governed by Berry curvature in momentum space. After considering the disorder in the theoretical calculation, the calculated intrinsic AHC due to momentum space Berry curvature is in good agreement with the experimental intrinsic AHC. The disorder affects the electronic band structure, which modulates the associated momentum space Berry curvature and further enhances the intrinsic AHC.

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$LaFeSiO_{1-\delta}$: a Novel Superconducting Member of the Fe Silicides Family with Squeezed FeSi Layers

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Since their discovery in 2008, iron-based superconducting pnictides (As, P…) and chalocgenides (Te,Se…) are now a well-established class of unconventional superconductors, spanning multiple structural families, with T_c up to 55 K in bulk materials [1]. This category of superconductors has recently been extended to other layered materials where pnictogen/chalcogen atoms are replaced by crystallogen elements: either with Ge in YFe_2Ge_2 ($T_c \sim 2$ K) [2] or Si in LaFeSiH ($T_c \sim 10$ K) [3].

In this work, we present the discovery of a new compound obtained by oxygenation of LaFeSi [4]. The resulting unexpected crystallogenide, $LaFeSiO_{1-\delta}$, showed very interesting properties. Our detailed study based on complementary experimental probes reveals that this crystallogenide is superconducting with a relatively high $T_c \sim 10$ K, regarding its strongly squeezed Fe-Si anion height, below 1 Å, challenging the usual relationship between structure and superconductivity in Fe-based compounds (Fig.1.).

Its unique crystal structure has a strong impact on its electronic properties. Just above T_c, its resistivity shows a non-Fermi liquid behavior, a signature of its electronic correlations. This correlated behavior is also visible in the NMR data which evidences weak antiferromagnetic fluctuations. The calculated electronic structure of LaFeSiO is significantly changed compared to the one of the canonical LaFeAsO pnictide. Its Fe-related Fermi surface, consisting almost uniquely of hole pockets, suggests another kind of electronic correlations and then a different related superconducting mechanism than the usual the s±-mechanism. Finally, the location of $LaFeSiO_{1-\delta}$, LaFeSiH and $LaFeSiF_x$ [5] superconductors in the phase diagram points towards the existence of a new emerging superconducting dome related to Fe-silicides.

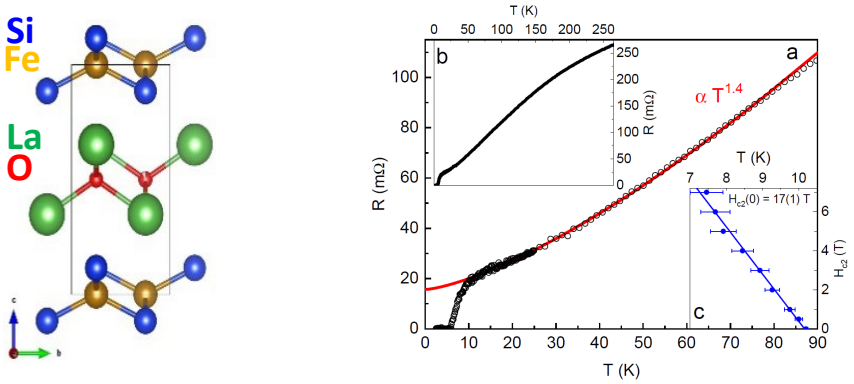

Figure 1: **Left:** crystal structure of $LaFeSiO_{1-\delta}$. **Right:** resistivity measurement of $LaFeSiO_{1-\delta}$ (full temperature range dependence in left inset and related H_{c2} critical field as a function of temperature in right inset).

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