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International Conference on Complex Orders in Condensed Matter: aperiodic order, local order, electronic order, hidden order

27 September - 2 October 2026
Evian-Les-Bains (France)



GENERAL INFORMATIONS

- Conference room :** The conference will take place at the seminar room located in the main building (same as the reception) on the ground floor
- Poster :** All posters are displayed on the Chablais room (ground floor) Monday 28 and Tuesday 29
- Restauration :** Breakfast, lunch and dinner are all served in the Restaurant located on the first floor of the main building
Breakfast served from 7h to 9h
Lunch served at 13h
Dinner served at 20h
- Welcome cocktail :** It will be served on the Sunday 27 September at 19h00 in the Bar (second floor, near reception)
- Excursion :** Wednesday 30 September 14h30
Evian visit including "Buvette Cachat"
- & Cheese tasting :** It will be served at 19h at the bar and terrace, followed by diner at 20h
- Conference dinner :** Thursday 1 October
A cocktail with jazz band concert will be served from 19h to 20h at the bar and terrace
The dinner served at 20h15 will consist of a cheese fondue. Alternative meal will be provided
- WIFI :** WIFI connection is only available in the common building of the vacation center (reception, bar and conference room). Connect to vvf clientèle. Go to your web browser and register with your first name and name. The connection is then valid for the all stay.

The ICCOCM 2026 conference is the second in a series that began in [Evian](#) in 2023. The conference aims to foster collaborations in the study of complex orders in condensed matter, with a particular focus on aperiodic order, local order, electronic order, magnetic order, and “hidden” order, as well as their influence on physical and chemical properties. At the atomic scale, complexity is characterised by two main parameters: periodic or aperiodic long-range order, and disorder and local order. Structural complexity and its influence on physical and chemical properties is encountered in a broad range of systems and requires an interdisciplinary approach. The conference will review recent advances in this field, with a particular focus on the study of incommensurately modulated phases, quasicrystals and approximants, strongly correlated electron systems, disordered and amorphous systems, high-entropy alloys and magnetically frustrated systems. Particular attention is given to highlighting the interdisciplinary approach and the common concepts, experimental methods, and theoretical frameworks used across these different fields.

This conference is being organised jointly by Tokyo University of Science, Université Grenoble Alpes, CNRS and ILL. It has received support from the CREST and the Japan Science and Technology Agency. It follows the [IRN Aperiodic conferences](#) organized in Octobre 2021 in Carry le Rouet, France. It is a successor to previous meetings held in [Nagoya](#) (2015), [Annecy](#) (2017), [Sendai](#) (2019), and [Evian](#) (2023) bringing together aperiodic and correlated electron communities.

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Program

Sunday 27 September 2026

16h30	Registration
19h00	Welcome Party

Monday 28 September 2026

8 h 30	Welcome and Introduction		
Session 1 chair: Ryuji Tamura			
8 h 50	Shinya Hosokawa - Soft X-ray Fluorescence Holography for Atomic Structure Characterizations around Light Elements	Invited	30 min.
9 h 20	Natalia Dubrovinskaia - The Beauty of Complexity and the Simplicity of Compressed Solid Matter Revealed by High-Pressure Crystallography	Contributed	20 min.
9 h 40	Florent Pawula - Turbostratic Stacking Faults : A Structural Lever for Modulating Quantum Phases in Misfit Chalcogenides	Contributed	20 min.
10 h 00	Nobuhisa Fujita - Axial rattling and soft phonon modes in a novel Al-Pd-W compound with WAl ₁₂ icosahedra	Contributed	20 min.
10 h 20	Tadashi Furuhashi - Chemical and structural complexities caused by elemental interaction in structural metallic materials	Contributed	20 min.
10 h 40	Break		
Session 2 chair: Anuradha Jagannathan			
11 h 15	Sylvain Petit - Magnetic frustration and complex orders	Invited	30 min.
11 h 45	Kaoru Kimura - Self-compensation and Bonding Conversion in Semiconducting Quasicrystalline Approximants, Related Crystals and Amorphous	Contributed	20 min.
12 h 05	Olivier Pagès - Percolation scheme for the very basic understanding of the optical phonon mode behavior of disordered semiconductor alloys	Contributed	20 min.
12 h 25	Emily Meekel - Disorder as a Design Principle in Framework Materials	Invited	30 min.
12 h 55	End of session 2		
13 h 00	Lunch		
Session 3 chair: Keichi Edagawa			
14 h 20	Olivier Perez - Tungsten phosphate bronzes as a model system for structural and electronic complexity	Invited	30 min.
14 h 50	Laura Cañadillas-Delgado - Insights into modulated nuclear and magnetic structures in metal-organic coordination polymers	Contributed	20 min.
15 h 10	Stefan Förster - Two-dimensional oxide quasicrystals : A model system linking periodic and aperiodic structures	Invited	30 min.
15 h 40	Flash presentation of posters session 1 (odd numbers) - 1 min/poster		20 min.
16 h 00	Poster Session 1 (odd numbers), including coffee break		
18 h 30	End of Poster session		

Tuesday 29 September 2026

Session 4 chair: Thierry Klein			
8 h 30	Farid Labib - Lattice Parameter as a Universal Design Principle for Magnetic Ground States in Tsai-type Icosahedral Intermetallic Compounds	Invited	30 min.
9 h 00	Sander van Smaalen - Chiral charge density waves in EuAl ₄ and related compounds	Contributed	20 min.
9 h 20	Maria Diaz-Lopez - Reimagining Interface Processing in Solid-State Batteries via Electrochemical Flash Sintering : Spatial Insights and Millisecond Structural Dynamics from Total Scattering	Contributed	20 min.
9 h 40	Kazuhiko Deguchi - Quantum magnetism of icosahedral Yb quasicrystals and approximants	Contributed	20 min.
10 h 00	Andrea Fantin - Probing chemical short-range order in high-entropy alloys : from large-scale facilities to the laboratory scale	Invited	30 min.
10 h 30	Coffee Break		
Session 5 chair : Kaoru Kimura			
11 h 10	Karen Frieze - Wadsley-related vanadium oxides under extreme conditions : incommensurate V _{0.92} O ₂ with a peculiar modulated structure and unexpected properties	Invited	30 min.
11 h 40	Yann Alexanian - Collective magnetic state induced by charge disorder in the non-Kramers rare-earth pyrochlore Tb ₂ ScNbO ₇	Contributed	20 min.
12 h 00	Anuradha Jagannathan - Electronic properties of the metallic mean family of one-dimensional quasicrystals	Contributed	20 min.
12 h 20	Iwao Matsuda - Periodic or quasi-periodic atomic chains in the surface copper boride	Invited	30 min.
12 h 50	End of session 5		
13 h 00	Lunch		
Session 6 chair: Nayuta Takemori			
14 h 20	Junmo Jeon - Quantum hyperuniformity and quantum weight	Invited	30 min.
14 h 50	Yuqing Yin - High-Pressure Synthesis and Crystal Structures of H ₃ Cl ₇ Phases	Contributed	20 min.
15 h 10	Marco Scavini - From genesis to application : In situ and in operando structural studies on rare-earth doped ceria phases.	Invited	30 min.
15 h 40	Flash presentation of posters session 2 (even numbers) - 1 min/poster		20 min.
16 h 00	Poster Session 2 (even numbers), including coffee break		
18 h 30	End of Poster session		

Wednesday 30 September 2026

Session 7 chair: Emilie Gaudry			
8 h 30	Mikito Koshino - Quasiperiodicity and Emergent Topology in Moiré Materials	Invited	30 min.
9 h 00	Nicolas Rougemaille - Fragmented phases in artificial frustrated magnets	Contributed	20 min.
9 h 20	Diana Quintero Castro - Comparing intrinsic and extrinsic contributions to phonon anharmonicity in the thermoelectric systems Mg ₂ Si and GeBi ₂ Te ₄	Contributed	20 min.
9 h 40	Cristhian David Hinostroza - Correlated disorder in a Garnet-type superionic conductor	Contributed	20 min.
10 h 00	Kaori Tanaka - Gapless superconductivity in two-dimensional quasicrystals and its real-space topology	Contributed	20 min.
10 h 20	Break		
Session 8 chair: Marek Mihalkovick			
11 h 00	Yuki Tokumoto - Superconductivity in Ta–Te-based van der Waals layered quasicrystal	Invited	30 min.
11 h 30	Pierre Bouvier - Polar instability at high-pressure in KNbO ₃	Contributed	20 min.
11 h 50	Noemi Gallucci - From chaos to order : programming nanocrystal superlattices for tailored optical function	Contributed	20 min.
12 h 10	Akira Sekiyama - High-energy photoemission study of strongly correlated rare-earth-based quasicrystal approximants	Contributed	20 min.
12 h 30	Olivier Delaire - Dynamic and static disorders in complex materials, probed with scattering experiments and simulations	Invited	30 min.
13 h 00	Lunch		
14 h 30	Guided tour of Evian including the ‘Buvette Cachat’		
18 h 30	Cheese tasting		

Thursday 1 October 2026

Session 9 chair: Ron Lifshitz			
8 h 30	Peru d'Ornellas - Fractons in the fractional Hall effect	Invited	30 min.
9 h 00	Nayuta Takemori - Analysis of band gaps and hyperuniformity in two-dimensional photonic quasicrystal approximants	Contributed	20 min.
9 h 20	Lilian Prodan - Disorder-controlled magnetism in polar antiferromagnets	Contributed	20 min.
9 h 40	Shinji Watanabe - Theoretical studies of magnetism in icosahedral quasicrystals and 1/1 approximants	Contributed	20 min.
10 h 00	Eteri Svanidze - Imperfections as a measure of exotic superconductivity?	Invited	30 min.
10 h 30	Break		
Session 10 chair: Thomas Doert			
11 h 10	Yasushi Ishii – Phasons in quasicrystals	Invited	30 min.
11 h 40	Yevheniia Kholina - Responsive disorder in framework materials	Contributed	20 min.
12 h 00	Xingyu Su - Element-Specific Ultrafast Probing of Electronic and Magnetic Orders with Time-Resolved Soft-X-Ray Spectroscopy	Contributed	20 min.
12 h 20	Laurent Guerin - Complex orders in molecular crystals probed by 3D-ΔPDF and superspace crystallography	Contributed	20 min.
12 h 40	<u>Group Photo</u>		
13 h 00	Lunch		
Session 11 chair: Leonid Dubrovinski			
14 h 30	Matthieu Le Tacon - Signatures of Electron-Phonon Coupling in the Unconventional CDW of Kagome Superconductor CsV ₃ Sb ₅	Invited	30 min.
15 h 00	Helen Walker - Exploring the disorder driving barocalorics using inelastic neutron spectroscopy	Contributed	20 min.
15 h 20	Ireneusz Buganski - Quasicrystals in ZnMg(Dy, Er, Ho, Tm)Li system	Contributed	20 min.
15 h 40	Jonas Wolber - n=1 Aurivillius and other 2-dimensional magnets	Contributed	20 min.
16 h 00	Break		
Session 12 chair: Koji Kimura			
16 h 40	Masato Matsuura - Study of Lattice and Phason Dynamics in i-AlPdMn Quasicrystal and its Approximants	Invited	30 min
17 h 10	Yui Ishii - Can a glass-like aperiodic structure coexist with a periodic crystal structure?	Contributed	20 min.
17 h 30	David Serban - Imaging Topologically Protected Strings in Dysprosium Indate using Bragg Coherent X-ray Diffraction	Contributed	20 min.

Friday 2 October 2026

Session 13 chair: Laetitia Laversenne			
8 h 30	Yoshihiro Okamura - Optical detection of nonlinear magnetoelectric coupling in multiferroic altermagnet	Invited	30 min.
9 h 00	Makito Aoyama - Pseudogap properties of quasicrystal-related materials in the quaternary Al-Pd-TM-Fe (TM=Cr, Mo, W) systems	Contributed	20 min.
9 h 20	Jonathan Bulled - Hierarchical structure of disordered metal-organic frameworks and growth-directed symmetry breaking	Contributed	20 min.
9 h 40	Thomas Doert - Hydroxyperovskites – Correlated Proton Disorder and Spin Dynamics	Contributed	20 min.
10 h 00	Break		
Session 14 chair: Laszlo Pusztai			
10 h 30	Laureline Porcar - Shape Memory alloys for multicaloric properties	Invited	30 min.
11 h 00	José-Enrique Rodríguez Fernandez - Influence of phase and structural ordering on the electrochemical performance of multiphase Na-layered oxides as positive electrodes	Contributed	20 min.
11 h 20	Andrii Syrota - Amorphisation by Structural Disorder and Its Effects on Topological Phases	Contributed	20 min.
11 h 40	Koji Kimura - Anharmonic Phonons in Rutile TiO ₂ Investigated by Inelastic X-ray and Neutron Scattering	Contributed	20 min.
12 h 00	<u>Concluding remarks</u> : Sander van Smaalen		
12 h 30	End of the conference		
13 h 00	Lunch		

LIST OF POSTERS - ICCOCM 2026

#	Name	Surname	Contribution Title
1	Ireneusz	Buganski	The electronic structure of ZnMg(Hf, Zr, Ti) periodic approximant phases
2	Timoth��	Courtial	Attempt to nano-engineer flat bands to enhance superconductivity
3	Matteo	d'Astuto	Paramagnon softening with doping in oxychloride cuprate superconductors
4	Leonid	Dubrovinsky	Peierls Physics and Crystal Chemistry of High Pressure Polymorphs of Na ₄ X ₅ (X = I, Br, Cl) Compounds
5	Naoki	Fujioka	First-principles study of 4 at.% Pd-doped Al ₁₃ Fe ₄
6	Erina	Fujita	Multi-descriptor analysis based on HYPOD-X, an open database of quasicrystals and approximants
7	Tomoyo	Fukuda	Wide e/a Control in Tsai-Type Approximants by Heterovalent Substitution
8	Gaston	Garbarino	New opportunities on the studies of condensed matter systems under extreme conditions at the ESRF-EBS
9	Emilie	Gaudry	First-Principles and Machine Learning Investigation of Adsorption and Hydrogen Dissociation on Graphene-Supported Single-Atom Catalysts
10	Satoshi	Kameoka	Creation of novel catalyst materials utilizing phason engineering
11	Thierry	Klein	Thermodynamic Evidence for Multiple Field-Induced Phases in a Slightly Distorted Kagome Antiferromagnet
12	Sian	Landi	Investigations on Xanthine Solid State
13	Laetitia	Laversenne	Study of Short-Range Order in TiVCr-Based Multiple Principal Element Alloys for Hydrogen Storage
14	Ron	Lifshitz	Detecting dislocations using Bragg-peak vortices
15	Marek	Mihalkovic	High-pressure synthesis of Al ₁₁ Fe ₄ and its DFT-assisted structure refinement
16	Goran	Nilsen	Collinear spin nematic phase in the breathing pyrochlore spinel LiGa _{0.95} In _{0.05} Cr ₄ O ₈
17	Andrea	Piovano	Crystal field and spin fluctuation in heavily doped nickelates
18	Laszlo	Pusztai	Understanding disordered structures: a paradigm shift due to Reverse Monte Carlo modeling
19	Sitaram	Ramakrishnan	Tracing the Horizon of Tetragonal–Monoclinic distortion in trilayer nickelate La ₄ Ni ₃ O ₁₀
20	Masanori	Sato	DFT analysis of pentacene adsorption on the surfaces of the Tsai-type Ag-In-Yb quasicrystal
21	Seki	Yusuke	Numerical Study of the NMR Coherence Peak in Quasicrystalline Superconductors
22	Yeong-Gi	So	Formation of Mn-based dodecagonal quasicrystals

23	Ayaka	Takahashi	Search for Superconductivity in Os-Based Decagonal Hypermaterials
24	Ryuji	Tamura	Magnetism of Tsai-type Icosahedral Quasicrystals
25	Hiroshi	Taniyama	Structure and magnetism of a new phase in the Ga–Pd–Tb system
26	Ren	Uchimoto	Fabrication and superconductivity of Ta–TM–Te van der Waals layered quasicrystals
27	Zhiyi	Wang	Atomistic Investigation of Martensitic Transformations in Cu-Based Shape Memory Alloys Using a Machine-Learned Interatomic Potential
28	Ya	Xu	Hydrogen Absorption Behavior of Hypermaterials Containing Hydrogen-Affinity Elements
29	Tsunetomo	Yamada	Non-Fermi-liquid behavior in a quasicrystal and its 2/1 cubic approximant
30	Yuki	Yamamoto	Correspondence between exact eigenstates on distinct electron site configurations with identical quasiperiodicity
31	Subaru	Yoshimoto	Relaxation of Magnetic Structure in the Regularly Ordered Frustrated Magnet DyRu ₂ Si ₂

ICCOCM 2026

Invited presentations abstracts

Dynamic and static disorders in complex materials, probed with scattering experiments and simulations

Olivier Delaire* ¹

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Abstract

A detailed view of the atomic structure and atomic motions in complex materials is needed to refine microscopic theories of transport and thermodynamics, and to design next-generation materials for energy technologies or computing devices. Many useful properties of complex materials arise from, or are tuned by, sources of disorder in their structure, which can be either static or dynamic. For instance, understanding the temporal and spatial correlations of ionic disorder in superionic conductors – solid materials with ionic diffusivities approaching those of liquids – is critical to improve their functional performance in solid-state batteries or fuel-cells. In parallel, the vibrational dynamics of the structure (phonons) controls properties ranging from ferroelectrics for sonar, to thermoelectrics for waste-heat harvesting, or phase-change materials for information storage and neuromorphic devices. To understand these phenomena in complex materials, one needs to identify and separate multiple possible sources of disorder: compositional fluctuations, spontaneous off-centerings, tilts or distortions of structural subunits, and numerous phonon modes – and their couplings. This has remained a daunting challenge. This presentation will highlight results from our investigations of atomic dynamics and disorder in complex materials with neutron and x-ray scattering experiments, combined with modern atomistic simulations. We seek insights into the atomic structure and dynamics by combining multimodal inelastic and diffuse neutron / x-ray scattering measurements to map the full energy (E) and wavevector ($\mathbf{Q}$) dependence of the dynamical structure factor, $S(\mathbf{Q}, E)$, the space-time Fourier transform of the van Hove correlation function [1],

$$G(\mathbf{r}, t) = \frac{1}{N} \left\langle \sum_{i,j} \delta(\mathbf{r} - \mathbf{R}_j(t) + \mathbf{R}_i(0)) \right\rangle \quad (1)$$

which gives the probability of finding a particle at position $\mathbf{r}$ at time t , given that a reference particle was located at the origin at $t = 0$. We rationalize our observations with first-principles atomistic simulations coupled with machine learning techniques and instrument digital twins, and utilize this microscopic information to inform models of thermodynamics and transport properties.

References

- [1] Van Hove, Léon, *Physical Review*, **95**, 249, 1954.

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Keywords— disorder, lattice dynamics, neutron and x-ray scattering, atomistic simulations

Fractons in the fractional Hall effect

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Charles Stahl³ Adolfo G. Grushin^{1,2,4}

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Abstract

In interacting systems, topology often depends on translational symmetry. The canonical example, the fractional Hall effect, emerges only in extremely clean samples. Efforts have been undertaken to extend such fractionalised phases to disordered contexts, however it is an open question whether interacting topological phases exist which have no crystalline analogue. We propose an exactly-solvable model that realises such a phase. This is done by coupling together a patchwork of Laughlin fractional Hall phases, each with a different fractionalisation. The model is presented via a coupled-wire construction, where we can tune the topology in real space by adjusting the spatial positioning of each wire. We show non-crystalline structure allows us to couple differently fractionalised phases together into a single gapped phase. Remarkably, this phase appears to realise a gapped fractonic order in 2D—violating a prominent no-go theorem which supposedly prohibits such a phase emerging in fewer than three dimensions. We show how the system has a ground state degeneracy that is exponential in system size, a signature of a fracton phase. We find a rich phenomenology of excitations, containing both anyons which behave as conventional fractional Hall excitations, and lineons which are constrained to move only in one dimension, where no physical fermionic operator can be written down which violate the fractonic constraints. Finally, time permitting, we will provide a discussion of the stability of this phase against arbitrary perturbations, and what needs to be done to declare victory against the no-go theorem that has guided the last years of research into fractonic physics.

References

- [1] Schirrmann, J., d’Ornellas, P., Stahl, C., Grushin, A.G. (2025). Fractonic Fractional Quantum Hall Effect. *arXiv preprint arXiv:2504.18337*, 2025.

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Keywords— Fractons, fractional Hall effect, disorder

Probing chemical short-range order in high-entropy alloys: from large-scale facilities to the laboratory scale

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Abstract

Chemical short-range order (CSRO), although thermodynamically driven, is usually the kinetically frozen imprint of an alloy's cooling history. Interest in its study has expanded markedly over the last decade (Figure 1), especially in compositionally complex alloys (CCAs, including medium- and high-entropy alloys) and in connection with mechanical properties. Yet, CSRO remains an elusive feature that is difficult to characterize unambiguously. This contribution highlights a few laboratory-accessible probes of CSRO in single-phase solid solutions that complement large-scale facility-based structure determination. After a concise overview of the main scattering and spectroscopy methods useful for resolving local structures and chemical ordering –such as X-ray absorption spectroscopy– the talk focuses on differential scanning calorimetry, dilatometry, and electrical resistivity measurements performed on benchmark ternary (e.g. CrCoNi) compositions. These laboratory-based experiments register subtle CSRO-related signatures in heat capacity, thermal expansion and charge-carrier scattering, enabling rapid screening, in-situ thermal cycling and kinetic studies.

Typical hurdles in multicomponent systems –weak scattering contrast among neighboring elements and an excess of refinable parameters– are mitigated when laboratory data are incorporated into the analysis alongside complementary large-scale facility data. Emerging evidence shows that CSRO has a measurable impact on thermophysical responses, whereas its effect on bulk mechanical performance appears modest, if not negligible. Rigorous control and reproducible formation of CSRO, coupled with reliable structural determination, remain the ultimate goal of a multimodal approach to untangle processing–local-structure–property relationships and guide future alloy design.

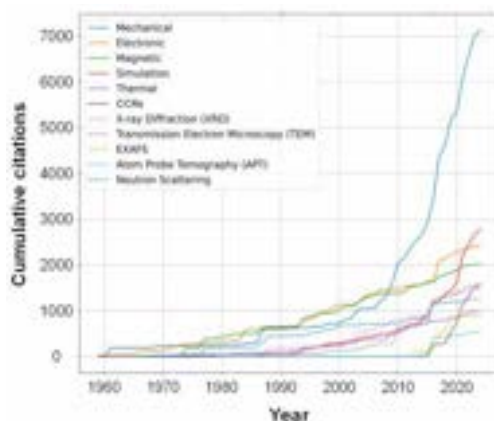


Figure 1: Cumulative citations of CSRO papers broken down by research sub-topic and characterization technique. Example: blue line represents “CSRO & mechanical”.

References

- [1] Courty F.G. *et al.*, “On the nature of chemical short-range order evolution”, *Research Square*, **rs-7339299** (2025). Available at <https://www.researchsquare.com/article/rs-7339299/v1>.
- [2] Bacurau V.P. *et al.*, *Nature Communications*, **15**, 7815 (2024).
- [3] Andreoli A.F. *et al.*, *Materials & Design*, **238**, 112724 (2024).
- [4] Li Y. *et al.*, *Nature Communications*, **14**, 7410 (2023).
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- [6] Fantin A. *et al.*, *Small Science*, **4**, 2300225 (2024).

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Keywords— chemical short-range order, high-entropy alloys, thermophysical methods

Two-dimensional oxide quasicrystals: A model system linking periodic and aperiodic structures

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Abstract

2D materials are widely investigated model systems for exploring structure-property relations with a special emphasis on microelectronic and catalytic applications. The advent of oxide quasicrystals (OQCs) broadened the family of 2D materials to include aperiodically ordered materials [1].

The prototypical OQC is formed in Ba-Ti-O on a hexagonal Pt(111) support [1]. On the atomic scale, scanning tunneling microscopy resolves a dodecagonal triangle-square-rhombus tiling of Ba atoms decorating the rings of a titanium oxide network [2]. Low-energy electron diffraction shows an ideal dodecagonal structure, which aligns with the high-symmetry directions of the substrate. The direct access to the real-space tiling allows for a statistical analysis, which revealed the ideal triangle : square : rhombus ratio of the dodecagonal Niizeki-Gähler tiling of $(1 + \sqrt{3}) : 1 : 1/(1 + \sqrt{3})$. Additionally, from lifting the tiling in the 4D periodic hyperspace, the hyperslope of the Ba-Ti-O OQC was proven to correspond to that of an ideal dodecagonal structure [3].

In this talk, we will focus on two links of the OQC to periodic structures by presenting the wealth of approximant structures that occur in these two-dimensional oxide networks and by discussing the interplay of the OQC with its periodic support.

The alignment of the OQC along the main substrate directions points to a quasicrystal-crystal heteroepitaxy in this system. So far, no evidence for an epitaxial stabilization by common components in reciprocal space has been found. Instead, by analyzing the vertex positions upon lifting into the internal space, we identify phason fluctuations as the stabilization mechanism. Mapping these fluctuations into the physical space reveals that the system maximizes the number of particularly lattice-matched approximant motifs to adapt to the substrate [4].

Periodic approximant phases are formed in the two-dimensional oxide layer when the Ba content is altered. At Ba coverages between 50% and 100% of the titanium oxide rings, seven periodic approximant phases are observed. This allows us to examine the structure-property relations in this system. As an example we explore the impact of the aperiodic surface potential on the electronic structure of freely propagating electrons by comparing the image potential state signature in the OQC with that of an approximant phase. The flexibility of the network furthermore allows us to grow OQCs from a metal-oxide honeycomb (HC) template [5]. The successive adsorption of guest atoms, such as Ba, Sr, or Eu, onto the HC layer triggers the network to reorganize. At a coverage of 73% of the honeycomb rings, the network adopts the dodecagonal structure. Using this approach, we have successfully incorporated the 4f element europium into the OQC aiming for imprinting magnetic properties into this dodecagonal phase.

References

- [1] S. Förster, K. Meinel, R. Hammer, M. Trautmann & W. Widdra, *Nature*, **502**, 215, 2013.
- [2] S. Schenk, O. Krahn, E. Cockayne, H. L. Meyerheim, M. de Boissieu, S. Förster & W. Widdra, *Nat. Commun.*, **13**, 7542, 2022.
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Wadsley-related vanadium oxides under extreme conditions: incommensurate $V_{0.92}O_2$ with a peculiar modulated structure and unexpected properties

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Abstract

Wadsley vanadium oxides form a homologous series with general composition V_nO_{2n+1} between the end members α - V_2O_5 and $VO_2(B)$. They are oxygen deficient with different ordered vacancies in an oxygen cubic close-packing array and exhibit a variety of crystal structures due to different polyhedra around the V^{4+} and V^{5+} cations and polyhedral connectivity. Members of this series exhibit a rich variety of structural, electronic, magnetic, and metal–insulator phase transitions. Starting from the Wadsley-phase V_6O_{13} , corresponding to $V_{0.92}O_2$, we synthesized a peculiar rutile-related phase at 10 GPa and 1273 K, which we subsequently studied with single-crystal X-ray diffraction. $V_{0.92}O_2$ starts to decompose at 470 K and atmospheric pressure. When heated to temperatures above about 350 K, the material transforms to an incommensurate phase. Measurements of electronic transport properties provide evidence that the incommensurate phase is insulating. In the incommensurate phase, the oxygen sublattice is essentially rigid. Amplitudes of the displacive modulation of the V atoms are also hardly significant and V—V distances are almost constant. The absence of significant displacements of the atoms in the modulated structure is attributed to the fact that the atoms are disordered over several split atom positions. For the modeling, an anharmonic description of the displacement parameters and their corresponding modulation was used for the V atoms to reach satisfactory agreement factors for main and first-order satellite reflections. On compression at room temperature, $V_{0.92}O_2$ reaches the ideal rutile structure at about 5.0 GPa.

Our results show that the structural and electronic behaviour of $V_{0.92}O_2$ at extreme conditions is distinctly different from that of stoichiometric VO_2 and that synthesis under extreme conditions can lead to new materials with unexpected properties and peculiar structural features.

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Keywords— Wadsley phases, vanadium oxides, incommensurate phases

Soft X-ray Fluorescence Holography for Atomic Structure Characterizations around Light Elements

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Abstract

To solve a fundamental difficulty in atomic structure characterizations around light elements, we have developed a soft x-ray fluorescence holography equipment of our own design available for the elements in the third period beyond Na. The experimental setup is shown in Fig. 1, which is composed of a compact vessel for flowing He gas, two stepping motors to change the crystal angles with respect to the incident x-ray beam, and an energy-resolved Si drift detector to collect the corresponding fluorescent soft x-rays [1]. We show atomic images around S in a ZnS single crystal with a zinc blende structure as an example. The neighboring Zn atoms are clearly observed at the ideal atomic positions in the distant range of about 1 nm from the central S atom. Based on the success of the soft x-ray fluorescence holography, we will be able to extend the measurable elements in the second period from C to F in the near future by changing the Si drift detector to that with a special polymer window and performing the experiments under vacuum condition.

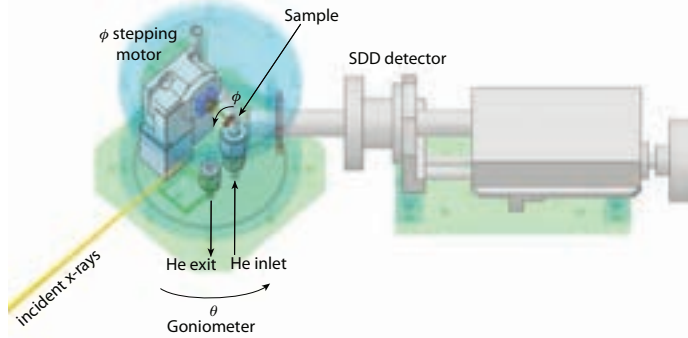


Figure 1: A schematic view of the vessel of our own design to carry out SXFH experiments in He gas atmosphere.

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Keywords— Atomic structures, Light elements, Soft x-rays

Phasons in Quasicrystal

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Abstract

Quasicrystal (QC) is a long-range-ordered solid with rotational symmetry incompatible with periodicity, where aperiodicity arises from competing incommensurate length scales inherent in the non-crystallographic rotational symmetry. One of the most generic properties of QC is an excitation called "phason", which is associated with phase difference of incommensurate density waves in QC. As an incommensurate length scale in QC arises from non-crystallographic rotational symmetry, the phason degrees of freedom lead to much more variety in structural modifications than ordinary low-dimensional incommensurate solids. In addition, thanks to accurate information on the atomic structure for some families of QC, the phason in the atomic scale is understood more precisely than before. The phason in the atomic scale is characterized by a local rearrangement of atoms, which yields characteristic *structural flexibility* in QC. In this lecture, I will try to illustrate the phason in QC as a basic concept for understanding diversity of real materials and discuss dynamic aspect including the characteristic vibrational spectrum.

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Keywords— quasicrystal, phason, incommensurate

Quantum hyperuniformity and quantum weight

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Abstract

Hyperuniformity provides a powerful framework to characterize the vanishing of long-wavelength density fluctuations, and has been widely used to achieve a unified understanding of quasiperiodic and disordered systems [1, 2, 3]. More recently, there have been growing efforts to understand phase transitions in quasiperiodic or disordered systems by employing generalized notions of hyperuniformity [3, 4, 5, 6]. However, since previous studies on hyperuniformity have focused only on classical fluctuations, they miss intrinsic quantum fluctuations. As a result, the conventional hyperuniformity classification framework has clear limitations in understanding quantum phase transitions, and in particular leaves several important open questions in distinguishing gapped versus gapless phases and extended versus localized phases in quasiperiodic systems.

In this talk, we introduce the concept of quantum hyperuniformity and show how its classification, defined through the scaling of the long-wavelength structure factor including its quantum contributions, offers a direct probe of quantum phases and phase transitions [7]. Using the Aubry–André model as a concrete example of quasiperiodic systems with extended-to-localized quantum phase transition [5, 8], we demonstrate that quantum hyperuniformity classes sharply distinguish gapped, gapless, and localized-extended phases, while at the quantum critical point the structure factor exhibits anomalous scaling beyond conventional linear or quadratic behavior. This anomalous scaling originates from multifractal critical wave functions and directly reflects an anomalously slow decay of long-range charge–charge correlations, providing a clear fingerprint of quantum criticality in real space.

Beyond classification, we will show that in gapped phases the quantum hyperuniformity framework naturally connects to quantum geometry through the quantum weight [7, 9]. In this regime, the structure factor exhibits universal quadratic scaling, whose coefficient—the quantum weight—directly encodes an effective length scale of the many-body state associated with the gap. This relation is further sharpened into universal scaling law, where the quantum weight provides a quantitative measure of spectral gap sizes in quasiperiodic systems, enabling one to extract gap information purely from ground-state correlations without explicit spectral calculations.

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Keywords— Hyperuniformity, Quantum criticality, Quantum weight

Quasiperiodicity and Emergent Topology in Moiré Materials

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Abstract

Moiré materials formed by twisted two-dimensional crystals provide a highly tunable platform for emergent electronic and structural phenomena arising from long-period interference patterns. While early studies mainly focused on electronic flat bands in periodic moiré patterns, recent developments have revealed a much broader landscape involving quasiperiodic structures.

In this talk, I will review recent theoretical studies on dynamical and quasiperiodic aspects of moiré materials. I will first briefly review the basic physics of periodic moiré materials, focusing on twisted bilayer graphene and related systems. I will then discuss recent developments beyond periodic moiré superlattices toward quasiperiodic moiré quantum matter. A prominent example is 30-degree twisted bilayer graphene, where the system lacks translational periodicity and forms a dodecagonal quasicrystalline electronic structure. I will introduce recent theoretical developments on the electronic structure of this system, including quasi-band descriptions and emergent momentum-space organization beyond the conventional Bloch framework. [1,2]

Finally, I will discuss twisted moiré trilayer systems containing multiple interacting moiré patterns. The interference between distinct moiré structures gives rise to moiré-of-moiré textures, emergent long-scale structures, and novel topological phenomena unique to quasiperiodic multilayer systems. [3,4]

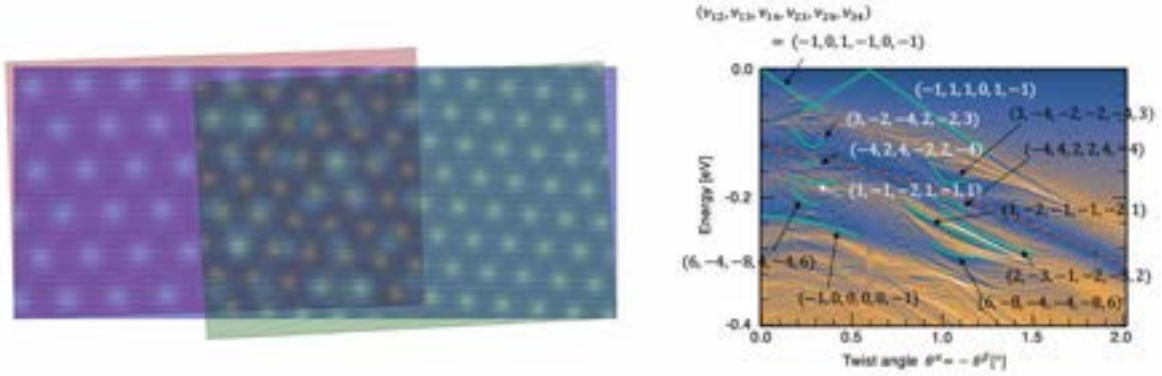


Figure 1: Graphene/hBN moiré trilayer and its energy spectrum with topological gap indexes [3,4]

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Keywords— Graphene, 2D materials, moiré superlattices

Lattice Parameter as a Universal Design Principle for Magnetic Ground States in Tsai-type Icosahedral Intermetallic Compounds

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Abstract

Among aperiodic crystals, quasicrystals (QCs) represent a unique class of structurally ordered solids exhibiting sharp Bragg reflections and non-crystallographic rotational symmetries such as tenfold [1]. Long-range magnetic orders in QCs [2–4] and their periodic counterparts, called approximant crystals (ACs), have been experimentally realized in a number of alloy systems, as summarized elsewhere [5].

Despite significant progress that has been made in understanding unique magnetic orders in QCs and ACs, their systematic design and synthesis remains a challenging task due to the lack of universal design principles. The electron-per-atom (e/a) ratio based on the Slater–Pauling concept, has widely been used to guide the design of magnetic orders in metallic systems, including Tsai-type QCs and ACs [5], yet accumulated evidence shows that e/a alone lacks universality in controlling magnetic ground states across different alloy families.

In this talk, a new design axis based on **lattice parameter** for controlling long-range magnetic order in Tsai-type QCs and ACs will be presented. The latest results on both Heisenberg (magnetically isotropic) and non-Heisenberg (magnetically anisotropic) systems will be discussed in terms of lattice parameter, e/a , and the correlation between the two quantities. Figure 1 shows a nearly monotonic relationship between lattice parameter and e/a in non-Heisenberg Au-based 1/1 ACs, together with the corresponding magnetic ground states.

Based on these results, a comprehensive picture of magnetism in Tsai-type QCs and ACs governed by the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction and crystalline electric field (CEF) effects is unveiled. This provides a practical guideline for the design and discovery of hidden magnetic orders not only in QCs and ACs, but also in other complex aperiodic systems.

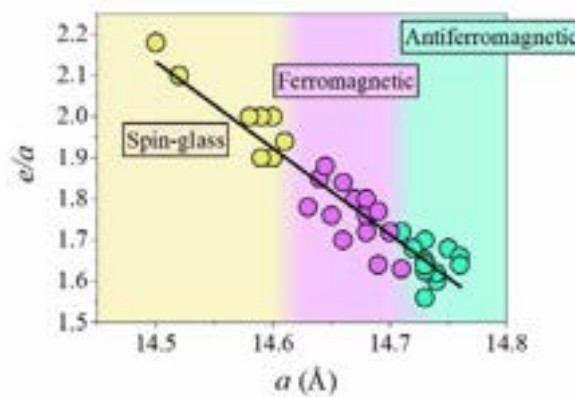


Figure 1: The lattice parameter dependence of e/a in non-Heisenberg Tsai-type compounds revealing a near-monotonic correspondence between these quantities.

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Keywords— quasicrystals, approximant crystal, magnetic order, Tsai-type compounds

Signatures of Electron-Phonon Coupling in the Unconventional CDW of Kagome Superconductor CsV_3Sb_5

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Abstract

The recent discovery layered Kagome superconductors AV_3Sb_5 ($\text{A}=\text{K}, \text{Cs}, \text{Rb}$) has sparked considerable excitement. These materials are characterized by an electronic structure featuring flat bands, van Hove singularities (vHs), Dirac cones, and non-trivial band topology, and offer a unique platform for exploring novel electronic states of matter with intertwined orders. At temperatures well above their superconducting T_c (2.7K in CsV_3Sb_5), an electronic superlattice commonly associated with a CDW. To date, no Kohn-anomalies associated with the formation of this CDW have been observed in their phonon dispersion, whereas chirality, time-reversal symmetry breaking or electronic nematicity have been reported, indicating that the underlying electronic order might be substantially more complex. High pressure studies have revealed a double superconducting dome structure associated with the changes in the nature and disappearance of the CDW inferred from indirect measurements.

I will present a detailed high pressure x-ray diffraction study of these materials showing in detail how the lattice superstructures evolve across the phase diagram. Previously unreported anomalies in the lattice dynamics across the CDW formation will also be presented. These results bring novel insights on the nature and origin of the CDW, challenging in particular scenario in which it arises from a Peierls-like nesting of occupied van Hove Singularities and point to strong electron-phonon interactions and significant anharmonic effects. Understanding these phenomena is crucial for uncovering the microscopic mechanisms underlying exotic quantum phases in correlated materials.

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Keywords— kagome, CDW, electron-phonon coupling

Periodic or quasi-periodic atomic chains in the surface copper boride

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A crystal surface, sandwiched between a vacuum and a substrate, is a unique platform to synthesize novel two-dimensional (2D) materials. Surface layers can be grown on substrates commensurately or incommensurately, depending on a balance between adsorbate–adsorbate and adsorbate–substrate interactions. Such a degree of freedom, being specific to a surface, results in the formation of exotic long-range ordered phases that cannot be realized in pure 2D systems [1-2].

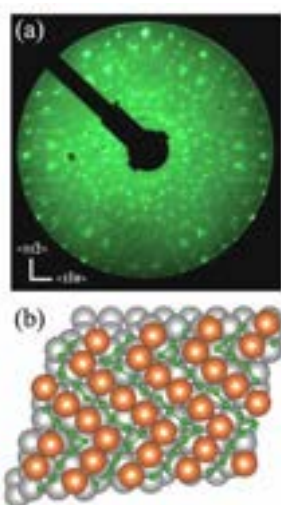


Figure 1 (a) Low-energy electron diffraction pattern and (b) a structure model of the $\sqrt{73} \times \sqrt{39} R \pm 5.8^\circ$ -B phase on Cu(111) [1-2]. Surface copper and boron atoms are colored in orange and green, respectively. The substrate copper is colored in gray.

When boron deposition is made on Cu (111), a 2D crystal phase of $\sqrt{73} \times \sqrt{39} R \pm 5.8^\circ$ is formed at the surface (Fig.1). Structure determination by the positron diffraction method unveiled that the surface layer is composed of alternating rows of zigzag Cu and B chains (Fig.1) [1-2]. The well-defined chemical stoichiometry (Cu_8B_{14}) indicates that the material is copper boride. It is worth mentioning that no copper boride has been reported in 3D boron compounds. The 2D copper boride is uniquely formed only in the environment of surface or interface.

Keeping in mind the knowledge of a possible formation of copper boride at a surface of the copper crystal, we attempted the boron deposition on Cu(110) and discovered the $3 \times 1'$ -B phase [3]. With scanning tunneling microscope, we found, as shown in Fig.2, that the surface was a periodic array of quasi-periodic atomic chains of copper boride [4]. The 1D structure of the individual chain is composed of two types of segments that are commensurate or incommensurate with the substrate Cu lattice. Such a surface system has theoretically been proposed to be the 1D quasicrystal by Aubry [5]. The structural characters, described in the paper [5], were identified in the $3 \times 1'$ -B/Cu(110) surface. The surface copper boride is likely to be a suitable playground to conduct science of quasicrystals.

The B/Cu(110) system at the higher boron coverage results in formation of the $7 \times 1'$ -B phase at the surface [6]. In the new 2D crystal phase, a width of the 1D structure has become atomically large enough to form the local 2D chiral structures in the chain. The structural variation traces the birth of chirality during the dimensional crossover of surface copper boride from 1D to 2D.

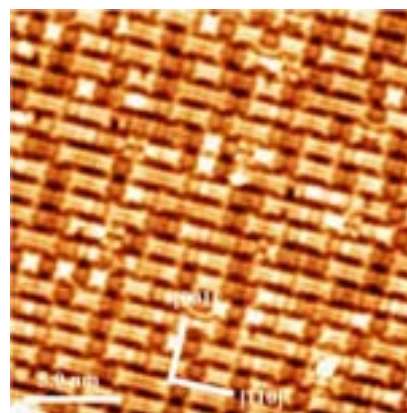


Figure 2 A microscopic image of the $3 \times 1'$ -B phase on Cu(110), observed by scanning tunneling microscope [4]. Each 1D structure has the two-atom width and bright protrusion corresponds to locations of boron atoms.

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Keywords—quasi-periodic, boron, one-dimensional, surface, boride

Study of Lattice and Phason Dynamics in i-AlPdMn Quasicrystal and its Approximants

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Quasicrystals, characterized by aperiodic long-range order, exhibit unique physical properties that stem from their lack of translational symmetry. While their static structures are well-described in higher-dimensional spaces, the understanding of their dynamic responses—comprising phonons (real-space excitations) and phasons (complementary-space excitations)—remains a significant challenge in condensed matter physics. In this presentation, we report our recent progress in investigating both phason and phonon dynamics in the icosahedral i-AlPdMn quasicrystal and its approximants using state-of-the-art neutron scattering techniques at J-PARC.

Regarding phason dynamics, we focused on the low- Q region to overcome the limitations of the Debye-Waller factor at high temperatures. We performed quasielastic neutron scattering (QENS) measurements on i-AlPdMn and its approximants (1/1 and 2/1 phases) using the cold-neutron disk-chopper spectrometer AMATERAS. In particular, we utilized a flat-shaped powder sample to obtain high-quality data over a wide temperature range. While previous studies primarily reported atomic jumps at high temperatures and high Q [1], our latest results at moderate resolutions (~ 0.1 meV) reveal fast dynamics that persist from $T = 300$ K down to $T = 3$ K. We will discuss the origin of this persistent fast QENS by comparing the signals among the quasicrystal and its approximants.

In parallel, we have deepened our understanding of lattice dynamics. Our recent work [2] revealed singular continuous states in i-AlPdMn, evidenced by a hierarchical gap structure in acoustic modes and nonreciprocal phonon propagation. To further verify these features, we performed high-resolution measurements using the near-backscattering spectrometer DNA (BL02). By employing the newly installed Si311 analyzers, we achieved an energy resolution of $\Delta E \sim 20 \mu\text{eV}$, allowing us to investigate phonons around strong Bragg peaks at high Q which were previously limited by instrument resolution. We also examined the detailed balance equation, $S(-Q, -\omega) = \exp(-\hbar\omega/k_B T) S(Q, \omega)$, in single crystals to clarify the observed asymmetry in phonon intensities.

In this talk, we will report our latest experimental results obtained from both AMATERAS and DNA, discussing the characteristic dynamics of quasicrystals—from persistent atomic motions at low temperatures to collective lattice vibrations—originating from their aperiodic order.

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Keywords— phason, phonon, inelastic neutron scattering, quasielastic neutron scattering

Disorder as a Design Principle in Framework Materials

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Abstract

Structural complexity – arising from disorder, aperiodicity, and local correlations – is increasingly recognised as a key factor governing the behaviour of functional materials [1]. However, establishing clear links between structure and properties remains challenging, particularly when deviations from periodic order dominate.

In this talk, I will show how metal-organic frameworks (MOFs) provide a versatile platform to investigate and manipulate structural disorder in a controlled manner. By combining total scattering with three-dimensional difference pair distribution function (3D- Δ PDF) analysis, we access real-space signatures of local and correlated structural distortions beyond the average crystallographic structure.

Through a series of case studies, I will highlight distinct manifestations of disorder, including the aperiodic network topology in TRUMOF-1 [2,3], orientational disorder of metal nodes in lanthanide-based frameworks [4], and correlated tilting distortions in van der Waals Framework-type materials. Across these systems, we demonstrate how synthetic design enables systematic variation of disorder, providing insight into its structural origins and its influence on material behaviour.

These results illustrate that disorder can be deliberately introduced and tuned, offering new opportunities to explore structure-property relationships in complex materials. More broadly, this work highlights common experimental approaches and conceptual frameworks for understanding structural complexity across diverse material classes.

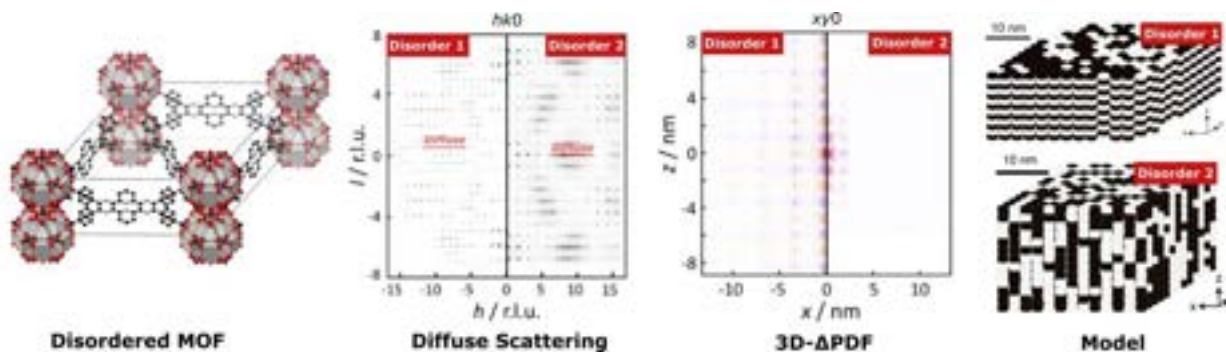


Figure 1: Outline of disordered MOF analysis and the observation of different local structures.

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Keywords— Disorder, diffuse scattering, 3D- Δ PDF, Metal-organic framework, structure-property, aperiodicity

Optical detection of nonlinear magnetoelectric coupling in multiferroic altermagnet

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Abstract

Magnetoelectric (ME) coupling, which enables mutual control between electric and magnetic properties of solids, has attracted significant attention as a key functionality emerging from simultaneous breaking of inversion and time reversal symmetries. Beyond its fundamental interest, ME coupling provides a promising route toward energy-efficient and dissipationless control of magnetic states, and has been widely studied in various material systems, including complex magnetic textures such as skyrmions. Therefore, the realization and exploration of ME coupling in functional magnets is of particular importance. In this context, the altermagnet is one important target, which has recently emerged as a novel class of magnetic materials characterized by antiferromagnetic order that breaks time-reversal symmetry without net magnetization. This unconventional order originates from the arrangement of nonmagnetic ions surrounding magnetic sites, leading to remarkable properties such as large spin splitting in electronic bands even in the absence of spin-orbit coupling, as well as anomalous Hall effects [1,2]. While most previous studies have focused on metallic or semiconducting systems, recent theoretical work predicts that insulating altermagnets can host a new type of ME coupling. In particular, *multiferroic altermagnets*, where ferroelectricity coexists with altermagnetic order, are expected to exhibit strong coupling between spin-dependent electronic structure and electric polarization, enabling dissipationless control of magnetic properties. However, experimental realization of this material class remains an open challenge.

In this talk, we demonstrate a giant nonlinear ME coupling in the multiferroic altermagnet $\text{Fe}_2\text{Mo}_3\text{O}_8$. While conventional linear responses are insensitive to the altermagnetic order, optical second harmonic generation (SHG) directly visualizes time-reversal twin domains. The nonlinear susceptibility is among the largest reported, exceeding those of topological semimetals despite zero net magnetization. This strong ME coupling also gives rise to a nearly perfect nonlinear optical diode effect, with an order-of-magnitude change in SHG intensity upon reversing the light propagation direction. If time permits, we further discuss nonlinear ME responses resonant with electromagnon excitations in the terahertz regime. These results reveal a strong interplay between magnetic order, electronic structure, and polar lattice degrees of freedom, establishing a novel route toward dissipationless control of altermagnetic systems.

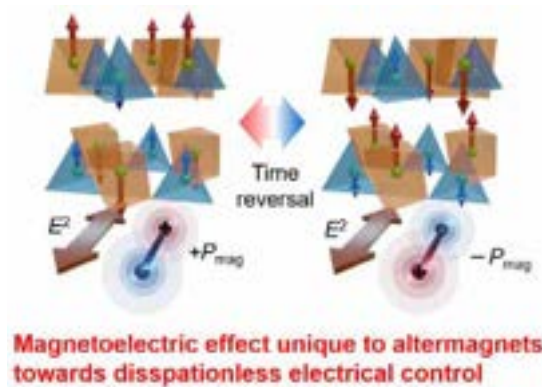


Figure 1: Schematic illustration of multiferroic altermagnet.

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Keywords— altermagnet, magnetoelectric effect, multiferroics

Tungsten phosphate bronzes as a model system for structural and electronic complexity

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Tungsten phosphate bronzes $(\text{PO}_2)_4(\text{WO}_3)_m$ provide a remarkable model system for exploring the interplay between structural and electronic complexity. Their crystal structures consist of WO_3 slabs built from corner-sharing WO_6 octahedra, separated by single PO_4 tetrahedral layers¹. The thickness of the WO_3 slabs is defined by the parameter m ranged from 2 to 14. Varying m therefore provides a direct means of tuning the structural dimensionality of the WO_3 framework. Recently, the discovery of ordered intergrowths between consecutive members has extended the family beyond integer values of m . Regular sequences of WO_3 slabs of different thicknesses generate well-ordered compounds with fractional average m values, introducing an additional degree of structural control. Rather than simply expanding the family, these fractional members provide a finer tuning of the WO_3 slab dimensionality and open the possibility of exploring the electronic phase diagram with a structural resolution inaccessible to the integer series alone.

This structural dimensionality has profound consequences for the physical properties. Across the series, metallic and poor-metal regimes are observed³⁻⁵, together with a rich sequence of temperature-driven electronic instabilities. Their evolution can be followed simultaneously through electrical transport and diffraction: resistivity anomalies accompany the appearance of satellite reflections or diffuse scattering, directly revealing the structural response associated with the electronic transitions. The nature of this response evolves markedly with m . Structural modulations involve, depending on the member, octahedral tilting, modulations of W–W distances associated with charge-density-wave instabilities, and correlated tungsten displacements giving rise to antiferroelectric ordering between neighboring WO_3 chains. Several of these mechanisms may coexist and compete, producing complex modulated states. Moreover, the sharpness of the electronic transitions appears closely related to the degree of structural coherence observed by diffraction, ranging from well-defined satellite reflections to short-range correlations characterized by diffuse scattering.

Tungsten phosphate bronzes thus provide a unique model system in which a single structural parameter — the thickness of the WO_3 slabs — governs not only electronic dimensionality, but also the nature of the collective instabilities and even the thermodynamic character of the resulting phase transitions. The recent discovery of ordered fractional members provides a finer tuning of this structural parameter, opening new possibilities for exploring how structural dimensionality controls the crossover between competing electronic states.

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Magnetic frustration and complex orders

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Abstract

Magnetism is a field that has contributed significantly to the discovery of complex orders in matter. These exotic orders are particularly favored by magnetic frustration, that is, by a system's inability to simultaneously satisfy all of its ipair-wise interactions. This phenomenon may be linked to the topology of the crystal lattice and is the source of new exotic states of matter, whose description goes beyond classical models. “Spin ice” and its quantum analogue are a prime example of this physics [1]. The crystallographic structure of these materials is based on a pyrochlore lattice, formed by a set of tetrahedra connected at their vertices, with each node occupied by a magnetic rare-earth ion (Tb, Dy, Ho, Pr, Nd ...). In other cases, magnetic frustration arises from the competition between several conflicting interactions. This often results in helical or cycloidal orders, which are frequently associated with unique physical properties, such as multiferroicity. In both cases, diffraction provides valuable insights, but the study of dynamics also allows for the testing of theoretical models by seeking to identify exotic excitations. Using examples taken from the literature, we will present a non-exhaustive overview of these systems, highlighting in particular the contribution of neutron scattering.

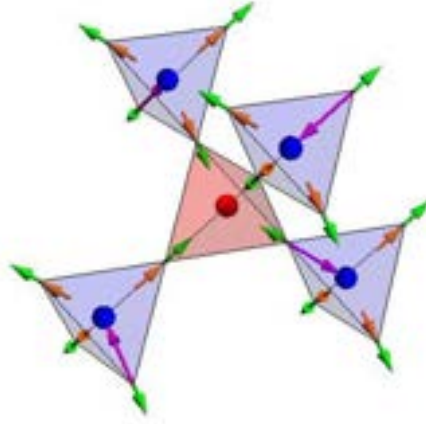


Figure 1: Fragmented state in spin ice

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Keywords — magnetic frustration, neutron scattering

Shape Memory alloys for multicaloric properties

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Abstract

Shape Memory Alloys (SMA) are multifunctional materials where a non-diffusive, reversible phase solid-solid transition (austenite $\leftrightarrow$ martensite) is driven by shear displacement and can also be induced by mechanical stress, temperature, or magnetic fields. These multiferroic materials, exhibiting coupled magnetic and structural orders, are particularly promising for applications such as sensors, actuators, heat-pumps (...), thanks to their significant entropy changes during the transition. However, fatigue behavior, essential for devices used in real-world conditions, remains a challenge due to lattice mismatch and defect accumulation. Our aim is to optimise the compatibility between martensite and austenite, in order to extend fatigue life.

In this work, we focus on NiMnIn-based ferromagnetic/ferroelastic SMAs. Firstly, we will briefly present the properties of the martensite-austenite phase transition studied using electrical, magnetic, mechanical and optical measurements (sometimes coupled), which allow us to indirectly deduce the thermodynamic properties of the transition, as well as the strong influence of composition and microstructure. Secondly, in order to better understand the relationship between macroscopic properties and the structural complexity of the material, we will present the results of our investigations with high quality single crystals in contrast to literature using thin films and polycrystalline materials. Neutron diffractions and crystallographic analysis were carried out : the monoclinic structure is described as $I2/m(\alpha\gamma)00$ with a modulation vector derived using the superspace formalism, in agreement with the literature [1]. However, our results reveal a discrepancy in the modulation vector between the single crystals ($q_M \approx \pm 0.11 \text{ \AA}^{-1}$) and the powders ground from the same single crystals ($q_M \approx \pm 0.33 \text{ \AA}^{-1}$), which suggests that the apparent incommensurability observed in the powders may arise from defect density rather than true incommensurable modulation.

An alternative structural description based on a phase exhibiting arrangement of stacking faults has been explored to provide a more physical interpretation of the diffraction patterns, in which the variation of the modulation vector could result from averaging over domains in polycrystalline samples. This description could indicate that the conventional superspace model may not fully account for the complexity of the microstructure and, in particular, the role of stacking faults in accommodating complex strain fields (e.g., epitaxy or ground powders). This suggests that the average structure observed in powder diffraction masks a more complex defect-driven reality.

We are extending our methodology to more ductile copper-based SMAs (CuZnAl), from the production of single crystals to property measurements and defect-driven crystallographic analyses.

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Keywords — *shape memory alloys, adaptive martensite, modulated martensite crystal*

From genesis to application: In situ and in operando structural studies on rare-earth doped ceria phases.

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Abstract

Functional materials based on pure and rare earth (RE³⁺)-doped ceria find application in a variety of fields, from catalysis to energy, thanks to their easy oxygen exchange and storage capacity and fast ionic charge transport.

These properties largely arise from their complex defect architecture, which depends on the composition and evolves with particle size and varying the external conditions.

For instance, in microcrystalline phases oxygen vacancies and dopant ions form defect rich droplets which increase in size on progressive RE³⁺ doping, inducing strong structural relaxations around oxygen vacancies and their trapping. This mechanism seems to be somewhat frustrated in nanoparticles and varies as a function of T and pO_2 making in situ and in operando characterizations essential for a meaningful comprehension of the compounds properties.

This contribution presents an in situ structural characterization of pure and rare-earth-doped ceria, ranging from the synthesis of nanoparticles using a wet method to their growth to form bulk phases, and their structural evolution under severe operating conditions. Synchrotron radiation powder diffraction and pair distribution function analysis will be the chosen method for this purpose.

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Keywords— Defects architecture, In situ X-ray diffraction, Pair Distribution Function Analysis.

Imperfections as a measure of exotic superconductivity?

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Abstract

The extreme fascination with uranium-based superconductors has once again come to light as a result of the many peculiar facets of UTe_2 [1]. In an effort to unify the chemical and physical understanding of this peculiar material, our previous work highlighted the minute crystallographic imperfections that drive differences in the superconducting state – from complete suppression to the emergence of one or even two superconducting transitions – whose origin lies in two types of defects [2]. The more important role is played by uranium deficiencies, which can completely suppress superconductivity of UTe_2 with an abundance of only 4%. A subtler imperfection arises due to local variations of translation symmetry, which amount to only 0.01%, splitting one superconducting transition into two [2].

In a related unconventional superconductor UBe_{13} , the sensitivity to imperfections is even higher [3]. This cage-like structure hosts uranium atoms in the center of each cage, surrounded by 24 beryllium atoms. In our recent study, we find that removal of just a few beryllium atoms in one unit cell drastically changes the critical temperature by nearly 30% [3]. The volume of the lattice stays the same, which signals that this change is miniscule, even when comparing to systems with strong structure-property relationships. We also consider what happens in another uranium-based unconventional superconductor UPt_3 – both in bulk and on the micro-scale [4]. Overall, the extreme sensitivity to imperfections in uranium-based systems likely originates in the flexibility of the uranium oxidation state, which is easily affected by the small changes to the crystallographic environment of uranium. Currently, only a few uranium-based superconductors are known, with nearly half of them exhibiting various degrees of crystallographic defects [5]. This talk, I will compare the effects of various chemical features to the resultant superconductivity and related phenomena.

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Keywords - superconductivity, cage structures, crystallographic defects

Superconductivity in Ta–Te-based van der Waals layered quasicrystal

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Abstract

A van der Waals (vdW) layered dodecagonal quasicrystal (dd-QC) in the Ta–Te system has recently been found to exhibit superconductivity with $T_c \sim 1$ K [1]. Owing to the predicted unconventional features of superconductivity in quasiperiodic systems, this material provides a promising platform to explore novel superconducting states. Here, we report the synthesis and superconducting properties of Ta–Te-based vdW layered dd-QCs, including ternary systems.

Polycrystalline samples were synthesized by reaction sintering, and powder X-ray diffraction confirms the formation of nearly single-phase dd-QCs. By introducing various third elements, ternary Ta–X–Te samples were obtained [2].

Some Ta–X–Te ternary systems exhibit improved crystallinity compared to the Ta–Te binary system. The temperature dependence of electrical resistance in single-phase quasicrystalline samples shows superconducting transitions at ~ 1 K for all samples, with the highest T_c reaching 1.35 K.

Specific heat measurements for the Ta–Cu–Te system show a clear jump at T_c , and the electronic contribution is well described by a full-gap model [3].

In NMR measurements, the nuclear spin–lattice relaxation rate $1/T_1T$ shows a clear coherence peak just below T_c and an exponential decrease at lower temperatures, supporting fully gapped superconductivity [4]. However, the coherence peak is much smaller than that in conventional superconductors, consistent with the theoretical predictions that the Bogoliubov peak in the quasiparticle density of states is smeared out by quasiperiodicity [5]. In addition, the decrease in the Knight shift is anomalously small compared to that in conventional superconductors, which may result from spin–orbit scattering.

For single-grain samples of the Ta–Nb–Te system, angular-dependent measurements of the upper critical field H_{c2} reveal surface superconductivity on the c -plane. The in-plane H_{c2} exceeds the Pauli limit, and for both in-plane and out-of-plane fields, the temperature dependence of H_{c2} shows an unusual increase down to 0.1 K, significantly exceeding the prediction of the conventional WHH theory in the dirty limit. These results suggest an important role of spin–orbit coupling in this system.

Furthermore, recent STM/STS measurements have achieved atomic-resolution imaging over areas of several hundred nanometers squared, revealing a spatially uniform superconducting gap. This result is consistent with theoretical studies [5] predicting that, although the superconducting order parameter is spatially inhomogeneous, the gap in the local density of states remains uniform.

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Keywords— van der Waals layered quasicrystal, superconductivity

ICCOCM 2026

Contributed presentations abstracts

Collective magnetic state induced by charge disorder in the non-Kramers rare-earth pyrochlore $\text{Tb}_2\text{ScNbO}_7$

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Abstract

The pyrochlore lattice featuring corner-sharing tetrahedra has long been a rich playground for geometrical frustration. A prominent example is the spin-ice state [1], where on each tetrahedron two spins point inward and two outward. This highly degenerate phase is a prototypical realization of a classical spin liquid phase, characterized by strong short-range correlations and the absence of long-range magnetic order. Disorder is a subtle ingredient that can modify the nature of such exotic non-ordered phases, as frustrated magnets are often highly sensitive to small perturbations. In spin-ice systems based on non-Kramers rare-earth ions, it breaks the local symmetry and splits the non-Kramers ground-state doublet. Theoretical works have predicted that this may induce quantum entanglement and stabilize either a quantum spin liquid or a spin-glass state, depending on the magnitude and distribution of the splitting relative to the magnetic interactions [2].

In this presentation, I will focus on the new pyrochlore oxide $\text{Tb}_2\text{ScNbO}_7$ and discuss the interplay between magnetic frustration on the Tb^{3+} pyrochlore sublattice and $\text{Nb}^{5+}/\text{Sc}^{3+}$ charge disorder on the non-magnetic site. Using a combination of electron, X-ray, and neutron diffraction, we first quantified the structural disorder and estimated the distribution of the splitting of the Tb^{3+} non-Kramers ground-state doublets, which we compared with magnetic excitations measured by inelastic neutron scattering. Combining macroscopic and neutron scattering measurements, we then showed that a partial spin glass transition occurs around 1 K while strong spin liquid correlations persist. These results suggest that $\text{Tb}_2\text{ScNbO}_7$ realizes one of the disorder-induced frozen quantum spin-liquid phases recently proposed theoretically [3].

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Keywords— Geometrical frustration, Charge disorder, Spin glass, Spin liquid, Synchrotron-based X-ray diffraction, Neutron scattering

Pseudogap properties of quasicrystal-related materials in the quaternary Al-Pd-TM-Fe (TM=Cr, Mo, W) systems

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Abstract

Al-based icosahedral quasicrystals (i-QCs) are known to exhibit low thermal conductivity (1-2 W/mK) due to their structural complexity, along with a relatively high Seebeck coefficient ($\sim 100 \mu\text{V/K}$), attributed to a pronounced pseudogap near the Fermi energy [1]. These characteristics render Al-based i-QCs promising candidates for future thermoelectric (TE) materials. However, the nature of the pseudogap in i-QCs remains largely elusive, as the absence of translational symmetry hinders precise theoretical analysis of their electronic structures.

Higher-order periodic approximants (PAs), which exhibit pseudogap properties similar to those of i-QCs due to structural similarity [2], serve as valuable platforms for understanding the nature of the pseudogap. In the Al-Pd-TM-Fe alloys (TM = Cr, Mo, W), i-QCs and two variants of 3/2 PAs (cubic; $Pa\bar{3}$, $a \sim 40 \text{ \AA}$, trigonal; $P\bar{3}$, $a \sim 29 \text{ \AA}$, $c \sim 35 \text{ \AA}$) are stably formed within a narrow compositional range [3-5]. In this study, we aim to experimentally clarify the effects of these icosahedral structural order and the constituent elements (TM = Cr, Mo, W) on the pseudogap properties.

TE measurements reveal that all samples exhibit low electrical ($\sigma_{RT} = 200\text{-}800 \text{ S/cm}$) and thermal ($\kappa_{RT} = 1\text{-}2 \text{ W/(m}\cdot\text{K)}$) conductivities, along with non-metallic transport behavior. The electronic specific heat coefficients estimated from the low-temperature specific heat measurements are significantly lower compared to those of conventional metals ($\gamma = 0.2\text{-}0.7 \text{ mJ/(mol}\cdot\text{K)}$). These features are attributed to the presence of a pronounced pseudogap near the Fermi energy.

Fig. 1 shows the temperature dependence of the Seebeck coefficient. Notably, the maximum values significantly differ depending on the crystal structures, following the order i-QC > cubic 3/2 PA > trigonal 3/2 PA, regardless of TM species. Such a systematic variation cannot be explained solely by differences in γ . Assuming that Mott's formula can be applied to these materials, this trend suggests that the slope of pseudogap at the Fermi energy differs depending on the structural order.

To directly probe the pseudogap structures, we recently performed hard X-ray photoelectron spectroscopy (HAXPES) measurements at SPring-8, Japan, on i-QCs and two variants of 3/2 PAs. In the presentation, we will discuss the effects of the icosahedral structural order and the constituent elements (TM = Cr, Mo, W) on the pseudogap properties, incorporating the recent HAXPES results.

Acknowledgements:

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Keywords— Quasicrystal, 3/2 Periodic Approximant, Thermoelectric Material, Pseudogap

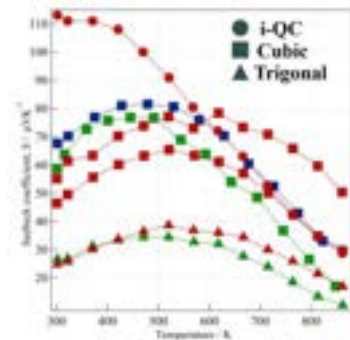


Fig. 1 Temperature dependence of the Seebeck coefficient in quasicrystal-related materials in the Al-Pd-TM-Fe system. TM = Cr, Mo, and W are indicated by blue, green, and red, respectively.

Polar instability at high-pressure in KNbO_3

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Abstract

Ferroelectric instabilities in perovskites are known to be suppressed by a moderate hydrostatic pressure. The prediction of their re-entrance in a much higher-pressure regime is well-accepted theoretically [1] but a conclusive experimental confirmation is still elusive. Here, we investigate another ferroelectric perovskite KNbO_3 [2]. It reaches a paraelectric cubic phase by ~ 12 GPa, but experimental investigations beyond that regime are scarce. We use single crystal X-ray diffraction, infrared and Raman spectroscopy and second-harmonic generation to explore the phases transitions up to 63 GPa. We show that a first transition occurs at 37 GPa from cubic to a non-polar $I4/mcm$ phase with a classical $a^0a^0c^-$ octahedra tilt patterns. This happens in many perovskites (including PbTiO_3) as a result of the enhancement of the tilting instability under pressure. Much more remarkably, at 43 GPa, a second transition occurs to a monoclinic phase with an incommensurate modulation that combines polar cation displacements with additional in-phase tilting and slight distortions of the octahedra (see Fig. 1). The absence of SHG signal shows that this phase remains macroscopically non-polar. Yet we understand this phase as the result of a tight competition between the zone-boundary tilting instability and the zone-center polar instability, which in turns shows that the latter is also enhanced by hydrostatic pressure. Raman spectra display very clearly the presence of multiple soft modes associated to the tilts and to the modulation. Interestingly, they also display persistent order-disorder signatures suggesting that local disorder plays an important role in mediating the competition between tilts and polar cation displacements. Finally, infrared spectroscopy allows us to identify the activation of the mode consisting of Nb anti-polar displacements, which is found here to have unusual strength.

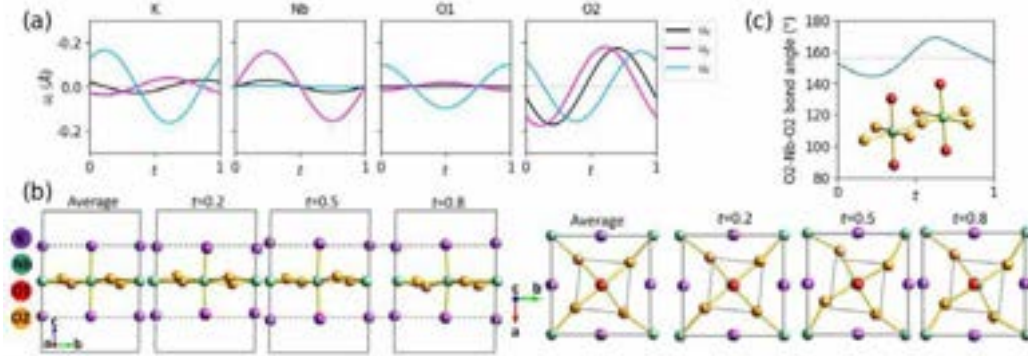


Figure 1: Atomistic depiction of the modulation at 58 GPa (a) t-plots (b) Projections of the crystal structure of KNbO_3 onto the bc and ab planes at selected t values. (c) Nb-O-Nb bond angle as a function of t. The dashed horizontal line represents the bond angle for the average structure.

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Keywords— Perovskite, polar displacements, single crystal X-ray diffraction, Raman, IR, SHG

Quasicrystals in ZnMg(Dy, Er, Ho, Tm)Li system

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Abstract

Long-range magnetic order, both ferromagnetic and antiferromagnetic, was discovered in Tsai-type icosahedral quasicrystals [1]. Inspired by this research, we started searching for magnetic order in remaining classes of icosahedral quasicrystals, particularly Zn-Mg-RE (RE - Rare-Earth) Bergman-type family. The magnetic long-range order in Tsai quasicrystals could be discovered by searching for the quasicrystal with a particular e/a ratio, controlling the strength of the exchange energy in RKKY interaction. Since all Zn-Mg-RE quasicrystals are spin-glass phases, we incorporated this idea and made a substitution of Mg(II) to Li(I) what should result in decreasing number of valence electrons.

Samples of ZnMg(Dy, Er, Ho, Tm)Li were prepared with self-flux method by replacing 5 at.% of Mg in the original melt with Li [3]. That resulted in the formation of the faceted quasicrystals exhibiting icosahedral morphology (Fig. 1). By means of the single-crystal X-ray diffraction, we could determine that the substitution site is the RE atom located in the center of local Tsai cluster that can be found alongside Bergman clusters. Therefore, the addition of Li does not only replace the magnetism-bearing atom, but also decreases the number of valence electrons as $RE^{3+} \rightarrow Li^{1+}$. Magnetic properties are now under study.

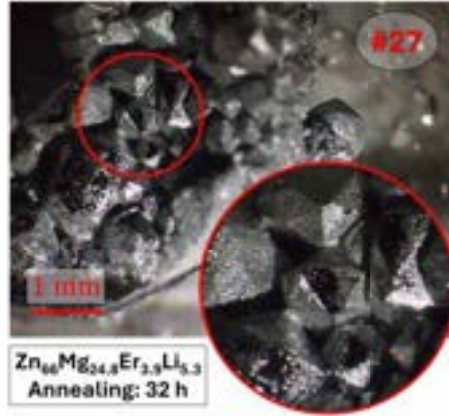


Figure 1: The ZnMgErLi #27 sample photo showing icosahedral grains.

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Keywords— Quasicrystals, Bergman phase, Crystal Growth

Hierarchical structure of disordered metal-organic frameworks and growth-directed symmetry breaking

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Abstract

Complex structures which emerge in nature from short-range interactions can often be described with a hierarchy of length-scales, a notable example is protein structure [1]. We examine the hierarchical structure found in some metal-organic framework (MOF) crystals using polarised light microscopy and spatially resolved diffuse scattering measurements. We consider in particular the CU27 series, which are important photocatalytic materials due to the combination of their inherent porosity and the optical properties of the organic linker [2, 3].

By analogy with the hierarchical structure of proteins, this MOF can be understood to have primary, secondary, tertiary, and sometimes even quaternary structures. The primary structure (~ 0.5 nm) of CU27 MOFs is the organic and inorganic building units from which they are built [Fig. 1(a)]. The secondary structure (~ 2 nm) is the local arrangement which is driven by short-range interactions [Fig. 1(b)]. On zooming out further one finds the nanodomains (10 – 40 nm). In some members of the CU27 series, we find that these nano-domains are elongated along the growth direction, in a way which breaks the hexagonal symmetry of the primary and secondary structure [Fig. 1(c-d)]. Since the symmetry breaking is along the growth direction, it leads to a quaternary structure of the same size of the crystal (20 – 200 μ m) [Fig. 1(e)]. The symmetry breaking leads to birefringence which is different in each of the domains, allowing for visible light imaging of the domain structure [Fig. 1(f)]. We will discuss the implications of this complex structure for the functionality of such MOFs.

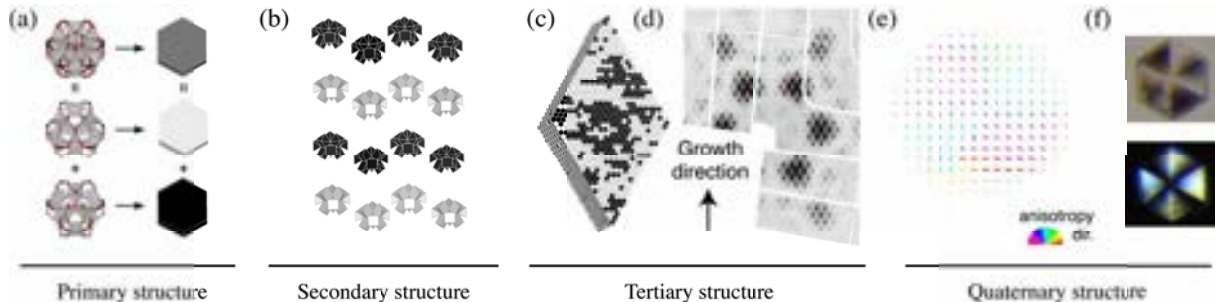


Figure 1: (a) The disordered cluster of a CU27 MOF (top left) can be understood as a combination of two orientations, which are represented with white and black tiles. (b) A simplified representation of the local CU27-Er structure, derived from refinement of the total scattering. (c) Snapshot of a model for the nanodomains of CU27, showing anisotropy along the growth direction. (d) Diffuse scattering measurement from a single domain of CU27, showing broken hexagonal symmetry. (e) Map of the diffuse scattering anisotropy across a whole crystal.

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Keywords— Disorder, Metal organic framework, Diffuse scattering

Insights into modulated nuclear and magnetic structures in metal-organic coordination polymers

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Abstract

Reports of molecular frameworks that exhibit modulated phases are still limited. This is particularly remarkable since weak interactions commonly observed in coordination polymers are equivalent to the forces that usually generate aperiodic systems. This would suggest that many of the published compounds might have unreported modulated phases. However, the study of these systems is of potential interest because the intrinsic properties of the material, such as phonon, electric, magnetic, photonic or molecular transport properties, are likely to be different from those of periodic materials. This is important in the sense that in many cases a more comprehensive review of the literature is necessary to identify novel structure–property relationships.

The methylammonium metal formates, $[\text{CH}_3\text{NH}_3]\text{M}(\text{HCOO})_3$, where $\text{M} = \text{Fe}, \text{Co}$ and Ni , are more unusual, as all undergo phase transitions from unmodulated to modulated structures on cooling.[1-4] These compounds exhibit a finely balanced system driven by subtle interplay of weak interactions within the hydrogen-bond network. The formate anion serves as a hydrogen bond acceptor, while the methylammonium counterion, located within the cavities, acts as a potent hydrogen bond donor. These competing interactions result in crystal structures with nearly equivalent energies. Consequently, subtle alterations in the hydrogen bonding network can induce structural phase transitions, giving rise to modulated phases that are closely related with variations in the electric properties of the compounds. In the case of the Fe and Ni, these modulated phases remains even below the magnetic ordering temperature, providing a unique opportunity to study magneto-structural coupling, giving rise to improper or proper magnetic modulated structures.

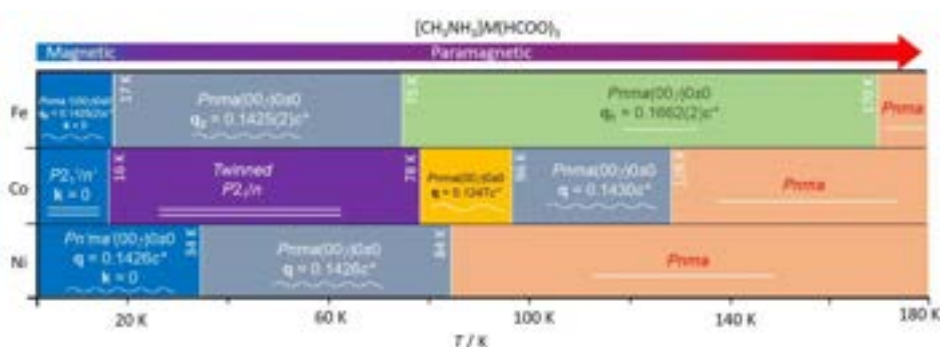


Figure 1: Temperature-induced phase transitions of the $[\text{CH}_3\text{NH}_3]\text{M}(\text{HCOO})_3$ compounds.

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Keywords— modulated structures, neutron diffraction, phase transitions.

Quantum magnetism of icosahedral Yb quasicrystals and approximants

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Abstract

Strongly correlated electron systems have attracted a great deal of interest in the study of unconventional superconductivity and non-Fermi liquid states, related to magnetic quantum criticality. Until very recently, quantum criticality has been intensively studied in only crystalline materials. The Au-Al-Yb quasicrystal with Tsai-type cluster exhibits novel quantum critical phenomena [1]. Quasicrystals possess long-range, quasi-periodic structures with diffraction symmetries forbidden in crystals. The valence of the Yb ion in the Yb icosahedral quasicrystals and approximants is intermediate between Yb^{2+} and Yb^{3+} [2], suggesting that valence fluctuations (spin and charge transfer fluctuations) are closely related to the quantum critical state of the Au-Al-Yb quasicrystal [3]. By investigating the (Au,Cu)-Ga-Yb icosahedral quasicrystals and approximants through the substitution of Yb ligands, we have found that the Yb icosahedral quasicrystals and approximants are actually located near the border of the valence change. In this study, we will discuss the variation of magnetism and mean Yb-valence by the chemical pressure effect and itinerant-electron concentration (e/a) control in the Yb icosahedral quasicrystals and approximants, supporting that the valence fluctuations play a crucial role in the unconventional quantum magnetism. We will also discuss magnetism and non-Fermi liquid behavior in the Yb icosahedral quasicrystals and approximants.

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Keywords— Quasicrystal, Quantum Magnetism

Reimagining Interface Processing in Solid-State Batteries via Electrochemical Flash Sintering: Spatial Insights and Millisecond Structural Dynamics from Total Scattering

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Flash sintering has emerged as a powerful route for the rapid densification of ceramics, but its application to solid electrolytes remains challenging because purely ionic conductors are limited by blocking electrodes, strong thermal gradients, and interfacial degradation. In this work, we investigate electrochemical flash sintering (EFS) as a route to fabricate self-supported, monolithic all-solid-state battery (ASSB)-type architectures composed of $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ – $\text{Li}_{1.4}\text{Al}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$ (LVP–LATP) composite electrodes and an LATP electrolyte layer. By operating under alternating-current conditions, densification is achieved in both composite and electrolyte layers while maintaining coherent electrode–electrolyte interfaces without preferential cracking or secondary-phase enrichment at the boundaries.

To understand the structural mechanisms governing this ultrafast process, we combine spatially resolved total scattering with automated large-scale diffraction analysis. Bragg diffraction and pair distribution function (PDF) analysis reveal pronounced heterogeneities generated by current localization and Joule heating, including hotspot formation, localized decomposition, amorphization, and phase redistribution. Analysis of large diffraction datasets using non-negative matrix factorization (NMF) enables efficient identification of minor and spatially localized impurity phases, providing a statistical view of phase evolution across the pellet.

To probe transient reaction pathways, in-situ total scattering experiments were performed in an adapted cell^[2] at the XPDF/i15-1 beamline of the Diamond Light Source using the newly commissioned ARC detector^[3], achieving ~50 ms time resolution. This enables direct observation of structural dynamics during the 2s-long flash event, including the rapid formation of metastable and amorphous intermediates, their crystallization within seconds, and the coupled evolution of local and average structure during the pulse. By correlating these transformations with processing variables such as frequency, current density, and hold time, we identify the parameters controlling densification, hotspot formation, and decomposition pathways.^[4]

These results demonstrate how advanced scattering methods can resolve both spatial and temporal complexity in non-equilibrium field-assisted processing. More broadly, they provide design rules for the rapid fabrication of dense solid electrolytes, robust interfaces, and next-generation solid-state battery architectures

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Hydroxyperovskites – Correlated Proton Disorder and Spin Dynamics

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Abstract

Perovskites ABX_3 and structurally related compounds are undoubtedly among the most thoroughly investigated classes of materials due to their chemical and structural flexibility and the respective tunability of their properties. Complex oxidic perovskites have been in the focus as potential high- T_c superconductors, as spintronic materials, catalysts, or possible energy conversion materials, see e.g. [1, 2]. Single $B(OH)_3$ or double hydroxyperovskites $BB'(OH)_6$ have received much less attention. These compounds can be described as A -site vacant perovskites in which the hydrogen atoms are located in the larger voids of the perovskite network. The majority of the naturally occurring minerals of this family are cation ordered double hydroxyperovskites like burtite, $CaSn(OH)_6$, mushistonite, $CuSn(OH)_6$, wickmanite $MnSn(OH)_6$, or stottite $FeGe(OH)_6$ [3]; their structures can be described as superstructures of dzhalindite, $In(OH)_3$, which crystallizes in space group $Im\bar{3}$. For most of these compounds, the precise crystal structure, especially with respect to the hydrogen position, is not known to date.

Like in water ice, the hydrogen atoms in the hydroxide perovskites show correlated structural disorder. Depending on the tilt system of the octahedra, the compounds can host a hydrogen bond network that is either local and ring-like, i.e., solely oriented around the vacant A site of the perovskite, or extended in a zig-zag or crankshaft-like chain. Structures with extended H-bond networks raise the question of whether these materials qualify as low-temperature proton conductors. Recent neutron scattering data on $CuSn(OD)_6$ with localized and $MnSn(OD)_6$ with crankshaft-like hydrogen bonding network, suggest that no fully ordered structure is adopted even at temperatures below 1 K [4, 5]. At the same time, no long-range magnetic order was observed for these compounds in magnetization and neutron scattering data even in the sub-Kelvin regime. Instead, muon spin resonance experiments evidence short-range spin fluctuations which might indicate the existence of a spin liquid ground state. Hydrostatic pressure induces a structural transition due to rearrangement of the proton sites in $CuSn(OD)_6$.

In this contribution we present results addressing the proton disorder and spin dynamics on synthetic $B\text{Sn}(OH)_6$ and $B\text{Sn}(OD)_6$ hydroxyperovskites with $B = 3d$ transition metals, including chemical analysis, spectroscopy, X-ray and neutron diffraction, magnetization, specific heat, and muon spectroscopy experiments. Moreover, first results on new compounds with $5d$ transition metals are discussed.

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Keywords: hydroxyperovskites; hydrogen bonds, correlated disorder, magnetism

The Beauty of Complexity and the Simplicity of Compressed Solid Matter Revealed by High-Pressure Crystallography

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Abstract

Materials under extreme compression exhibit a striking duality: increasing structural complexity can give rise to unexpected simplicity in their underlying chemical and physical principles. In contrast to behavior observed at ambient conditions, confined environments fundamentally reshape bonding, reactivity, and phase stability.

In this talk, we explore high-pressure and high-temperature crystallography as a powerful in situ approach to uncover this interplay between complexity and simplicity in solid matter. Our experimental investigations span a wide range of compound classes, including oxides, borides, carbides, nitrides, halides, and hydrides. These studies reveal how extreme pressure–temperature conditions reorganize matter, leading to emergent structural motifs and simplified governing principles that challenge conventional chemical intuition.

A central highlight is the synthesis of compounds featuring homoatomic anions, representing a significant step forward in the design of novel materials under extreme conditions. These findings illustrate how compression can stabilize unexpected bonding arrangements while reducing apparent chemical complexity.

We will also discuss the methodological and technical advances enabling these discoveries, including state-of-the-art devices and software for X-ray diffraction data acquisition and analysis. The broader implications of high-pressure crystallography extend across physics, chemistry, materials science, and the Earth and planetary sciences. Ultimately, this work demonstrates how extreme conditions reveal both the richness and the underlying simplicity of solid-state behavior, offering new perspectives on the fundamental nature of matter.

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Keywords— high-pressure crystallography, synthesis, in situ analysis

Axial rattling and soft phonon modes in a novel Al-Pd-W compound with WAl_{12} icosahedra

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Abstract

We report the discovery of axial rattling in a novel hexagonal $Al_{68}Pd_{14}W_{10}$ compound (space group $P6_3/m$). The crystal structure of this compound was recently solved using single-crystal X-ray diffraction [1,2], revealing a rigid network of WAl_{12} icosahedra forming one-dimensional (1D) channels along the c -axis. Within these channels, Pd and Al atoms are arranged in an alternating array along the central axis. Moreover, these atoms exhibit thermal ellipsoids significantly elongated along the c -axis, suggesting structural flexibility and the presence of anharmonic low-energy excitations characteristic of axial rattling.

Low-temperature specific heat measurements were performed on this compound and revealed an excess specific heat component below 6 K that deviates from the Debye model (indicated by the arrow in Fig. 1, left). To investigate the potential origin of this anomaly, we performed first-principles calculations using the Vienna Ab initio Simulation Package (VASP, ver.5.4) [3].

We first performed structural relaxation calculations with the space group fixed to $P6_3/m$, confirming that the ground state of this compound is non-magnetic. Based on this result, we subsequently carried out phonon spectrum calculations within density functional perturbation theory (DFPT), revealing flat soft modes in the a^*b^* plane, as indicated by the arrow in Fig.1 (right). These modes are associated with axial rattling of atomic columns within 1D channels. The axial displacement of these atoms induces a symmetry-broken structure with space group $P6_3$, which is stabilized by an energy gain of approximately 7.6 meV/u.c. Accordingly, the soft phonon modes associated with the 1D atomic columns are most likely responsible for the low-temperature specific-heat anomaly observed in the hexagonal $Al_{68}Pd_{14}W_{10}$.

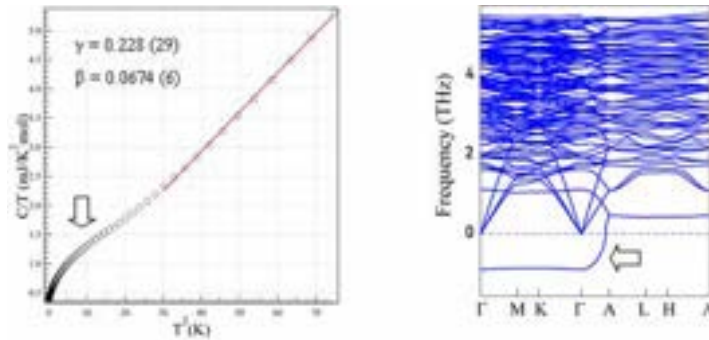


Figure 1: (left) Low-temperature specific heat of the hexagonal Al-Pd-W compound plotted as C/T versus T^2 . The arrow indicates an excess specific heat at below 6K. (right) Calculated phonon band structure of the high-symmetry phase. The arrow points to the flat soft-mode branch along the a^*b^* plane, associated with the axial rattling of the Al-Pd columns.

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Keywords— icosahedron, axial rattling, soft phonon mode

Chemical and structural complexities caused by elemental interaction in structural metallic materials

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Abstract

Interstitial alloying elements (i), such as carbon (C) or nitrogen (N), effectively strengthen steels by addition of small amounts via nanoscale clustering/precipitation. When a substitutional alloying elements (s) having strong carbide/nitride forming tendency, atomic i-s clustering occurs as a precursor of stable carbide/nitride precipitation. Such phenomena are resulted from interplay of ordering and phase separation (spinodal decomposition) and seen more obviously in ferritic and martensitic alloyed steels because solubility of C or N is quite low in bcc solid solution. However, even in fcc austenitic steel with large solubility of C or N, i-s clustering is expected to occur under strong attractive i-s interaction.

In this presentation, nanoscale clustering/precipitation and resulting hardening behaviors are discussed based on “sublattice alloy design” concept in ferritic [1] and austenitic steels [2,3] with nitriding.

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Keywords— Steel, ordering, phase separation, precipitation strengthening

From Chaos to Order: Programming Nanocrystal Superlattices for Tailored Optical Function

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Abstract

The self-assembly of nanocrystals (NCs) into ordered hierarchical structures offers a powerful route to tailor emergent collective properties yet remains fundamentally challenging due to the complexity of nanoscale interactions governing organization, stability, and function. Here, we discuss how surface chemistry, ligand-mediated interactions, and compositional control can be exploited to direct the formation of ordered supramolecular architectures and tune their optical response.

We demonstrate how the fabrication of ordered superlattices can be achieved through a bottom-up approach by engineering a soft organic corona around cerium oxide (CeO₂) NCs. In particular, the use of amines with different alkyl chain lengths (C8–C18) enables systematic tuning of interparticle forces, driving a transition from disordered aggregates to hierarchically ordered superlattice structures. Structural and energetic considerations highlight the central role of ligand-mediated interactions in governing assembly pathways and final organization, as well as their impact on the resulting optical properties.^{1,2} Building on these principles, we extend the same design strategy to metal NCs (Au, Ag, Pt), where ligand density and solvent–ligand interactions are shown to play a critical role in directing supramolecular organization. Using a microemulsion-based functionalization approach with oleic acid and oleylamine ligands, we demonstrate that increasing surface coverage promotes the formation of more ordered nanocrystal assemblies, while the external environment strongly modulates aggregation behavior and the associated optical response.³

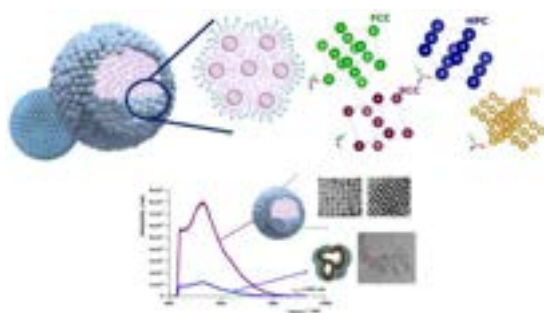


Figure 1: Schematic representation of ordered hierarchical structures and comparison of optical properties between ordered and disordered aggregates.

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Keywords— superlattice, optical enhancement, hierarchical organization

Complex orders in molecular crystals probed by 3D- Δ PDF and superspace crystallography

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Abstract

Molecular crystals host complex orders reminiscent of those observed in strongly correlated inorganic systems. We show how two crystallographic methodologies, three-dimensional difference pair distribution function (3D- Δ PDF) and superspace crystallography, give quantitative access to such orders in two molecular materials.

The bromide-bridged Pd chain compound $[\text{Pd}(\text{cptn})_2\text{Br}]\text{Br}_2$ (cptn = 1R,2R-diaminocyclopentane) develops a two-dimensional charge density wave (CDW) below room temperature, which conventional Bragg refinement cannot describe. Synchrotron diffuse scattering refined by 3D- Δ PDF resolves the $\text{Pd}^{\text{II}}/\text{Pd}^{\text{IV}}$ valence alternation and identifies the $\text{Br}\cdots\text{NH}_2$ hydrogen-bonding network as the interaction stabilizing the 2D CDW, while weak inter-plane coupling prevents three-dimensional locking [1].

The molecular Mott insulator $\text{Et}_2\text{Me}_2\text{Sb}[\text{Pd}(\text{dmit})_2]_2$ hosts a quasi-equilateral triangular lattice of $[\text{Pd}(\text{dmit})_2]_2$ dimers. High-resolution diffraction reveals an intermediate incommensurate phase between the frustrated room-temperature phase and the low-temperature charge-separated phase. Superspace refinement shows that the modulation leaves the intradimer Pd–Pd distance unchanged but couples interdimer transfer integrals to an arch distortion of the dimer through steric interaction, revealing a competition between geometric, electronic and spin frustration [2].

Both examples extend the toolbox of aperiodic and disorder-resolved crystallography from inorganic systems to molecular materials, where the same concepts of competing modulations, correlated disorder and frustration emerge from intermolecular interactions and electron–lattice coupling within molecular dimers.



Figure 1: how to make complex orders in molecular materials

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Keywords— 3D- Δ PDF, superspace crystallography, charge density wave, geometric frustration, molecular conductors

Correlated disorder in a Garnet-type superionic conductor

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Abstract

The solid superionic conductors $\text{Li}_{7-x}\text{La}_3\text{M}_{2-x}\text{M}'_x\text{O}_{12}$ ($\text{M} = \text{Ta}, \text{Nb}$; $x > 0.25$) has recently attracted attention due to its potential usage as solid-electrolyte materials. It presents an Ia-3d space group and a garnet-type framework for the diffusive Li atoms [1], with the number of stable Li-sites still on debate [2]. Previous works, with $\text{M} = \text{Ta}$ and $x = 0.5$, have found that anharmonic lattice vibrations contribute to a correlated motion of ions [3]. Yet, although the role of the electric repulsion between ions has been addressed [4] investigation of the short-range interaction and their influence has not been fully investigated. In this work we studied the single crystal neutron diffuse scattering of the $\text{Li}_{6.5}\text{La}_3\text{Zr}_{1.5}\text{Nb}_{0.5}\text{O}_{12}$ solid solution, obtained on the SXD instrument, at ISIS. Simulations of the static $S(Q)$, obtained using Machine-learned molecular dynamics, are in close agreement with our experimental results (Fig. 1) except for the presence of additional Bragg peaks, due to the use of an ordered supercell. Our experimental results and analysis of the MD trajectories suggest the presence of correlated disorder on the Li-sublattice.

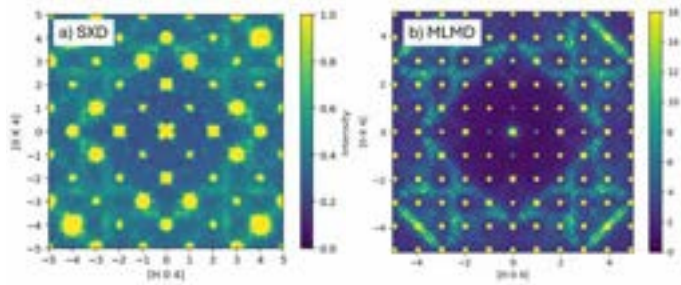


Figure 1: Neutron structure factor $S(Q)$ at 300 K obtained (a) on SXD and (b) using MLMD.

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Keywords— solid ionic conductors, correlated disorder, neutron diffuse scattering

Can a glass-like aperiodic structure coexist with a periodic crystal structure?

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Abstract

Glass-like aperiodic structure and long-range crystalline periodicity are generally regarded as mutually exclusive. Here I demonstrate that such an apparently contradictory state emerges at a structural quantum critical point (sQCP), where a soft-mode-driven second-order structural phase transition is suppressed down to the absolute zero temperature. Using the ferroelectric oxide $\text{Ba}_{1-x}\text{Sr}_x\text{Al}_2\text{O}_4$ as a model system, I show that a glass-like short-range correlation develops in the AlO_4 network, while the periodic arrangement of Ba/Sr ions remains robust.

BaAl_2O_4 undergoes a second-order ferroelectric structural phase transition driven by an acoustic soft mode [1, 2]. This compound comprises a corner-shared AlO_4 network with six-membered cavities occupied by Ba ions. The structural phase transition is suppressed by substituting Sr for Ba, and a sQCP appears approximately at $x = 0.1$ [3]. Inelastic neutron scattering experiments on powder samples reveal that the number of low-energy phonons increases as the system approaches the sQCP [4]. Simultaneously, all phonon peaks become strongly damped, resulting in a vibrational spectrum reminiscent of a boson-peak. Pair distribution function analysis demonstrates that a glass-like AlO_4 network is realized at the sQCP while the periodic arrangement of Ba/Sr ions is preserved [4]. This behavior manifests in glass-like low-temperature physical properties, including excess specific heat, a plateau in thermal conductivity, and a reduced Debye temperature [4, 5]. I will discuss the microscopic mechanism how the glass-like structure is introduced in the periodic atomic arrangement.

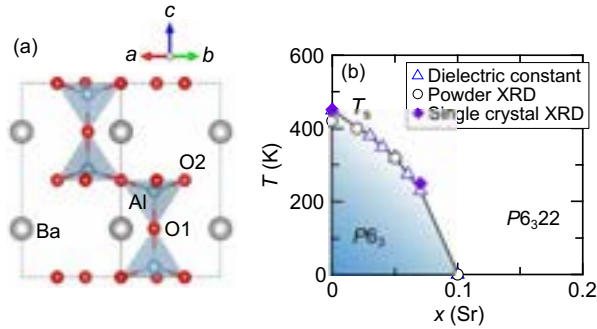


Figure 1: (a) Crystal structure of BaAl_2O_4 (high-temperature phase). (b) Structural phase diagram of $\text{Ba}_{1-x}\text{Sr}_x\text{Al}_2\text{O}_4$.

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Keywords— structural quantum critical point, acoustic soft phonon, glass-like physical properties

Electronic properties of the metallic mean family of one-dimensional quasicrystals

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Abstract

The metallic mean family of one-dimensional quasicrystals includes the well-known Fibonacci chain, which corresponds to the golden mean. The series of metallic mean chains tends towards the periodic crystal in a certain way that can be described simply using the cut-and-project scheme. In higher dimensions too, analogous metallic mean lattices have been proposed, such as in [1]. I will discuss electronic properties of the family of metallic mean chains as a function of k , the metallic mean index. One of the interesting properties studied are the values of topological invariants of the model, which lead to the quantization of certain transport properties, such as the Hall conductivity in a 2D system. In 1D systems, the same invariants can be measured in a topological pump experiment. The combined electronic spectra of the set of metallic mean quasicrystals form a subset of the Hofstadter butterfly [2]. For fixed k , the Hall conductivity has a distinctive non-monotonic behavior as a function of filling (see Fig.1). I will discuss how, as k gets very large, one tends towards the standard Landau level physics as for periodic crystals under a magnetic field. It is commonly accepted that electronic states in quasicrystals are typically multifractal - or critical - states. However, very few such wavefunctions are explicitly known. One such exact solution for such a critical wavefunction is the zero-energy eigenstate of the hopping Hamiltonian in a Fibonacci chain. I will discuss how it generalizes to other members of the metallic mean family.



Figure 1: Hall conductivity σ_H versus energy E for a silver mean 2D system, showing quantized values in the gaps (only the lower half of the spectrum is shown). Note the non-monotonicity of σ_H as band filling (or E) is increased, unlike the behavior of electrons in a periodic lattice under a field. The dotted lines joining plateaux are just guides to the eye.

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Keywords— topological invariants, critical states, quasiperiodic chains

Responsive disorder in framework materials

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Abstract

The field of disordered crystals has evolved from treating defects as random isolated bits to discovering exciting phenomena when correlations between these defects appear. Now we explore pathways for controlling the assembly of these correlated defects. Another frontier we explore is the responsive disorder – the correlated disorder that rearranges between distinct configurations in response to external stimuli including temperature, solvent exchange, and gas loading. Using in situ single-crystal diffuse scattering, we reveal how this disorder reorganizes, uncovering multiple hidden structural transitions undetectable by conventional Bragg diffraction.

In Prussian blue analogues (PBAs), flash-freezing produces a metastable phase characterized by network corrugation driven by water freezing within pores [1]. Dehydration triggers irreversible vacancy reorganization from checkerboard patterns to connected diagonal channels, dramatically altering mass transport [2]. Gas loading (H₂, CO₂, noble gases) reveals framework adaptation with flexibility to guest molecules.

In the flexible MOF DUT-8, controlled solvent exchange drives transitions between distinct disordered configurations [3], each with unique diffuse scattering signatures. Differential diffuse scattering methods (*3D- ΔPDF*) allow separating framework-guest and framework-framework correlations, providing atomic-scale insight into switching mechanisms and intermediate states.

Beyond traditional applications in gas storage and separation, responsive disorder enables information storage—Truchet-tile patterns encode information like atomic-scale QR codes that can be rewritten by transforming the disorder.

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Keywords— Correlated disorder, diffuse scattering, responsive disorder

Self-compensation and Bonding Conversion in Semiconducting Quasicrystalline Approximants, Related Crystals and Amorphous

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Abstract

Understanding how carrier doping affects electronic states is a central issue in semiconductors. In many systems, doping introduces free carriers and leads to metallic conduction. However, in some materials, the introduced carriers are compensated by intrinsic structural or electronic mechanisms, preventing metallization. This phenomenon, known as self-compensation, is particularly prominent in boron-based crystals/amorphous and amorphous semiconductors, but its microscopic origin differs significantly among material classes.

The α - and β -rhombohedral phases of pure boron are considered to be 0/1–2/0 rhombohedral approximants of icosahedral quasicrystals [1]. In β -rhombohedral boron, the ideal crystal structure contains holes in the valence band and is expected to be metallic. In reality, however, interstitial atoms and atomic vacancies are spontaneously introduced so as to balance the electron count, resulting in a semiconducting state. Even when electron doping is attempted using Li or Mg, these defects rearrange to cancel the added carriers, and metallization is suppressed [2]. Similar self-compensation also occurs in the related crystal α -tetragonal phase. In the case of electron doping via carbon substitution in these boron crystals, similar self-compensation is expected; however, due to solubility limits of substitution, the situation remains unclear [3].

In boron carbide, $B_{13}C_2$ is expected to be metallic due to one hole in the valence band. However, in practice, it can be considered that self-compensation occurs because, in some unit cells, the three-atom chain is replaced by a four-atom cluster, which is considered to be adding one interstitial atom, resulting in semiconducting behavior [4].

In contrast, amorphous semiconductors exhibit different mechanisms. In chalcogenide glasses, flexible coordination environments prevent stable carrier introduction. In amorphous Si, a large number of dangling bonds generate localized states within the band gap, which trap doped carriers and inhibit conduction.

Besides self-compensation, bonding conversion induced by transition-metal addition shows also a marked contrast between boron-based systems and amorphous Si. In β -rhombohedral and amorphous boron, a small amount of transition-metal atoms converts covalent bonding into metallic bonding, leading to a semiconductor-to-metal transition at low concentrations [5]. This behavior is closely related to the B_{12} cluster units common to these systems [6]. In amorphous Si, however, much higher metal concentrations are required to achieve a similar transition.

These results demonstrate that both self-compensation and bonding conversion are strongly governed by local atomic structure and bonding characteristics, with boron-based materials exhibiting unique behavior associated with icosahedral cluster-based structures.

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Keywords— quasicrystalline approximant, amorphous, self-compensation, bonding conversion

Anharmonic Phonons in Rutile TiO₂ Investigated by Inelastic X-ray and Neutron Scattering

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Abstract

Anharmonic lattice vibrations strongly influence the physicochemical properties of transition-metal oxides. Rutile TiO₂ is a representative anharmonic oxide system, in which the softening of the polar A_{2u} phonon mode has been discussed in relation to incipient ferroelectricity [1]. However, the anharmonicity of the lowest-energy optical phonon, namely the B_{1u} mode, and its relationship to physicochemical properties remain less understood.

In this study, we investigated the optical phonons in rutile TiO₂ using inelastic X-ray scattering (IXS) and inelastic neutron scattering (INS) in combination with first-principles calculations. IXS measurements were performed at BL35XU and BL43LXU of SPring-8 [2], and INS measurements were carried out using the triple-axis spectrometer installed at 6G TOPAN in JRR-3 [3]. Single-crystalline samples were measured over a temperature range between 15 and 300 K.

Figure 1 shows representative IXS spectra of the transverse optical phonon branch derived from the B_{1u} mode (denoted as TO(B_{1u})) measured at 300 K and 15 K. The TO(B_{1u}) branch exhibits pronounced phonon softening and linewidth narrowing upon cooling. Similar temperature dependences were also observed for the polar TO(A_{2u}) branch.

The observed softening of the TO(B_{1u}) branch cannot be explained within the conventional picture of ferroelectric soft modes. The results suggest that higher-order anharmonic interactions play an important role in the TO(B_{1u}) branch. The implications of the anharmonic phonons for the physicochemical properties of rutile TiO₂ will also be discussed.

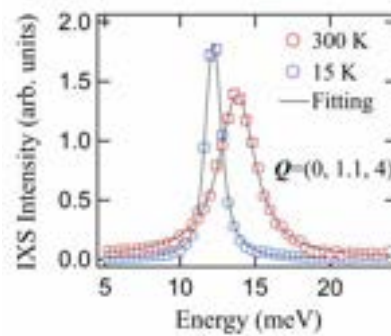


Figure 1: Representative IXS spectra of the TO(B_{1u}) branch in rutile TiO₂ measured at 300 K and 15 K.

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Keywords— TiO₂, anharmonic phonons, inelastic X-ray scattering, inelastic neutron scattering

Percolation scheme for the very basic understanding of the optical phonon mode behavior of disordered semiconductor alloys

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Abstract

Due to their simplicity (two chemical bonds arranged at random on a high-symmetry/cubic lattice), the pseudo-binary $A_{1-x}B_xC$ disordered semiconductor alloys with zincblende structure are a benchmark to explore at which length scales operate various kinds of disorders introduced by alloying. The lattice dynamics offers a convenient platform for doing so in that the wavelength of the studied vibrations ranges from quasi-infinite for phonon-polaritons, “averaging” over the alloy disorder, down to ultimately small for phonons, of merely twice the lattice constant, “zooming” into the alloy disorder. Two atoms per primitive cell generate both the bond-collective acoustic modes and the bond-specific optical ones. Our approach is to focus on the latter that potentially offer a more local (bond-related) insight into the alloy disorder. The transverse optical (TO) modes are especially attractive in that they exhibit both a phonon-polariton regime plus a phonon regime, contrasting with the basic invariance of the longitudinal optical (LO) regime. The TO diversity offers the possibility to probe the alloy disorder from different angles, which is potentially rich of information. Over the past two decades our group has developed a so-called percolation model in which the TO modes distinguish *homo* from *hetero* environments per bond (1-bond→2-TO scheme), and hence are not only bond-specific/sensitive but also environment-sensitive [1]. The latter virtue is denied by the historical modified-random-element-isodisplacement (MREI) model [2] in which the like bonds of a given species vibrate at the same frequency at a given composition x , whatever their local environment (1-bond→1-TO scheme). The percolation scheme has been successfully tested on various semiconductor alloys with cubic (zincblende, diamond) and hexagonal (wurtzite) structures at all length scales, from quasi-infinite ones probed by forward-Raman scattering down to ultimately small ones accessed by inelastic X-ray/neutron scattering, with *ab initio* phonon calculations in support. This suggests the universality of the percolation scheme. Some meaningful examples, *i.e.*, concerned with cubic- $Zn_{1-x}Be_xSe$ and/or hexagonal- $Zn_{1-x}Mg_xS$, addressed within our ViSA (Vibrations of semiconductor alloys, <https://lcp-a2mc.univ-lorraine.fr/projet-visa/>) consortium are reviewed in this communication.

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Keywords—Lattice dynamics, mixed crystals

Turbostratic Stacking Faults: A Structural Lever for Modulating Quantum Phases in Misfit Chalcogenides

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Abstract

Misfit chalcogenide compounds are incommensurate layered heterostructures formed by the alternating stacking of two structurally distinct subsystems: a rock-salt-type quadratic layer (PbSe, SnSe, BiSe...) and a hexagonal transition metal dichalcogenide (TMDC) layer (NbSe₂, TaS₂...), whose lattice mismatch gives rise to inherent incommensurate modulations. Moreover, inter-subsystem charge transfer can stabilize emergent electronic phases, e.g. superconductivity inherited from or enhanced beyond the parent NbSe₂ [1,2]. Misfit chalcogenides harbor an intrinsic susceptibility to turbostratic disorder, i.e. interlayer rotations, whose impact on emergent electronic phases remains largely unexplored. In this work, we demonstrate that turbostratic stacking faults are a dominant structural feature of lead-substituted misfit selenides and play a decisive role in governing the onset and robustness of superconductivity across the solid solution. High-resolution transmission electron microscopy (HRTEM) on focused ion beam (FIB) prepared lamellae provides direct imaging of turbostratic fault distributions. Transport measurements reveal that increasing disorder systematically suppresses long-range crystallographic coherence, with direct consequences for Cooper pair formation and the competition between superconductivity and charge density waves. Elemental analysis by energy-dispersive X-ray spectroscopy (EDX) confirms that compositional inhomogeneities are negligible, isolating turbostratic disorder as the primary structural tuning parameter of the electronic ground state. Low-temperature electrical transport and heat capacity characterizations suggest that turbostraticity correlate with reduced critical temperatures. These results establish turbostratic disorder as a key lever for engineering superconductivity in incommensurate layered systems, contributing to new pathways for controlled modulation of quantum electronic phases through stacking sequence engineering.

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Keywords— Misfit, Chalcogenides, Turbostraticity, Superconductivity

Disorder-controlled magnetism in polar antiferromagnets

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Abstract

Antiferromagnetic materials are promising candidates for ultra-fast and energy-efficient spintronic devices [1]. To enhance and manipulate their functionality, it is essential to understand how their properties can be tuned by external stimuli or chemical composition. Here, we investigate the effect of controlled, site-selective substitution on the crystal structure and magnetism of polar antiferromagnets $M_2\text{Mo}_3\text{O}_8$ ($M = \text{Fe}, \text{Co}, \text{and Zn}$). We show that atomic-scale control of chemical composition enables systematic tuning of magnetic (see Fig.1) and electronic states, where chemical disorder acts as effective microscopic control parameters [2]. A key finding is the strong site preference of non-magnetic Zn, which significantly modifies both intra-layer and inter-layer exchange interactions, as well as the competing magnetic anisotropies associated with octahedral and tetrahedral magnetic M^{2+} sites [3, 4]. Our results demonstrate that chemical disorder in $M_2\text{Mo}_3\text{O}_8$ is not merely a perturbation but a controllable parameter. This enables direct correlations between structure and physical properties, opening new pathways for designing functional magnetic materials.

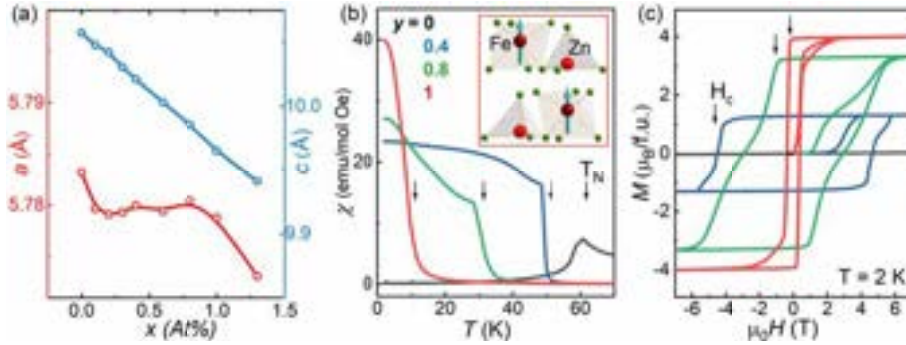


Figure 1: Effect of site-selective substitution on the structure and magnetism of polar $\text{Fe}_{2-y}\text{Zn}_y\text{Mo}_3\text{O}_8$. (a) Synchrotron powder X-ray diffraction patterns, (b) temperature dependence of the magnetic susceptibility χ , and (c) magnetic hysteresis loops for crystals with different Zn concentrations y . The inset in (b) illustrates the preferential site occupancy of magnetic ions at tetrahedral and octahedral positions.

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Keywords— Chemical disorder, polar magnets, functional materials

Comparing intrinsic and extrinsic contributions to phonon anharmonicity in the thermoelectric systems Mg_2Si and GeBi_2Te_4

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Abstract

Controlling lattice thermal conductivity through phonon engineering is a central challenge in thermal management and the development of efficient thermoelectric materials. In this work, we investigate the role of structural complexity and bonding anisotropy in governing phonon anharmonicity by comparing two contrasting systems: the cubic semiconductor Mg_2Si [4] and the layered van der Waals compound GeBi_2Te_4 (GBT), a topological insulator [3]. Phonon properties were probed using powder and single crystal inelastic neutron scattering, Raman spectroscopy and thermal conductivity. These experimental results are compared and complemented by temperature-dependent *ab initio* lattice-dynamical calculations within the stochastic temperature dependent effective potential (sTDEP) framework [2]. The layered structure in GBT necessitates inclusion of van der Waals-forces, for this the vdW-DF-cx functional was used [1].

The phonon density of states and dispersion relations reveal markedly different behaviors in the two systems. These are shown in Fig.1. Mg_2Si exhibits well-defined phonon modes, a high Debye temperature, and temperature-induced broadening, consistent with predominantly intrinsic anharmonic phonon-phonon interactions. In contrast, GBT displays strongly broadened phonon spectra, reduced Debye temperature, and early deviations from Debye behavior.

The phonon linewidth analysis from both neutron scattering and Raman spectroscopy further emphasizes this contrast. Acoustic phonons in Mg_2Si remain comparatively sharp at low temperature and broaden systematically with increasing temperature, accompanied by smooth phonon softening, in agreement with conventional three- and four-phonon decay processes. The Raman-active optical mode shows moderate temperature-dependent shifts and linewidth increase, characteristic of intrinsic anharmonicity. By contrast, GBT exhibits substantially larger linewidths already at low temperature and weakly defined dispersive modes.

These differences are directly linked to the underlying crystal structures. While Mg_2Si provides an isotropic reference system, the layered structure of GBT introduces strong anisotropy in bonding and structural disorder, which acts as additional scattering channels. As a result, phonon transport in GBT is dominated by extrinsic and disorder-driven effects, leading to significantly suppressed lattice thermal conductivity around room temperature. This comparative study highlights how lattice dimensionality and bonding hierarchy govern phonon dynamics and provides insights for designing thermoelectric materials with intrinsically low thermal conductivity.

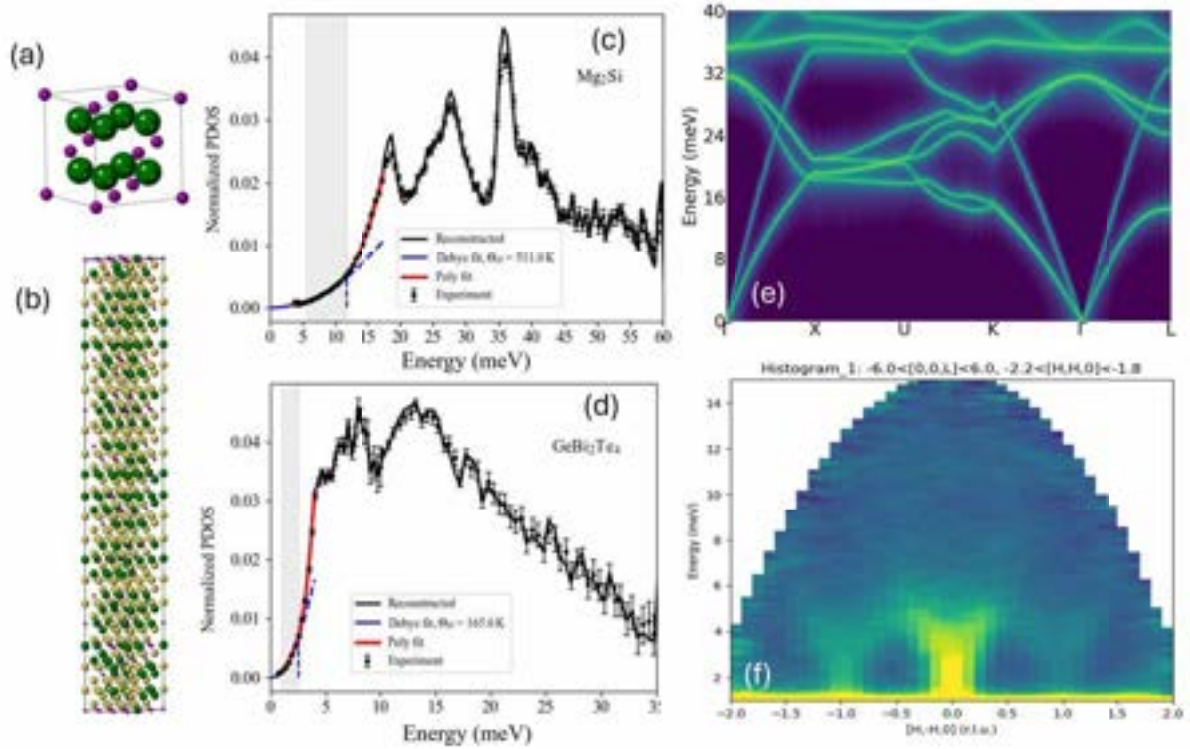


Figure 1: (a) Unit cell of Mg_2Si with Mg in green and Si in purple. (b) $3 \times 3 \times 3$ unit cell of GBT indicating atomic disorder showing Bi in green, Ge in purple and Te in yellow. (c,d) Experimentally extracted phonon density of states, along with the Debye fit and a polynomial fit, highlighting the deviation to the Debye model. (e) Phonon dispersion relation of Mg_2Si at 300 K calculated using sTDEP. (f) Measured phonon spectra of GBT at 300 K along the $[H - 2, -H - 2, 0]$ integrated in the L direction.

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Keywords— vdW materials, thermoelectrics, inelastic neutron scattering, anharmonic phonons

Influence of phase and structural ordering on the electrochemical performance of multiphase Na-layered oxides as positive electrodes

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Abstract

Next-generation Na-ion batteries are triggered by the development of new cathode materials that enable the maximum extraction of their capacities while compromising high energy density and long-term stability. Among the most promising cathode families, the layered oxides (2D materials) are the best candidates due to their compositional and phase tunability. Different phases have been reported in the literature to exhibit distinct kinetic and electrochemical properties [1]. These phases are classified under Delma's notation, which classifies phases as O3 (space group $R\bar{3}m$), P2 (space group $P6_3/mmc$) or P3 (space group $R\bar{3}m$), among others, depending on the crystallographic position of the Na in the unit cell (P for prismatic and O for octahedral) and the number of octahedra needed to describe the unit cell (2 or 3). Other phases with lower symmetry, such as O'3 (space group $C12/m1$) and *Pnma* (see **Figure 1a**), are also synthesised [2,3]. Here, we studied compositional systems with a general formula and composition of $\text{Na}_{2/3}\text{Mn}_{0.8}\text{Fe}_{0.1}\text{Ti}_{0.1}\text{O}_2$ (designated as NMFTO), featuring different structural ordering and phase ratios. The NMFTO system was crystallised under three different phases (pure P2, a biphasic P2 & *Pnma* and an O'3, see **Figure 1b**). As demonstrated by galvanostatic charge-discharge tests (see **Figure 1d**) and cyclic voltammetry (see **Figure 1e**), despite the same chemical composition, the crystalline phase of the material plays a key role in the final unlocking of the redox systems involved in Na de/intercalation. O'3 demonstrated to displace Mn redox pair to higher voltages, sluggish kinetics and lower presence in the electrochemical reaction, provoking lower capacities and higher irreversible processes. Meanwhile, a biphasic layered-tunnel system showed that although slightly lower capacity, diffusion and structural stability are improved, increasing capacity retentions up to 13% more than a pure P2 phase. Additionally, a second polymorphic system with the chemical formula $\text{Na}_{0.81}\text{Mn}_{0.52}\text{Ni}_{0.2}\text{Mg}_{0.08}\text{Fe}_{0.09}\text{Zn}_{0.11}\text{O}_2$, denoted as P3/P2/O3-Na0.81, was studied. This system enables tuning of the phase ratio among O3, P2, and P3 via the synthesis temperature (see **Figure 1c**) and provides an additional basis for correlating electrochemical performance with crystal ordering. A comparative analysis of both polymorphic systems allows direct correlation of structural features and crystal ordering with electrochemical performance. In summary, both systems demonstrate that the coexistence of multiple phases enhances electrochemical performance, confirming that the crystallographic phase influences not only the kinetics but also the thermodynamic properties of the material.

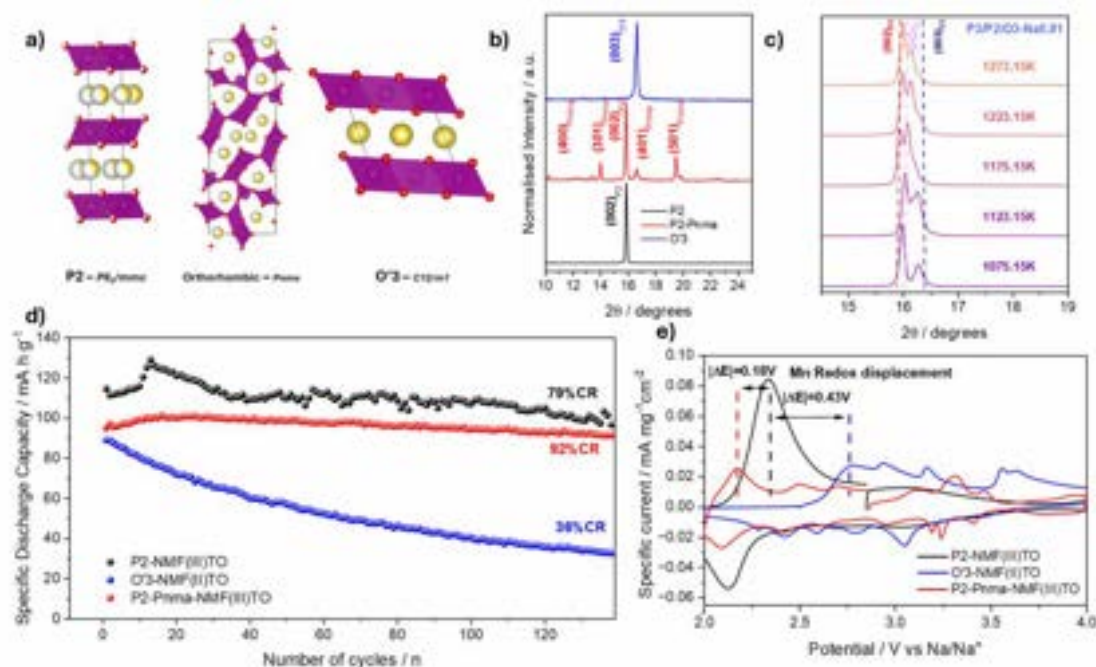


Figure 1: a) Unit cells of the NMFTO structures presented, b) XRD patterns for the pure P2, biphasic P2-Pnma and O'3 phase, c) XRD evolution upon temperature on P2/P2/O3-Na0.81 polymorphic system, d) Discharge curves for the mentioned materials at C/10, 4.0-2.0V, 20°C, EC:PC:FEC 1M NaPF₆, e) CV curves at 0.1mV s⁻¹ for the pure P2 material, biphasic P2-Pnma and the O'3 at 20°C, EC:PC:FEC 1M NaPF₆.

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Keywords— Multiphase layered oxides, Structural orderings, Na-ion batteries

Fragmented phases in artificial frustrated magnets

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Abstract

Artificial spin ice (ASI) systems have established themselves as a versatile experimental platform [1, 2, 3] for investigating the rich physics characteristic of classical frustrated magnets. By engineering two-dimensional (2D) lattices of interacting nanoscale magnetic islands, ASI systems not only emulate seminal models of statistical mechanics but also provide a "lab-on-chip" approach in which to visualize, in space and time [4, 5], collective behaviors and emergent properties of matter. These systems have recently enabled the realization of a diverse range of phenomena, including complex magnetic orders, liquid-like phases hosting topological quasiparticle excitations, reentrant transitions, and magnetic moment fragmentation.

The concept of fragmentation is particularly counterintuitive. In certain 2D ASI systems, order and correlated disorder coexist at thermodynamic equilibrium, giving rise to a state of matter that is simultaneously solid and liquid, everywhere in the lattice, anytime. This fragmented state, theoretically predicted about a decade ago [6], has now been observed both in bulk frustrated magnets [7] and ASI systems [8]. While probing such unusual phases of matter in arrays of interacting nanomagnets presents experimental challenges, ASI allows direct visualization and manipulation of fragmented states, down to the level of the individual spin degree of freedom.

By bridging abstract theoretical concepts with tangible experimental accessibility, ASI systems provide an unparalleled opportunity to study cooperative phenomena in frustrated magnets. Through a selection of recent examples, this presentation will highlight the pivotal role of ASI in advancing our understanding of fragmented phases of matter, exhibiting simultaneously magnetic order, Coulomb spin liquid physics and topological quasiparticle excitations carried by spin fragments.

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Keywords— Artificial spin ice, frustrated magnetism, magnetic moment fragmentation, topological quasiparticle excitations, liquid-like physics, emergent properties, cooperative phenomena

High-energy photoemission study of strongly correlated rare-earth-based quasicrystal approximants

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Abstract

Within a decade, strongly correlated electronic states in rare-earth-based approximant crystals (ACs) have attracted considerable attention following the discovery of exotic quantum states. Among them, Tsai-type Au-Al-Gd and Au-Al-Tb ACs show various magnetic ground states such as antiferromagnetic, ferromagnetic and spin-glass states as a function of Au concentration or electron-per-atom ratio [1]. On the other hand, Tsai-type $(\text{Ce}_x\text{Y}_{1-x})\text{Cd}_6$ ACs have been found to show anomalous magnetic transition [2]. For understanding these magnetic transitions, the local rare-earth $4f$ electronic states and the hybridization effects with neighboring sites or itinerant bands should be clarified. In order to reveal them, we have performed bulk-sensitive hard x-ray photoemission and rare-earth $3d$ -edge resonance photoemission studies of the Tsai-type Ce- [3, 4], Tb- [5] and Gd-based [6] ACs. In CeCd_6 , it is found that the Ce $4f$ orbitals are predominantly hybridized with the valence-band electrons far from the Fermi level (E_F) rather than at E_F , in sharp contrast to the hybridization seen for the intermetallic Ce-based crystalline compounds. On the other hand, for the Tb- and Gd-based ACs in which the $4f$ states are more localized than those in the Ce ions, the hybridization between the rare-earth and Au $5d$ orbitals are found to depend on the Au concentration, which could control the magnetic ground states. The degree of resonance enhancements near E_F in the $3d$ -edge resonance photoemission has been qualitatively different between the Tb- and Gd-based ACs, which reflects the different $4f$ -orbital asymmetry between the Tb and Gd ions.

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Keywords— photoemission spectroscopy, rare earth, quasicrystal approximants

Imaging Topologically Protected Strings in Dysprosium Indate using Bragg Coherent X-ray Diffraction

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Abstract

Topological defects, such as vortices and strings, play a critical role in determining the functional properties of ferroic materials^[1–3]. Recent studies demonstrate the potential of three-dimensional, non-destructive imaging of topological defects in multiferroic materials^[4], unlocking new capabilities for probing these features in complex systems. Here, we extend the application of Bragg Coherent Diffraction Imaging (BCDI)^[5, 6] to explore topological states in the indate systems. BCDI reconstructions of DyInO₃ show the three-dimensional internal phase distribution within nanocrystals, providing a direct volumetric visualisation of one-dimensional topologically protected strings. By reconstructing the internal phase distribution, we map the spatial trajectories of defect cores, revealing that spatially isolated strings propagating in parallel possess consistent winding directions, while looped or reconnected strings manifest as counter-winding pairs to satisfy topological conservation. Furthermore, we employ enhanced reconstruction methods that significantly improve the resolution of the collected data, allowing for unprecedented insight into these complex defect networks.

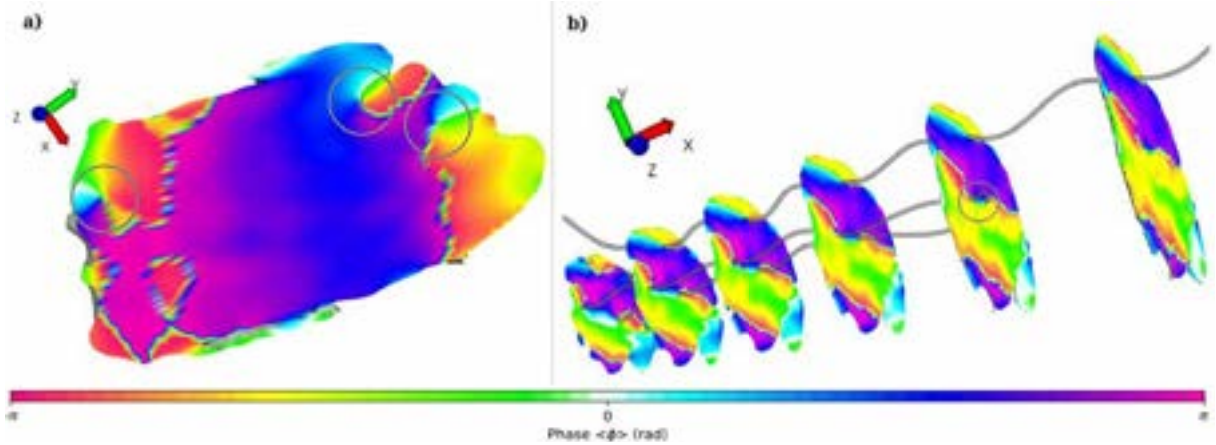


Figure 1: **a)** Clipped Phase through BCDI reconstruction of a DyInO₃ crystal displaying a complex topological state of three vortices winding in the same direction. **b)** Serial phase cross-sections through a DyInO₃ crystal, each slab 10 nm thick, arranged 600 nm apart, exhibiting complex string (curved grey rods) connectivity. One of the strings passes through several slabs before looping back (high-contrast circular indicator) through a different set of vortices.

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Keywords— Bragg CDI, X-ray imaging, Dysprosium Indate

Element-Specific Ultrafast Probing of Electronic and Magnetic Orders with Time-Resolved Soft-X-Ray Spectroscopy

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Abstract

Complex ordered states in condensed matter often emerge from the coupling among electronic, magnetic, and lattice degrees of freedom. Understanding how these coupled orders evolve on ultrafast timescales is essential for clarifying the microscopic mechanisms behind photoinduced phase transitions, magnetization dynamics, and emergent functionalities in quantum materials. However, conventional optical probes often lack the element specificity and interface sensitivity required to disentangle the roles of different atomic species in complex materials and heterostructures.

Here, we discuss the potential of time-resolved soft-X-ray spectroscopy as an element-specific probe of ultrafast electronic and magnetic order dynamics. By tuning the probe photon energy to core-level resonances, soft-X-ray techniques can selectively access transient responses associated with specific elements and electronic states. In particular, time-resolved soft-X-ray magneto-optical Kerr effect and nonlinear optical probes such as soft-X-ray second-harmonic generation provide complementary sensitivity to magnetization, symmetry breaking, and interfacial electronic structures [1, 2]. These techniques are especially powerful for complex systems in which multiple order parameters are strongly coupled. Time-resolved soft-X-ray measurements can reveal how photoexcitation redistributes electronic density, modifies magnetic order, and drives transient symmetry changes on femtosecond-to-picosecond timescales. The element specificity of these probes is particularly valuable for functional heterostructures, multicomponent compounds, and materials with hidden or interfacial orders. Such approaches provide a powerful route to disentangling ultrafast charge, spin, and lattice dynamics at interfaces in semiconductor, ferroelectric, and magnetic heterostructures.

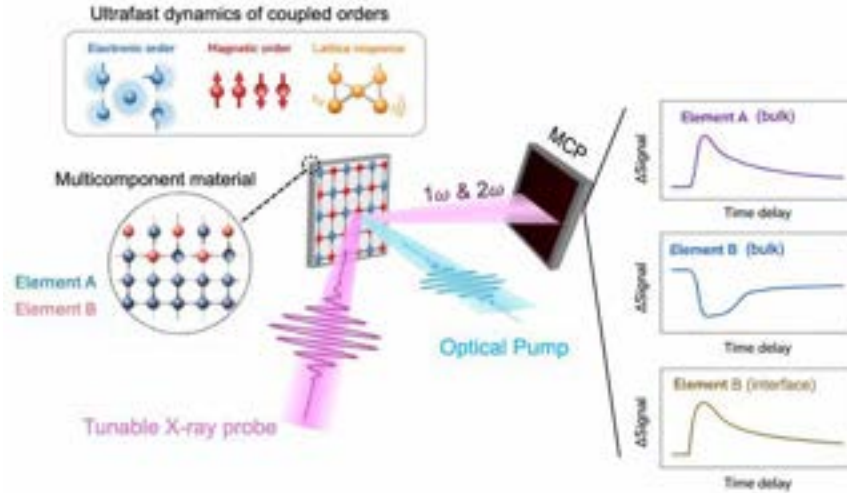


Figure 1: Schematic illustration of element-specific time-resolved soft-X-ray spectroscopy and nonlinear optical probing of coupled orders in a multicomponent material. A femtosecond optical pump drives the system out of equilibrium, while a delayed tunable soft-X-ray probe detects transient responses at selected core-level resonances. Detection at the fundamental and second-harmonic frequencies provides complementary sensitivity to bulk and interfacial electronic, magnetic, and lattice dynamics.

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Keywords— time-resolved spectroscopy, soft X-ray, electronic order, magnetic order, ultrafast dynamics, element specificity

Amorphisation by Structural Disorder and Its Effects on Topological Phases

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Abstract

Topological phases of matter exhibit robust conducting edge states tied to invariants such as the Chern number. While well understood in crystalline systems due to presence of symmetries, their realization in disordered or amorphous materials remains less explored[1].

Here we study the evolution of a decorated honeycomb crystalline lattice to a hyperuniform amorphous system by introducing Stone–Wales[2] (SW) defects (Fig.1) that disrupt long-range order. Using the topological Weaire–Thorpe Hamiltonian for electrons[3, 4], we show that these defects can induce pseudo-band inversions and reverse the Chern number. With adiabatic arguments we predict the topological phase of the amorphous system and explain the band-inversion mechanism via effective hopping renormalization.

We also reveal the possibility of structural disorder destroying the topological phase of the crystal. In certain regimes, SW defects generate bound states, leading to eventual closure of the mobility gap. This drives the system through an insulator-metal transition via a percolation mechanism, for which we provide analytical and numerical estimates of the critical defect concentration and identify which crystalline topological phases are robust to amorphisation.

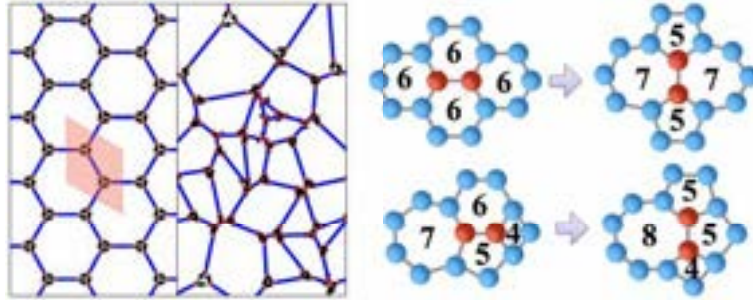


Figure 1: Left: comparison between crystalline and amorphous Chern insulators. Right: Stone-Wales defect via bond rotation.

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Keywords— Chern insulator, structural disorder, percolation

Analysis of band gaps and hyperuniformity in two-dimensional photonic quasicrystal approximants

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Abstract

Photonic quasicrystals provide a versatile and highly controllable platform to investigate wave phenomena in such aperiodic systems. In particular, they enable systematic exploration of the relationship between structural order and collective excitations, offering insight into general wave-mechanical principles beyond specific material constraints [1]. In two-dimensional dielectric systems with air cylinders, periodic structures such as the triangular lattice exhibit large complete photonic band gaps (PBGs), whereas square lattices do not support complete gaps due to the mismatch between TE and TM modes. For quasiperiodic structures, however, band-gap formation remains less understood, and complete gaps have not been established in canonical tilings such as Ammann-Beenker or Penrose [2], except for limited reports in square-triangle tilings [3].

In this study, we investigate the band structures of two-dimensional photonic quasicrystal approximants based on Ammann-Beenker (eightfold symmetry), square-triangle, and Hexagon-Boat-Star (HBS, tenfold symmetry) tilings using the plane-wave expansion method. We identify complete photonic band gaps in both the square-triangle and HBS tilings and demonstrate, for the first time, a complete gap in a tenfold-symmetric quasiperiodic structure. Furthermore, by introducing secondary air cylinders at the centers of star-shaped prototiles, we increase the point density and observe the emergence of a complete gap in the Ammann-Beenker tiling and a substantial enhancement of the gap in the HBS structure.

To clarify the structural origin of band-gap formation, we perform hyperuniformity analysis [4]. Our results show that structures combining high point density with low structural complexity systematically favor gap formation. This finding suggests that hyperuniformity serves as a unifying structural descriptor for wave propagation in aperiodic systems and provides a predictive design principle for band-gap engineering [5].

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Keywords— quasicrystals, hyperuniformity, band gap, aperiodic structures, wave propagation

Gapless superconductivity in two-dimensional quasicrystals and its real-space topology

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Abstract

Quasicrystals form a new class of topological materials, which lack translational symmetry yet possess long-range aperiodic order with scale invariance, and superconductivity has recently been discovered in quasicrystals [1]. We have previously shown the stable occurrence of topological superconductivity with broken time-reversal symmetry in two-dimensional quasicrystals by solving for the mean fields self-consistently [2]; however, the fundamental nature of topological superconductivity is not dissimilar to that in periodic systems. In this work, we perform self-consistent studies of superconductivity in Ammann-Beenker quasicrystals under magnetic field, and find gapless superconductivity at and near half filling, which arises from unique interplay of highly degenerate confined states and inherent inhomogeneity of quasicrystals. In the presence of Rashba spin-orbit coupling, the quasicrystalline gapless superconductor can be topologically nontrivial and characterised by a real-space topological invariant called a pseudospectrum index given by a spectral localizer. Signified by the pseudospectrum index, the gapless topological superconducting phase exhibits edge states with near-zero energy [3].

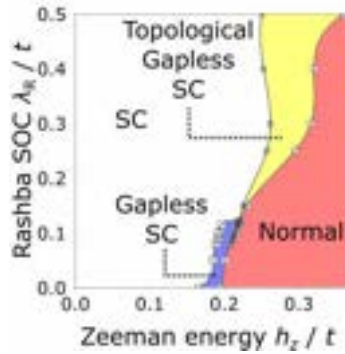


Figure 1: Topological phase diagram of Ammann-Beenker quasicrystals in terms of the Rashba spin-orbit coupling λ_R and the Zeeman energy h_z in units of the hopping amplitude t . The topological phase in the yellow region is characterised by the pseudospectrum index $C_L = 2$ in the bulk.

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Keywords — quasicrystals, gapless superconductivity, real-space topological index

Chiral charge density waves in EuAl₄ and related compounds

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Abstract

The BaAl₄ structure type has centrosymmetric, tetragonal symmetry, I4/mmm, with three crystallographically independent atom sites: Ba, Al1 and Al2. The compound EuAl₄ crystallizes in the BaAl₄ structure type [1]. Magnetic Eu²⁺ atoms are responsible for four, differently ordered, antiferromagnetic (AFM) states below T_{N1} = 15.4 K [2]. Metamagnetic states, with fields up to 1.8 T, include two skyrmion phases. Before reaching AFM order, a charge-density wave (CDW) develops in EuAl₄ at T_{CDW} = 145 K [2]. The symmetry of the CDW is a major issue, also in view of the symmetry of the magnetic interactions that define the AFM and skyrmion phases [3,4]. Here, we present the crystal structures of the incommensurate CDW of EuAl₄. In particular, the symmetry of the CDW is analyzed in view of x-ray diffraction data [5,6], results of transmission electron microscopy (TEM), density functional theory (DFT) calculations and inelastic x-ray scattering (IXS) [3,4]. The CDW is discussed in relation to its recently proposed chiral character, requiring a non-centrosymmetric symmetry [7].

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Keywords— EuAl₄, charge-density-wave, aperiodic crystal

Exploring the disorder driving barocalorics using inelastic neutron spectroscopy

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Abstract

As global warming prompts more people to use air conditioning, it is imperative that new environmentally-friendly cooling technologies are developed to break the vicious heating cycle. The most promising replacement technology uses barocalorics, which undergo a large isothermal entropy change associated with a pressure-induced solid-solid phase transition. Initially barocalorics were thought to be rather rare, but we now know that they can be found in a wide range of materials families, including metals, molecular crystals, molecular-ionic salts, and coordination frameworks of different dimensionalities. This is encouraging, but now means we have a large and chemically diverse parameter space to explore, making it even more important to develop principles for identifying and designing the best barocalorics.

The majority of the first-order phase transitions responsible for substantial barocaloric effects are structural order-disorder transitions, highlighting the significance of disorder to these materials' functionality. Traditionally the community interested in correlated excitations have either ignored or denied the existence of disorder, viewing it as a complication to the analysis. However, advances in simulating these lattice dynamics mean that the analysis is becoming tractable.

Disorder in crystals can be accounted for with large supercells in conventional lattice dynamics calculations, using band unfolding to determine the disorder-induced broadening of the phonons [1]. Adamantane is a barocaloric with an orientationally disordered high temperature high entropy phase. INS and super cell lattice dynamics (SCLD) revealed that the entropy change is 40% configurational and 60% vibrational, associated with a softening of the acoustic modes, which also gain a more substantial rotational component [2]. However, there are caveats to the use of SCLD for calculating the phonon spectrum in disordered crystals: 1) careful convergence testing is required to ensure a representative distribution; 2) these calculations are computationally expensive; and 3) the inevitable restrictions on finite supercell size mean they are unable to model very long wavelength excitations.

An alternative approach is to use molecular dynamics simulations. These have the advantages that structurally disordered materials are no more intrinsically difficult to model than any other system; and that the harmonic approximation is not necessary, so modelling temperature dependence or other effects of anharmonicity is straightforward. On the other hand, a very significant disadvantage is that molecular dynamics simulations must be large in size and run for long simulation times in order to achieve good resolution in Q and ω respectively. The advent of cheap and accurate machine-learned force fields is therefore making this method rapidly more accessible. MACE equivariant message-passing network interatomic potentials capture the full anharmonicity and achieve accuracy close to DFT at a fraction of the cost. This has allowed us to generate MD trajectories long enough to sufficiently sample phase space, and to validate these directly against inelastic and quasi-elastic neutron scattering data. We will present MACE simulations and experimental data collected from a series of orientationally disordered molecular-ionic barocalorics. We interrogate the trajectories to determine the atomistic origin of these materials' large pressure-driven entropy changes.

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Keywords— INS, QENS, Barocalorics

Theoretical studies of magnetism in icosahedral quasicrystals and 1/1 approximants

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Abstract

Ground-state properties of rare-earth based 1/1 periodic approximants of icosahedral quasicrystal are clarified theoretically on the basis of an effective model for magnetism taking into account uniaxial anisotropy arising from crystalline electric field [1]. By performing numerically-exact calculation on the 1/1 approximant crystal, we have determined the ground-state phase diagram for ferromagnetic interactions. The result shows that eight kinds of noncollinear and noncoplanar magnetic structures are stabilized, whose magnetic space groups are identified as $I_{\bar{4}}m' \bar{3}$, $C2'/m'$, and $R\bar{3}$. We have clarified the degeneracy of each ground state, corresponding to the numbers of the domains. By analyzing each state, the magnetic as well as topological properties are revealed. Our results are shown to explain the measured magnetic structures in the Tb-, Ho-, Dy-based 1/1 approximants and the effective model is discussed to be useful for understanding the magnetic structures and their topological properties in broad range of rare-earth based 1/1 approximants.

So far, theoretical studies of magnetism in quasicrystals were limited to low dimensional systems. Recently, we have *for the first time* clarified theoretically how magnetic-long-range order arises on three-dimensional quasicrystals [2,3]. By performing Monte Carlo simulations for the Heisenberg model on the Yb lattice of the quasicrystal $\text{Cd}_{5.7}\text{Yb}$ composed of regular icosahedrons [2] as well as the full Yb sites [3], we show that the ferromagnetic transition takes place as a continuous transition. We have revealed the ferromagnetic transition mechanism by showing that the difference in the local environment of each site is governed by cooperative evolution of spin correlations upon cooling, giving rise to the critical phenomena. In the presentation, we will discuss the universality class by comparing the critical exponents identified by the finite-size scaling analysis of the Monte Carlo data with the experimental identifications in the rare-earth-based quasicrystals and approximants.

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Keywords— icosahedral quasicrystal, 1/1 approximant crystal, magnetism

n=1 Aurivillius and other 2-dimensional magnets

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Abstract

As strong interest is given to functional materials in catalysis, energy storage, or micro-electronic applications, 2-dimensional materials are a promising platform for new compounds enhancing or tuning the properties of their bulk parent compounds. By adding anisotropy to their properties or showing different electronic/magnetic behavior, due to removed exchange couplings, they further act as an ideal probe in fundamental research on magnetic exchange and structures. Mixing oxide and fluoride anions moreover allow to reach lower transition metal oxidation states raising a wide range of different magnetic cations with different electronic configurations.

Accommodating cations with different sizes and charges the n=1 Aurivillius structure type with the general formula $[\text{Bi}_2\text{O}_2][\text{A}_{n-1}\text{M}(\text{O},\text{F})_{3n+1}]$ and its oxyfluoride members $\text{M} = \text{Nb}^{5+}$, Ta^{5+} , $\text{V}^{4+/5+}$, Zr^{4+} , Ti^{4+} , Mn^{2+} , $\text{Fe}^{2+/3+}$, Co^{2+} , and Ni^{2+} [1–5] is well adapted to investigate short and long range magnetic and nuclear order. Built of structurally resilient $[\text{Bi}_2\text{O}_2]^{2+}$ layers with fluorite structure and $[\text{M}(\text{O},\text{F})_4]^{2-}$ perovskite layers, which allow investigation of octahedral tilting but also flexibility to accommodate alternative tetrahedral or strongly distorted coordination depending on the specific, central cation and oxidation state.

For this communication main focus has been laid on the iron and vanadium case. The changes induced to magnetic order by mixing Co, Mn, or Ni into the Fe compound have been investigated by neutron powder diffraction [6] (compare Fig. 1d-g). The motivation for the V compound is to achieve and stabilize the lower V^{+4} oxidation state (see Fig. 1a-c) to investigate magnetic d^1 - d^1 exchange with possible photocatalytic activity. The influence of the exact synthesis conditions on mixed-valency of the products and connected disorder is analyzed by X-ray and neutron powder diffraction, single crystal X-ray and electron diffraction, V-K α -XANES, ^{57}Fe -Mössbauer, magnetic measurements and/or impedance spectroscopy.

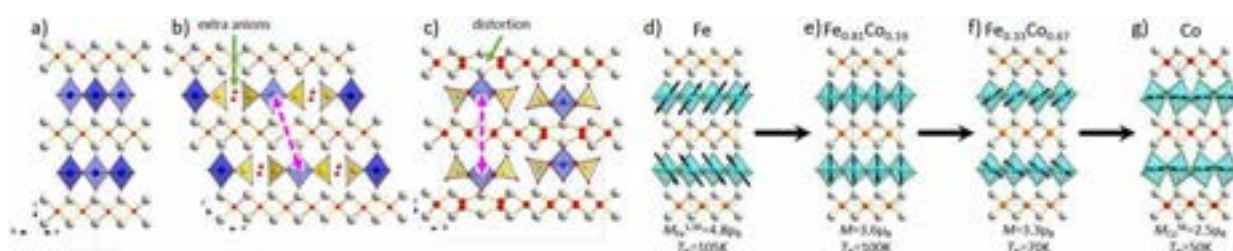


Figure 1: a) V-Aurivillius, b) V-vacancy ordered structure, c) $\text{Bi}_2\text{O}_2\text{VO}_{3.5}$ full-oxide [8],
d-g) $\text{Fe}_{1-x}\text{Co}_x$ magnetic structures [7].

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Keywords — neutron diffraction, local order, magnetism

High-Pressure Synthesis and Crystal Structures of H₃Cl₇ Phases

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Abstract

High pressure (HP) provides a direct route to engineer new chemistry and enables unconventional bonding motifs that are inaccessible under ambient conditions. Here, we investigate the chlorine-rich hydrogen-chlorine chemistry in the pressure range of about 40 to 75 GPa using laser-heated diamond anvil cells (DACs). The reaction products were studied using synchrotron single-crystal X-ray diffraction (SCXRD). We report the discovery of a previously unknown hydrogenated polychloride, H₃Cl₇, whose crystal structure contains layers of chlorine atoms with a distorted Kagome lattice topology.

Two distinct polymorphs of H₃Cl₇, H₃Cl₇-I and H₃Cl₇-II, coexist at 65(3) GPa. The arrangement of chlorine atoms in both structures can be derived from a hexagonal prototype structure (*P6/mmm*, #191; *hP7*), in which chlorine atoms form three distinct sublattices: honeycomb lattice layers formed by Cl1 atoms, Kagome lattice layers in the *ab* plane formed by Cl3 atoms, and dimers of Cl2 atoms aligned along the *c* axis (Figure 1).

H₃Cl₇-I exhibits many additional reflections relative to the *hP7* prototype. Its incommensurately modulated structure is described by a modulation wave vector $\mathbf{q} = \alpha\mathbf{a}^* + \beta\mathbf{b}^*$, with $\alpha = 0.782$ and $\beta = -0.391$. Transformation of the basic *hP7* cell to a pseudo-hexagonal setting ($a = a_0$, $b = \sqrt{3}a_0$, $c = c_0$) enables a (3+1)-dimensional superspace description, with the structure refined in the superspace group *Cmmm*($\alpha 00$)0*s*0 and $\alpha = 0.782(2)$ at 65(3) GPa.

In contrast, the structure of H₃Cl₇-II is commensurately modulated and can be described within a $2 \times 2 \times 1$ supercell with symmetry reduction to subgroup *P6/m* (#175). Density functional theory calculations support the experimental observations. Systematic evaluation of candidate hydrogen configurations establishes the H₃Cl₇ stoichiometry and reveals the electronic structures of the novel polymorphs.

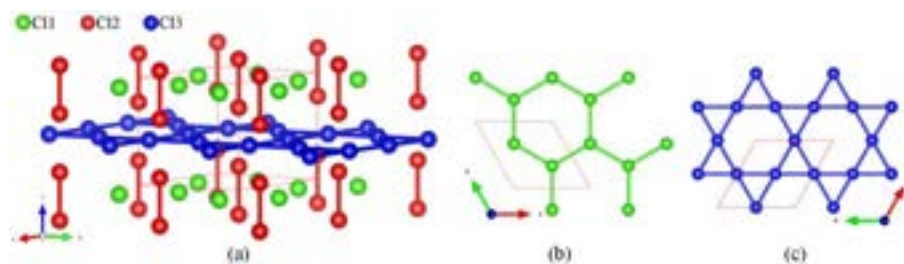


Figure 1. Hexagonal prototype structure of H₃Cl₇. (a) General view of the structure; (b) honeycomb lattice of Cl1 atoms; (c) Kagome lattice of Cl3 atoms, in projection on *ab* plane; dimers of Cl2 atoms, aligned along the *c* axis, are shown in (a). Cl1 atoms are green, Cl2 atoms are red, and Cl3 atoms are blue.

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Keywords— Kagome lattice, hydrogenated polychloride, high pressure crystallography

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Poster presentations abstracts

The electronic structure of ZnMg(Hf, Zr, Ti) periodic approximant phases

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Abstract

The similarity between Tsai and Bergman-type phases can be investigated in the Zn-Mg-(Hf, Zr, Ti) system. In the system, the Bergman F-phase is right next to the Tsai P-phase quasicrystal in the composition phase diagram. Also, there is 1/1 cubic approximant that shows all the structural variants have similar thermodynamical stability conditions. The approximant crystallizes in $Im\bar{3}$ space group and was modelled by Gómez, et al. [1]. The model puts partially occupied atoms in the sites forming triangle of two soccerball polyhedron vertices and one site that should be unoccupied in ideal Bergman-type phase. The site, however, is occupied in a Tsai-type phase allowing for the investigation of the role of the electronic structure in the stabilization of particular cluster variant, both being phason-flip related [2].

Calculations of the electronic structure were performed based on the density functional theory. Comparative study of approximant with Hf, Zr and Ti prove the role of orbital hybridization in structure stabilization, however is transition-metal dependent. For Ti, the hybridization contribution to the hamiltonian is surpassed by electrostatic contribution, explaining why Mg instead of Zn occupies the site extra in Bergman cluster model. Most stable structure version always involves additional site being occupied, signifying the importance of the deviation from ideal Bergman cluster.

All the considered models, exhibit elevated localization around Mg atoms, what contributed to low Mg-Mg distance ($\approx 2.8 \text{ \AA}$). In addition, the Fermi surface analysis confirms elevated nesting along 2-fold symmetry direction hinting a Peierls-like stabilization mechanism. The pseudogap, even though exists, is deeper in less-stable structure model, and shows prominent peak at Fermi level of most-stable version (Fig. 1).

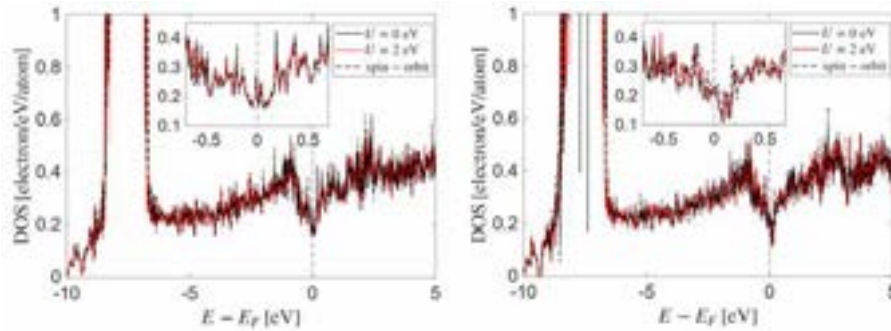


Figure 1: The density of states for ZnMgHf modelled with (left) and without(right) additional atom.

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Keywords— Quasicrystals, Bergman phase, DFT

Attempt to nano-engineer flat bands to enhance superconductivity

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The physics of flat band systems has recently emerged as a new field within condensed matter physics [1]. Due to the fact that electrons have zero velocity in these bands, the relevant energy scale is associated with electron-electron interactions. Theories then predict that the superconducting critical temperature, T_c , depends linearly on the pairing interaction, g , $T_c \propto g$ rather than exhibiting the conventional exponential scaling, $T_c \propto \exp(-1/g)$. Consequently, superconductivity could manifest in non-superconducting materials, such as magic-angle twisted graphene [2], and critical temperatures much higher than those of conventional superconductors can be envisaged [3].

Here, we present an experimental attempt to control the emergence of flat bands by nano-patterning aluminium and niobium thin films, and to explore their potential link with enhanced superconductivity. Inspired by theoretical works showing that fractal lattices may trigger the emergence of flat bands [4], we produced different superconducting structures using electron-beam lithography techniques. We then measured the evolution of the critical temperature and computed Fermi velocity using magneto-transport measurements. The Fermi velocity quantifies the emergence of flat bands. Our ultimate goal is to determine whether there is a correlation between the critical temperature and the Fermi velocity in nanostructures made from the same material.

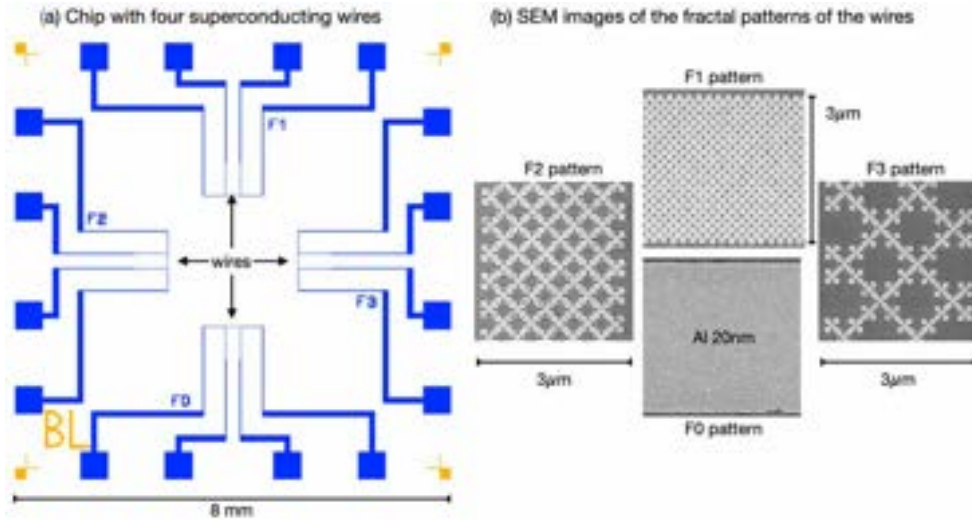


Figure 1: Chip design and realization to disentangle material defect from the patterning influence (a) Chip with four superconducting wires of the very same material. Each wire is connected in a four wires resistivity measurement configuration. (b) SEM images of the fractal-like patterns of the wires. The patterns are derived from the Vicsek's fractal. Light grey corresponds to 20 nm thick superconducting aluminium, dark grey correspond to the silicon substrate. The unstructured F0-wire is the reference material.

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Keywords— superconductivity, flat band, lithography

Paramagnon softening with doping in oxychloride cuprate superconductors

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Nicholas Brookes⁴, Victor Porée⁵, Alessandro Nicolaou⁵,
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Abstract

Understanding how magnetic excitations and exchange interactions evolve with doping is crucial for deciphering the physics that shapes the phase diagram of high-temperature cuprate superconductors. Here, we clearly determine the behavior of the paramagnon dispersion in the oxychloride cuprate up to the highest doping level. We find that the paramagnon bandwidth, defined by the energy at the X zone boundary ($\frac{1}{2}, 0, 0$), remains unchanged within experimental uncertainty, even though it exhibits significant broadening. In contrast, along the nodal direction $\Gamma - M$ (*i.e.*, from $(0, 0, 0)$ to $(\frac{1}{2}, \frac{1}{2}, 0)$), the paramagnon energy shows a marked softening with doping, with a shift of up to $\Delta E \sim 150$ meV at the midpoint of the zone for the highest doping, which is about half of its initial value in the antiferromagnetic phase. Calculations of the dynamical spin structure factor for a one-band Hubbard model, taking up to the third nearest-neighbor hopping term, t'' term (see Fig. 1) account for this behavior, accurately reproducing the observed wavevector dependence and directional variation in the Brillouin Zone.

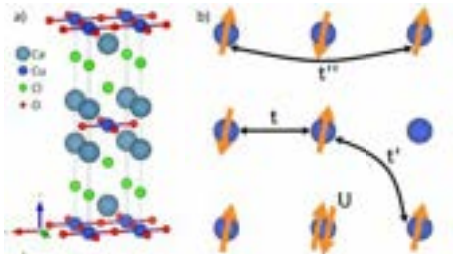


Figure 1: a) Tetragonal crystal structure of CCOC. b) Effective one-band Hubbard model for the CuO₂ layers. From Ref. [1].

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Keywords — High-Temperature-Superconductivity, paramagnon, cuprate

Peierls Physics and Crystal Chemistry of High Pressure Polymorphs of Na₄X₅ (X = I, Br, Cl) Compounds

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Abstract

One-dimensional materials have attracted great attention due to the possibility to study spin-charge separation, charge and spin-density waves, topological spin excitations, and other spectacular phenomena. Discoveries of quasi-one-dimensional materials made it possible to investigate at least some aspects of hypothetical theoretical models experimentally. Still, the synthesis of truly monoatomic chains remains elusive. We explore a novel path of experimental synthesis of monoatomic one-dimensional chains by their chemical stabilization in ionic compounds. We demonstrate that in synthesized at high pressure sodium halides Na₄X₅ (X = I, Br, Cl) with hP18 Ga₄Ti₅-type structures, transfer of valence electrons from cations to anions leads to the formation of halogen chains connected with other atoms only by ionic interaction and having one-dimensional electronic structure. The Peierls physics in the systems is confirmed by newly synthesized incommensurately modulated i-hP18-Na₄X₅ (X = I, Br, Cl) compounds, as well as by the discovered hP36 phases of Na₄Cl₅ and Na₄Br₅. Theoretical analysis suggest that at zero temperature, in agreement with what is expected for Peierls materials¹, the electron-phonon interactions destabilize the linear monoatomic metallic chains of halogen anions, leading to opening band gaps in the electronic structure. However, at finite temperature, anharmonic effects of lattice vibrations lead to stabilization of regular monoatomic chains of equidistant halogen anions, as experimentally observed in the hP18-Na₄X₅ polymorphs, closing the band gaps, and making the one-dimensional chains semi-metallic.

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Keywords— high-pressure crystallography, synthesis, in situ analysis, alkali metals halides

First-principles study of 4 at.% Pd-doped $\text{Al}_{13}\text{Fe}_4$

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Abstract

$\text{Al}_{13}\text{Fe}_4$ is a crystalline approximant to a decagonal quasicrystal containing numerous crystallographically inequivalent atomic sites in its monoclinic (mC102) unit cell [1]. Recently, it has been proposed as a platform for single-atom catalysts by adding trace amounts of catalytically active elements such as Pt and Pd [2,3]. The catalytic activity of 1–10 at.% Pd-doped $\text{Al}_{13}\text{Fe}_4$ for acetylene semihydrogenation has been experimentally investigated [3]. It was found that catalytic activity improved with increasing Pd content from 1 to 4 at.% and that the crystal structure underwent a transition from monoclinic to orthorhombic. In this study, we focused on 4 at.% Pd-doped $\text{Al}_{13}\text{Fe}_4$, which exhibited the highest activity, and used first-principles calculations to investigate the Pd substitution sites in both the monoclinic and orthorhombic phases.

The calculations were performed using the Vienna Ab initio Simulation Package (VASP). The projector-augmented-wave (PAW) method was used to describe the interaction between electrons and ionic cores, and the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation was used for the exchange-correlation functional. The cutoff energy for the plane-wave expansion was set to 350 eV. Sugiyama et al. reported that single-crystal X-ray diffraction of $\text{Al}_{13}\text{Fe}_4$ doped with approximately 4 at.% Pd revealed that Pd occupies the Fe(4) site in orthorhombic $\text{Al}_{13}\text{Fe}_4$ [4]. Both monoclinic and orthorhombic $\text{Al}_{13}\text{Fe}_4$ have 20 crystallographically inequivalent sites, namely Fe(1)–(5) and Al(1)–(15). Accordingly, 4 at.% Pd doping corresponds to substituting approximately 4 atoms per unit cell in the monoclinic phase and approximately 8 atoms per unit cell in the orthorhombic phase with Pd. In this study, all Pd substitutions were carried out at the same crystallographic site. Consequently, the Al(7) site in the monoclinic phase was excluded due to its multiplicity of 2, which is insufficient to accommodate the approximately 4 Pd atoms required per unit cell. A thermodynamic convex hull for the Al-Fe-Pd ternary system was constructed using the calculated formation enthalpies for Pd substitution at each site, together with structural data obtained from the Materials Project [5].

In the orthorhombic phase, the Al(15) site was the most energetically favorable for Pd substitution among Al sites, while the Fe(4) site was the most favorable among Fe sites. In the monoclinic phase, Pd substitution was energetically favorable at the Al(14) and Fe(1) sites. Further analysis using the thermodynamic convex hull revealed that the orthorhombic structure with Pd at the Fe(4) site is thermodynamically stable. This result is consistent with the experimental finding of Sugiyama et al. that Pd partially occupies the Fe(4) site in the orthorhombic phase [4].

Previous studies have reported that, in monoclinic $\text{Al}_{13}\text{Fe}_4$, the Fe(1) site has the largest Voronoi cell volume and that Pd, which has a larger atomic radius than Fe, preferentially occupies the Fe(1) site [3]. Applying a similar argument to the orthorhombic phase, we found that the Fe(4) site also has the largest Voronoi cell volume. In future studies, the stabilization mechanism of the Fe(4) site in the orthorhombic phase will be investigated from an electronic-structure perspective.

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Keywords— $\text{Al}_{13}\text{Fe}_4$, Pd single-atom catalyst, periodic approximant, DFT calculation, thermodynamic stability, acetylene semihydrogenation

Multi-descriptor analysis based on HYPOD-X, an open database of quasicrystals and approximants

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Abstract

Quasicrystals (QCs) and approximant crystals (ACs) are structurally related complex materials. We introduce HYPOD-X (Hypermaterials Open Datasets for X; HMs = QCs + ACs) [1] and demonstrate its application to a multi-descriptor analysis comparing HM compositions with ordinary crystal (OC) compositions derived from the Materials Project [2]. HYPOD-X includes a composition dataset (1,064 entries), a phase-region dataset covering 43 Al-based ternary systems, and a temperature-dependent properties dataset of 1,449 curves. The datasets were curated through manual and semi-manual extraction with expert supervision to ensure data quality (Fig. 1). Building on this resource, we carried out a multi-descriptor analysis, a generalization of the classical e/a approach [3], across eight element systems. For 59 weighted-average elemental descriptors (58 from XenonPy [4–6] plus e/a), we evaluated HM–OC differences using the Mann-Whitney U statistic, expressed as a z -value with FDR correction, where larger $|z|$ indicates a larger shift between the HM and OC distributions. We then combined this with a KDE-based score, where a higher score indicates a clearer and sharper peak for HMs than for OCs. These two measures were integrated into a quadrant classification, in which descriptors with both high $|z|$ and high score were identified as the informative descriptors for distinguishing HMs from OCs. The analysis suggests that polarizability-related and size-related descriptors, along with the Mendeleev number, tend to differ between HMs and OCs across multiple element systems. We expect HYPOD-X to serve as a shared foundation for data-driven research on quasicrystals and approximants.

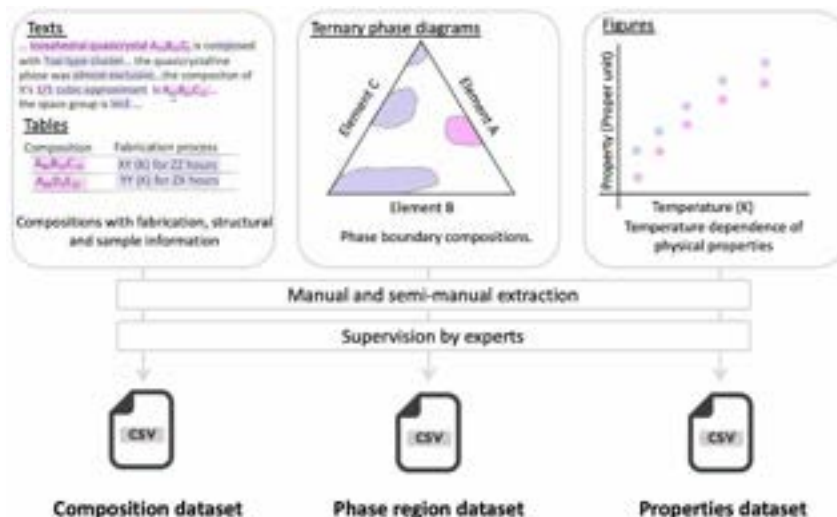


Fig.1 Workflow for extracting data from journal articles.

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Keywords— experimental dataset, materials science, data science

Wide e/a Control in Tsai-Type Approximants by Heterovalent Substitution

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Abstract

Quasicrystals (QCs) constitute a class of aperiodic crystals that exhibit long-range order without translational periodicity, often characterized by non-crystallographic rotational symmetries such as fivefold symmetry^[1]. Their periodic counterparts, known as approximant crystals (ACs), share identical local environments with QCs and provide a powerful platform for exploring unconventional physical phenomena in these complex structures.

Recently, a new materials design strategy based on heterovalent substitution has been established in Ga-Pt-Gd ACs, whereby trivalent Ga and zerovalent Pt are partially replaced by monovalent Au, resulting in quaternary Ga-Pt-Au-Gd ACs with a significantly extended electron-per-atom (e/a) ratio over a wide range (≈ 1.5 -2.0) without altering the underlying crystallographic symmetry^[2].

In the present study, we extend this strategy and reports the discovery of a new family of quaternary Tsai-type ACs by introducing tetravalent Sn and monovalent Au into the original Ga-(Pd,Pt)-Y 2/1 ACs containing non-magnetic Y. The effectiveness of substitution depends on the alloy system, leading to distinct structural evolution in the Ga-Pd-Y and Ga-Pt-Y systems, including a transition from the 2/1 AC to the 1/1 AC phase. As shown in Fig. 1, powder X-ray diffraction patterns confirm the formation of highly pure quaternary 1/1 ACs for representative compositions. These results demonstrate that heterovalent substitution provides a viable route to control both electron concentration and crystal structure in Tsai-type ACs. At the conference, we will present detailed structural analysis of these transformations and discuss how heterovalent substitution affects the physical properties.

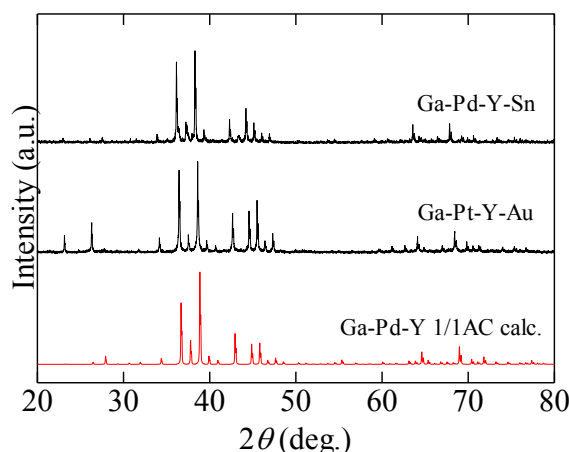


Figure 1: Powder X-ray diffraction patterns of representative synthesized samples with nominal compositions $\text{Ga}_{25.3}\text{Pd}_{35.2}\text{Y}_{14.5}\text{Sn}_{25.0}$ and $\text{Ga}_{44.0}\text{Pt}_{22.0}\text{Y}_{14.0}\text{Au}_{20.0}$. The calculated pattern of Ga-Pd-Y 1/1 AC is shown at the bottom.

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Keywords— quasicrystals, approximant crystal, Tsai-type compounds, physical properties

New opportunities on the studies of condensed matter systems under extreme conditions at the ESRF-EBS

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In the last decades, we have witnessed an unprecedented surge in high-pressure research that has greatly improved our fundamental understanding of materials under high compression. The X-ray investigations of matter under extreme conditions has become one of the major activities at the ESRF and other 3rd generation synchrotron sources. The array of techniques includes X ray diffraction, Inelastic X-ray Scattering, Nuclear Inelastic Scattering, X ray absorption and emission spectroscopy, X ray magnetic circular dichroism, X-ray Compton scattering, X-ray magnetic scattering, among many others. As a direct consequence, many scientific breakthroughs have been achieved across fields ranging from fundamental physics to Earth and planetary sciences, chemistry and materials research, and extending into biophysics/biochemistry including questions concerning life and biological function under extreme conditions. Since August 2020, the new ESRF-EBS (extremely brilliant source) opened to the user community a new generation of synchrotron light source with unprecedented characteristics. In particular, the crystallography beamlines dedicated to the studies of materials under extreme conditions (ID15B and ID27) benefit enormously of the beam focusing capabilities and the coherent fraction.

In this presentation, the new capabilities available on the newly upgraded ID15B and ID27 will be presented. Also, the strengthen of the user support capabilities on the High-pressure laboratory allow to prepare the most challenging crystallographic studies under extreme pressure ($P < 2\text{Mbar}$) and temperature ($3\text{K} < T < 1000\text{K}$) conditions.

We will discuss particular scientific problems regarding the studies of compounds with charge density in function of high pressure and at low temperature. Finally, the possibilities of collaborations and discussions on possible future beamtime access will be introduced.

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Keywords— single crystal XRD, extreme conditions

First-Principles and Machine Learning Investigation of Adsorption and Hydrogen Dissociation on Graphene-Supported Single-Atom Catalysts

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Abstract

Nitrogen-doped graphene single-atom catalysts (SACs) have shown remarkable promise in selective hydrogenation and hydrogen storage. However, the rationalization of hydrogenation reaction in these systems is still challenging. In this paper, by systematically calculating hydrogen adsorption and dissociation energies on active 3-fold sites $M-C_{3-x}N_x$, with x ranging from 0 to 3 and with $M = Co, Ni, Pd$, we show that hydrogen dissociation is endothermic – except for $Pd-N_3$ and $Pd-CN_2$ – and proceeds via two distinct mechanisms (Fig. 1a), depending on the nitrogen content of the site.[1] Furthermore, by expanding the range of transition metals tested and employing an interpretable machine learning algorithm (SISSO, Fig. 1b), we rationalize the influence of N-doping on the adsorption energies of small molecules (H_2 , C_4H_6 , C_4H_8 , N_2 , NH_3 , CO).[2] This study provides a comprehensive understanding of adsorption and hydrogen dissociation on graphene SACs, paving the way for the design of catalysts tailored to specific applications.

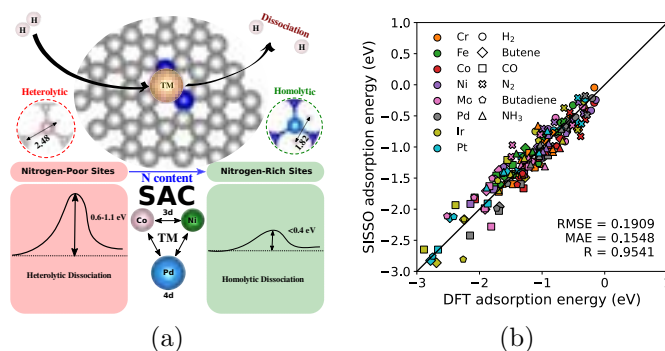


Figure 1: (a) Scheme for H_2 dissociation on M-N-C (b) Parity plot : SISSO prediction versus DFT.

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Keywords— Density Functional Theory, Interpretable Machine Learning, Single Atom Catalyst

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Creation of novel catalyst materials utilizing phason engineering

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Abstract

The objective of this research is to create novel catalytic materials and express novel functions through phason engineering. We investigated the catalytic properties of various Al-based crystals and approximate crystalline alloys by (1) introducing discrete phason strain through compositional control, and (2) doping with catalytically active elements (Pt, Pd, Ni) utilizing "non-equivalent sites" (comparing properties with existing conventional catalysts).

For catalytic property evaluation, we used industrially significant C₂H₂ selective hydrogenation (C₂H₂ + H₂ → C₂H₄) as a probe reaction to verify the effect of phason strain on catalytic properties. Regarding (1), we successfully fabricated quasicrystals (IQC), approximate crystals (P₄₀, C₁ phase), and crystals (ε, β' phase) in Al-Pd-Ru alloys. Comparison of their catalytic properties revealed that Pd contributes to activity and Ru contributes to selectivity [1]. Furthermore, it was found that for small molecules such as C₂H₂, the effect of local structure (ensemble sites) is greater than that of phason strain (arrangement of *m*BC and *p*MC). In addition, regarding (2), we succeeded in developing a novel 'single atom' catalyst material by utilizing the 'non-equivalent sites' of quasicrystals and approximate crystals, which are a characteristic of phason engineering. In particular, we found that extremely high selective hydrogenation ability for C₂H₂ was exhibited by doping Pd with Al₁₃Fe₄, one of the quasicrystal-related materials (Al₁₃Fe₄-Pd) as a platform. Theoretical calculations on the surface structure (thermodynamic convex hull, simulated cleavage method) suggested that the isolated dispersion of Pd atoms forms 'ensemble (geometric atom group) sites' that play an important role in activity [2].

This research was supported by JST CREST (JPMJCR22O3).

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Keywords— Quasicrystal-Approximant catalysts, C₂H₂ semi-hydrogenation, phason engineering

Thermodynamic Evidence for Multiple Field-Induced Phases in a Slightly Distorted Kagome Antiferromagnet

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Abstract

Frustrated kagome antiferromagnets are predicted to host exotic field-induced quantum phases, yet experimental identification of their thermodynamic signatures remains challenging. We combined specific heat and ultrasound measurements up to 36 T and down to 0.5 K to map the H-T phase diagram of the slightly distorted kagome magnet $\text{Y}_3\text{Cu}_9(\text{OH})_{19}\text{Cl}_8$ [1]. We show [2] that the suppression of long-range antiferromagnetic order with field coincides with the onset of the unconventional 1/6 magnetization plateau previously observed in this system, establishing a connection between magnetic order and fractional plateau formation. Our measurements confirm the opening of a spin gap ~ 3.5 K within the plateau and provide evidence for an additional low-energy excitation channel not coupled to lattice strain. Beyond the plateau, a further compressible phase emerges consistent with the supersolid state predicted by T. Picot *et al.* [3] hence revealing an unexpectedly rich sequence of field-induced phases in this quantum magnet.

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Keywords— magnetic orders, frustration, thermodynamic measurements

Investigations on Xanthine Solid State

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Abstract

Introduction

Xanthine is a pigment belonging to the purine family. It is a substance resulting from the metabolism of purine bases (adenine, guanine, and hypoxanthine). It is converted into uric acid by the action of xanthine oxidase. Methylxanthines such as caffeine, theophylline, and theobromine are commonly used as mild stimulants and for their bronchodilator properties, particularly in the treatment of asthma. Some animals used its high refractive index in a particular direction (100 plane, $n = 1.83$) and microstructure for camouflage or for reflecting photons onto ocular detectors [1].

Its crystal structure has been recently resolved [2] but its XRPD pattern shows an unusual ‘hump’ between 13° and ca. 30° (2 θ scale with Cu anode). This could be due to a single or a mix of the following reasons: presence of an amorphous part, extensive presence of defects [3], dynamic disorder just like in caffeine [4], static disorder, polytypism [5] or chemical impurities. The crystal structure shows no sign of extensive disorder and long maturation at high temperature in different solvents -supposed to get rid of fines and amorphous particles- did not change the XRPD pattern. Just may be 10% of the hydrogen atoms could lead to tautomerism and this is not enough to justify the anomaly of the XRPD pattern. Thus, we launched a collaborative study to understand the Xanthine (XT hereafter) solid state.

Results

The first step was to investigate a potential bias of the apparatus, but we demonstrated that for two other solid phases of xanthine (Na₂Xanthine-5H₂O & Na-Xanthine – 4H₂O) with the same data collection and data processing there is no physical problem with the diffractometer in the range 13° - 40° (2 θ scale). Pure xanthine is the only

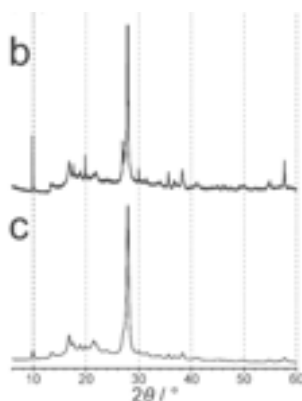


Figure 1: XRPD pattern of pure xanthine (b) with synchrotron radiation and (c) from single crystal diffraction

solid showing this “hump” on XRPD pattern (see figure below (b) with synchrotron radiation and (c) from single crystal diffraction). In order to investigate furthermore the xanthine solid-state, High-Energy Milling (HEM) has been applied at RT for 12 hours. The XRPD pattern became simply two broad peaks of low intensity centered at 14° and 28° (2 θ scale with Cu anode). The relaxation pathways at 5K/min depend on the presence of minute amount of water or not. Without drying, there are 2 exothermic events: one broad $\Delta H = -4\text{J/g}$ between 60 and 105°C and one sharp at 110°-120°C $\Delta H = -30\text{J/g}$, followed by a single endothermic event between: 120 and 145°C. With a preliminary drying at 80°C for 30 minutes, two well separated exothermic peaks are observed one centered at 150°C $\Delta H = -60\text{J/g}$ and a second one centered at 220°C $\Delta H = -30\text{J/g}$. They correspond to two sequences in recovery of crystallinity as demonstrated by temperature resolved XRPD (with a much slower average heating rate): at 150°C it is at

rather medium range, at 220°C it is at rather short range. In both cases, the ‘hump’ in the XRPD pattern remains unaffected.

Even though xanthine was put at high temperatures or was purified several times by recrystallization of its double and single sodium salt, the ‘hump’ on XRPD pattern did not disappear nor even decrease.

Although small, simple and rigid, xanthine molecules exhibit a complex solid state - including polytypism - whose understanding is a real challenge (5). The high-resolution SEM photo below shows the stacking of domains of ca 50-70 nm thickness consistent with polytypism.

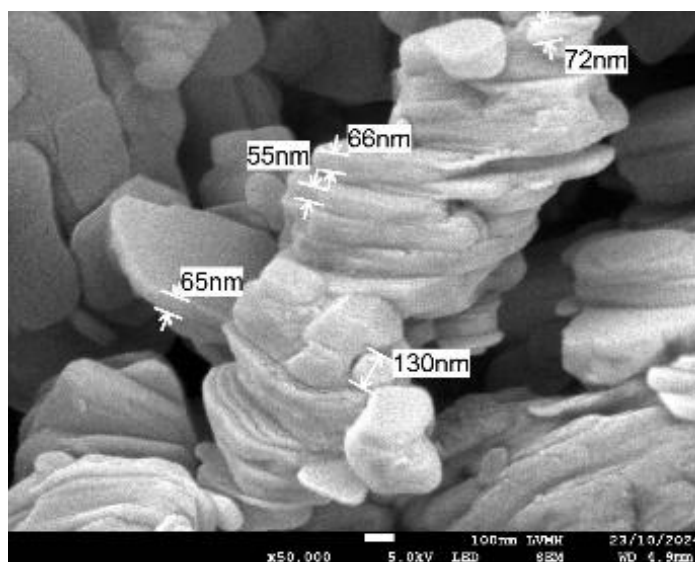


Figure 2: SEM photo of pure xanthine

Xanthine could also be a candidate for an orientational disorder phase associated with different tautomeric forms.

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Keywords— Xanthine, XRPD, Solid State, Disorder, High-Energy Milling, Crystallinity, Polytypism.

Study of Short-Range Order in TiVCr-Based Multiple Principal Element Alloys for Hydrogen Storage

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Abstract

Multiple principal element alloys (MPEAs) - composed of three or more elements with comparable concentrations - form stable single-phase solid solutions with simple crystal structures. Their stability arises from the balance between a high configurational entropy, which favors structural disorder, and enthalpy effects, which promote atomic ordering [1]. TiVCr-based MPEAs crystallize as body-centered cubic solid solutions in which the constituent atoms randomly occupy the 2a sites. However, atomic size mismatches and differences in bonding enthalpies between the elements give rise to short-range order (SRO). The local chemical correlations and concentration fluctuations may influence both the interaction of molecular H₂ with the alloy surface and the diffusion of atomic hydrogen, which are key processes governing hydrogen sorption and storage properties.

We have synthesized TiVCr-based MPEAs containing controlled additions of Mn, Fe, or both (up to 8 at.%), which exhibit remarkable hydrogen absorption and desorption behavior at room temperature, with equilibrium pressures above 1.5 bar and total hydrogen storage capacities ranging from 2.4 to 3.2 wt. %. In this work, we present the characterization of hydrided and dehydrided alloys using complementary techniques to elucidate the local atomic arrangement: (1) X-Ray total scattering combined with pair distribution analysis, (2) aberration-corrected high-angle annular dark-field scanning transmission electron microscopy coupled with atomic-resolution energy-dispersive X-ray spectroscopy mapping, and (3) neutron powder diffraction.

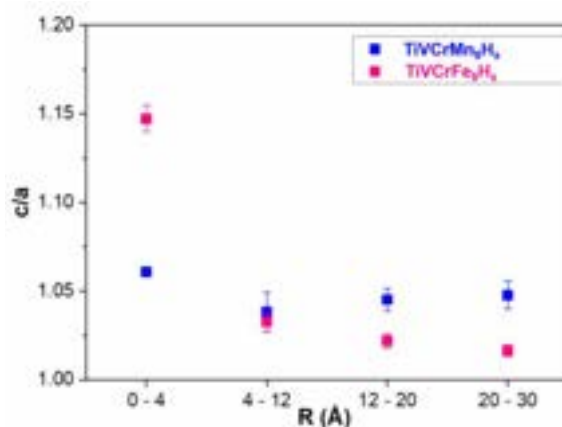


Figure 1: Evolution of the tetragonal distortion (c/a) as a function of R range in two hydrided MPEAs.

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Keywords— Multiple Principal Element Alloys, Short Range Order, Pair Distribution Function

Detecting dislocations using Bragg-peak vortices

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Abstract

We introduce a new Fourier-based method to characterize edge dislocations in two-dimensional quasicrystals, and apply it to the analysis of scanning tunneling microscopy (STM) data of dodecagonal Ba-Ti-O. The central result is that edge dislocations possess a distinct reciprocal-space signature consisting of Bragg peaks with winding complex-valued vortex-like profiles. We establish analytically, numerically, and experimentally that these Bragg-peak vortices encode the same topological information as the winding numbers used to define the Burgers vector of the dislocation. This reciprocal-space signature provides a simple and robust method for locating and classifying dislocations directly from local atomic-position data, without requiring an explicit tiling construction and a real-space tracing of a Burgers loop. This provides a practical framework for analyzing dislocations in both quasiperiodic and periodic crystals.

High-pressure synthesis of $Al_{11}Fe_4$ and its DFT-assisted structure refinement

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Abstract

High-pressure sintering (HPS) of $Al_{4.2}Fe$ composition at 6 GPa yields two new variants of the Al_5Fe_2 phase featuring channels with highly mobile Al atoms down to low temperatures. Upon quenching from 800 C, the channel-Al atoms freeze into previously unobserved structures characterized by Pearson symbols mC30 and oF120, with the same $Al_{11}Fe_4$ composition. High-pressure density-functional (DFT) molecular-dynamics study confirms the mC30 structure, while oF120 sub-phase is reinterpreted as a tweed-like coherent superposition of the triclinic aP15 domains.

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Collinear spin nematic phase in the breathing pyrochlore spinel



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Abstract

The combination of magnetic frustration and strong spin-lattice coupling can lead to a wide variety of novel magneto-structural behaviours. This is exemplified by the breathing pyrochlore spinels $\text{LiGa}_x\text{In}_{1-x}\text{Cr}_4\text{O}_8$, where the end-member compounds ($x = 0$ and $x = 1$) exhibit complex sequences of magnetic and structural phase transitions [1]. Here, we show that replacing 5% Ga with In ($x = 0.05$) suppresses this complexity, leaving only a single, apparently second order, transition. A combination of neutron diffraction and NMR allows us to identify the low-temperature state with a collinear nematic state (also known as antiferromagnetic spin ice) associated with an effective biquadratic spin-lattice coupling term [2]. Reverse Monte Carlo analysis of the diffuse magnetic neutron scattering indicates the presence of both Coulomb-like spin correlations at high temperature, and short range order between collinear local spin configurations at low temperature. The dynamical structure factor as probed by inelastic neutron scattering features a continuum centred around the (200) position, with a broad maximum at around 6 meV [3]. Landau-Lifshitz spin dynamics simulations combined with linear spin wave theory reveal that the latter is associated with ferromagnetic loop dynamics lifted to finite energy transfer by the biquadratic term [4].

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Keywords— frustrated magnetism, nematic order, spin ice

Crystal field and spin fluctuation in heavily doped nickelates

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Abstract

Hole-doped nickelates, isostructural to cuprates, are a strongly correlated electron system that exhibits charge order as well as peculiar spin dynamics associated with the doping level. The hole doping can be made with introduction of cations like Sr (quenched disorder), by oxygen overstoichiometry (annealed disorder) or both. The interest in focusing on O doped samples is the unique coexistence of 3D modulated spin and oxygen ordering. Such coexistence might support the picture of pinning the magnetic to the oxygen order in oxygen-doped samples. This would also imply that the quasi-2D nature of the spin correlations might not be the optimal model for heavily oxygen-doped nickelates.

In this study we present the latest result of our triple axis neutron spectroscopy investigation of crystal field and spin order and dynamics in A_2NiO_{4+d} samples (with $A=Nd, Pr$, $d=0.25$ or 0.23). The spin fluctuations were followed along the layers' plane, as well as out of plane and both revealed an evident dispersion with corresponding coupling strength much closer that what found at lower doping. The analysis in function of temperature also highlighted a marked difference between the onset of spin fluctuations and spin order as well as their intensity evolution. Crystal field analysis showed also a clear dependence of the energy of first CEF transition with respect to the O content (Figure 1) [1]. The strongly oxygen doped phase, bringing (ordered) interstitial oxygen in between NiO planes influences the 3D magnetic order, as well as CEF levels, and lattice order and dynamics [2]. The overall scenario seems supporting the picture of pinning the magnetic to the oxygen order in oxygen-doped samples.

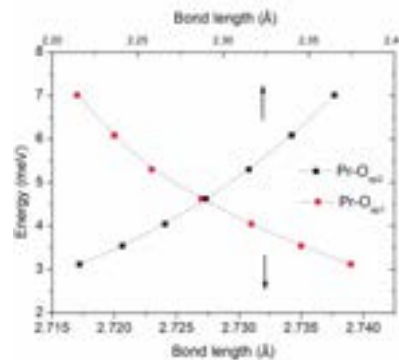


Figure 1: Trend of first CEF level energy obtained through point charge model calculations by varying the atomic positions of O_{ap} . From [1]

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Keywords— oxygen doping, oxygen superstructure, CEF-spin wave interaction

Understanding disordered structures: a paradigm shift due to Reverse Monte Carlo modeling

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Reverse Monte Carlo (RMC) [1] is a computer modeling tool that enables one to create large scale, three dimensional structural models, containing many thousands of atomic coordinates. These structural models are consistent, within errors, with experimental data from neutron and X-ray diffraction, EXAFS and anomalous X-ray scattering (AXS). The latest versions of the RMC computer code [2] make it possible to also include various constraints on, e.g., coordination numbers and angular distributions, as well as the simultaneous use of interaction potentials.

The appearance of RMC modeling has initially ignited hot debates concerning its usefulness, and indeed, even its validity – most notably, due to the ‘problem’ of ‘non-uniqueness’ of the structural models. I will discuss this issue in some detail and (try to...) demonstrate that ‘non-uniqueness’ is not a problem with RMC modeling, but the natural consequence of the fact that diffraction data on disordered materials contain direct information on two-body correlations only. RMC modeling has just remained an innocent victim that (unfortunately ?) is able to generate a multitude of structures that are equally consistent with a given set of experimental data.

In the summarizing part of the presentation, it will be shown how, over the years, Reverse Monte Carlo modeling (or, in a wider context, the need for creating a structural model) has changed the way of interpreting liquid/amorphous diffraction (and EXAFS, AXS) data -- so much that RMC has become indispensable for the purpose, particularly for multi-component systems.

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Keywords— liquid structure, amorphous structure, Reverse Monte Carlo

Tracing the Horizon of Tetragonal–Monoclinic distortion in trilayer nickelate $\text{La}_4\text{Ni}_3\text{O}_{10}$

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Abstract

Since the inception of research on superconductivity in the trilayer nickelate $\text{La}_4\text{Ni}_3\text{O}_{10}$, its structural symmetry has remained ambiguous. At ambient conditions, $\text{La}_4\text{Ni}_3\text{O}_{10}$ stabilizes in a twinned monoclinic structure ($P2_1/c$). Upon heating, it undergoes a transition to a tetragonal $I4/mmm$ phase at $T_s \approx 1030$ K [1], while a distinct low-temperature transition associated with density-wave (DW) ordering emerges below $T_{DW} \approx 135$ K [2]. Although previous reports suggested the presence of an intermediate orthorhombic phase [3], we find that the transition proceeds directly from the tetragonal to the monoclinic structure, forming a twofold superstructure. This is shown from the pressure–temperature phase diagram and supported by *ab-initio* density-functional theory calculations [4]. Furthermore, employing X-ray diffraction we report the first observation of incommensurate satellite reflections associated with DW ordering in flux-grown samples, extending earlier observations that were limited to floating-zone crystals. Raman spectroscopy corroborates the observation. Additional phonon modes below 130 K, suggest a breaking of monoclinic $P2_1/c$ symmetry.

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Keywords — Nickelates, High-pressure crystallography, Density-wave ordering

DFT analysis of pentacene adsorption on the surfaces of the Tsai-type Ag-In-Yb quasicrystal

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Abstract

Molecular adsorption on quasicrystal (QC) surfaces has attracted attention due to its potential for fabricating molecular materials with properties arising from quasicrystalline ordering. In recent years, scanning tunneling microscopy (STM) experiments have demonstrated that pentacene (Pn) molecules adopt positions and orientations on the twofold and fivefold surfaces of the Tsai-type Ag-In-Yb QC that are consistent with substrate ordering [1, 2].

We previously examined Pn adsorption on the twofold surface of the Tsai-type Ag-In-Yb QC using density functional theory (DFT) calculations [3], and subsequently investigated Pn adsorption on the fivefold surface. The QC surfaces were approximated using a disk-shaped cluster, and the adsorption energies of a single Pn molecule at various surface positions were calculated. The Tsai-type QC surface contains sites composed of acute rhombohedron units [4]. On both surfaces, the stable adsorption sites obtained from calculations correspond to these sites. However, the obtained adsorption configurations are not fully consistent with the Pn molecular arrangements observed in STM experiments [1, 2]. This discrepancy could stem from computational errors arising from approximating the QC surfaces with a disk-shaped cluster and an insufficient consideration of atomic defects on the QC surfaces.

In our subsequent work, therefore, the applicability of the cluster approximation in DFT calculations was examined by comparing it with the repeated slab model. The stability of the Pn molecule on the Cu(111) surface was evaluated as a benchmark system. We found that the cluster approximation yielded accuracy comparable to that of the slab model in predicting stable adsorption positions along the surface-parallel direction [5]. In this presentation, we report our recent investigation of atomic defects on the fivefold Tsai-type Ag-In-Yb QC surface by evaluating the desorption energies of surface atoms. The stable adsorption configurations of the Pn molecule on surfaces containing atomic defects were also analyzed. We will discuss the factors responsible for the discrepancy between our previous theoretical predictions and experimental observations of Pn adsorption on the QC surfaces [1, 2].

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Keywords— quasicrystal, pentacene, density functional theory calculation, surface, adsorption

Numerical Study of the NMR Coherence Peak in Quasicrystalline Superconductors

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Abstract

Since the discovery of quasicrystals by Shechtman *et al.* in 1984, their unique electronic properties have attracted significant attention in condensed matter physics. Recently, the second quasicrystalline superconductor, Ta_{1.6}Te, was discovered[1], and intensive research is underway to understand the unique physical properties of this superconductor. Notably, NMR experiments on this material have revealed that the height of the NMR coherence peak deviates from the behavior expected by the BCS theory[2].

In this study, we numerically investigate the nuclear spin-lattice relaxation rate $1/T_1$ using the real-space BdG equations on a Penrose lattice, considering the attractive Hubbard model. Our results confirm that the NMR coherence peak appears just below the superconducting transition temperature T_c even in the quasiperiodic model. However, a comparative analysis with a square lattice over a wide range of parameters reveals that differences arise in the height and shape of the NMR coherence peak. For instance, Fig.1(a) shows the results for the case of $U = 3.0$ at quarter-filling($n = 0.5$). To elucidate the origin of these differences, we further analyze the relationship between the spatial distribution of the local relaxation rates [Fig.1(b)] and the local density of states (LDOS).

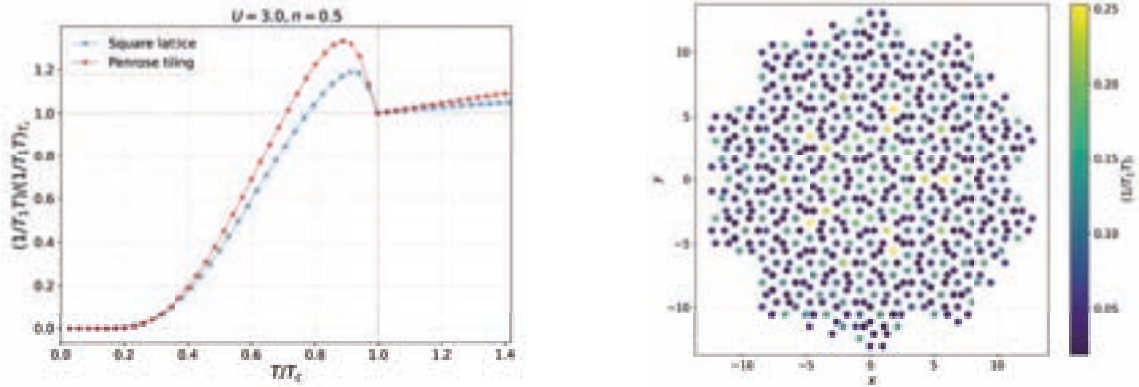


Figure 1: (a) Calculated temperature dependence of relaxation rate for the square and Penrose lattices($U = 3.0$, $n = 0.5$). (b) Spatial distribution of the local relaxation rate on the Penrose lattice at $T/T_c = 0.886$.

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Keywords— Quasicrystal, Superconductivity, Nuclear Magnetic Resonance (NMR), NMR coherence peak

Formation of Mn-based dodecagonal quasicrystals

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Quasicrystals are ordered matters characterized by quasiperiodicity and rotational symmetries that are forbidden in conventional crystals. Recently, the discovery of superconductivity in the Ta-Te dodecagonal quasicrystal, a two-dimensional system, has drawn significant attention to the structure and physical properties of dodecagonal quasicrystals [1]. In metallic alloys, reports of dodecagonal quasicrystals have been limited since their initial discovery in Ni-Cr particles in 1985 [2]; examples include melt-spun V-Ni(-Si) thin films [3], Mn-Cr-Ni-Si ingots [4], and Mn-Cr-Ni-Si-Al found in fulgurites [5]. Among these, the Mn-Cr-Ni-Si dodecagonal quasicrystal is the only one confirmed to exist in bulk alloys. Furthermore, this Mn-Cr-Ni-Si quasicrystal is unique as the only Mn-based quasicrystal—containing 50 at.% or more of Mn—among more than 100 quasicrystalline alloys reported to date. Given that manganese is known to exhibit a wide variety of magnetic behaviors in its elemental, alloyed, and compound forms, the magnetic properties of this system are of great interest. However, no studies on its physical properties have been conducted because single-phase samples of the Mn-based quasicrystal have not yet been obtained. Therefore, the objective of this study is to fabricate single-phase samples of the Mn-Cr-Ni-Si dodecagonal quasicrystal through the exploration of various alloy synthesis processes.

Starting with the composition $\text{Mn}_{72.0}\text{Cr}_{5.5}\text{Ni}_{5.0}\text{Si}_{17.5}$ reported by Ishimasa et al. [4], alloys of various compositions were prepared by arc melting in an argon atmosphere. For some of the prepared alloys, ribbon samples were fabricated using the single-roller melt-spinning technique. The arc-melted ingots and melt-spun ribbons were sealed in evacuated quartz tubes and subjected to appropriate heat treatments. All samples were characterized by powder X-ray diffraction (XRD). For selected samples, microstructural observation and compositional analysis were performed using scanning electron microscopy (SEM) equipped with energy-dispersive X-ray spectroscopy (EDS).

Currently, we are exploring the optimal conditions for both alloy composition and fabrication processes. Our results to date have confirmed an increase in the volume fraction of the quasicrystalline phase compared to previous studies. In this presentation, we will report the details of the fabrication processes and sample characterization, and discuss the formation conditions of the Mn-based dodecagonal quasicrystal.

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Keywords— dodecagonal quasicrystals, Mn-based alloys, formation conditions, synthesis

Search for Superconductivity in Os-Based Decagonal Hypermaterials

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Abstract

Materials possessing higher-dimensional periodic structures, including quasicrystals and their approximants, are referred to as hypermaterials (HM). Several HMs exhibiting superconductivity have been reported. Among them, the dodecagonal quasicrystal in the Ta–Te system exhibits high thermal stability and a relatively high superconducting transition temperature (T_c)^[1]. These characteristics have stimulated increasing interest in superconductivity in HMs with quasiperiodicity in two dimensions. Recently, superconductivity was observed for the first time in a decagonal HM in the approximant crystal $\text{Al}_{13}\text{Os}_4$. This compound is stable in air and exhibits a T_c of 5.45 K^[2], the highest reported among known HMs. These features enable precise physical property measurements that were difficult in previously reported superconducting HMs, further increasing interest in decagonal HMs.

However, in the Os-based system, reproducible preparation of high-quality superconducting decagonal HMs has not yet been achieved. In previous studies, synthesis conditions were not described in detail, and the compositional conditions required to obtain single-phase samples remain unclear. In addition, the Al–Os binary phase diagram is not well established, limiting guidelines for composition control and heat-treatment conditions.

In this study, we explore compositions in the Os-based decagonal HM system. We identify the optimal composition for obtaining the approximant phase and examine the thermal stability and superconducting properties of selected samples. In this presentation, we will report the details of sample preparation using arc melting and melt spinning, as well as the effects of heat treatment and the results of magnetization measurements.

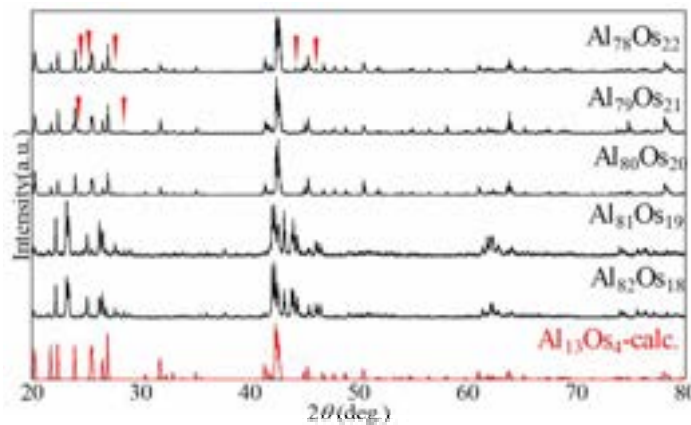


Figure 1: Powder XRD pattern of Al-Os samples after annealed

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Keywords— superconductivity, decagonal, Os-Based

Magnetism of Tsai-type Icosahedral Quasicrystals

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Abstract

Icosahedral quasicrystals were long believed to be unfavorable for long-range magnetic order owing to strong geometric frustration and aperiodicity. Recent studies on Tsai-type approximant crystals and quasicrystals, however, have demonstrated that quasiperiodic magnetism can be systematically designed through electron-mediated RKKY interactions and valence electron concentration (e/a) control [1]. In particular, composition-tunable ferromagnetic icosahedral quasicrystals with high phase purity have established ferromagnetism as an intrinsic bulk property of quasiperiodic matter [2]. Furthermore, bulk and annealable ferromagnetic quasicrystals have enabled quantitative investigations of intrinsic magnetic criticality inaccessible in metastable rapidly quenched quasicrystals [3]. These studies reveal unconventional critical behavior arising from the interplay between quasiperiodicity, long-range RKKY interactions, and spin anisotropy. Together with recent discoveries of antiferromagnetic order [4] and noncollinear spin structures, these findings establish quasiperiodic magnetism as a designable class of magnetic matter and open new perspectives on exotic magnetic textures and unconventional critical phenomena unique to quasiperiodic systems.

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Keywords— quasicrystal, approximant, magnetism

Structure and magnetism of a new phase in the Ga–Pd–Tb system

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Abstract

In rare-earth (RE) intermetallic compounds, the interplay between crystal structure and magnetism often leads to unconventional magnetic behavior. In layered RE systems in particular, the distinct atomic arrangements along the in-plane and out-of-plane directions give rise to strong magnetic anisotropy and complex magnetization processes, through anisotropic exchange interactions and crystalline electric field effects. Moreover, when structural modulation or disorder is present, the influence of such complex structural features on the resulting magnetic properties remains insufficiently understood.

We report the synthesis, crystal structure, and magnetic properties of a new Ga–Pd–Tb compound grown as single crystals by the Ga self-flux method. Single-crystal X-ray diffraction reveals that this phase adopts a layered structure in the space group R-3m. The Tb sites are partially occupied, and the Tb/Ga mixed layers exhibit structural modulation ^[1], as evidenced by satellite reflections and diffuse scattering. These structural features indicate the presence of multiple local environments for Tb ions, which may lead to non-uniform magnetic interactions.

Magnetization measurements show antiferromagnetic ordering below $T_N \approx 20$ K, together with a negative Weiss temperature. Under applied magnetic fields, the compound exhibits field-induced transitions, including a multi-step change in magnetization and pronounced hysteresis at low temperatures. These observations suggest that structural modulation and partial occupancy give rise to non-uniform magnetic interactions, which are likely responsible for the observed complex magnetic behavior.

This new Ga–Pd–Tb phase provides a platform for investigating how structural modulation and disorder influence magnetic properties in anisotropic rare-earth intermetallic systems. In this poster presentation, we will report on the detailed structural and magnetic properties of the new Ga–Pd–Tb phase, along with the results of the ongoing AC magnetization measurements.

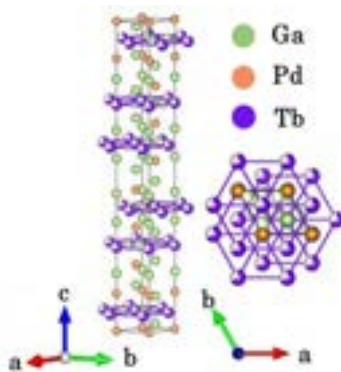


Figure 1: Crystal Structure of a new phase in the Ga–Pd–Tb system, represented by the VESTA software ^[2]. The Tb and Ga sites are partially occupied, respectively.

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Keywords— magnetism, layered structure, single crystal, anisotropy, structural analysis

Fabrication and superconductivity of Ta–TM–Te van der Waals layered quasicrystals

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Abstract

Ta–Te quasicrystals are dodecagonal quasicrystals. They are the only known van der Waals layered quasicrystals and the only transition-metal chalcogenide quasicrystals [1]. They are thermodynamically stable and allow the growth of large-grain single crystals. In 2024, our group discovered that Ta–Te quasicrystals undergo a superconducting transition at approximately 1 K [2]. This was the second reported superconducting quasicrystal. The first example, a metastable Al–Zn–Mg quasicrystal, exhibited a much lower transition temperature T_c of about 50 mK. Therefore, Ta–Te quasicrystals are currently the most experimentally accessible superconducting quasicrystals.

However, Ta–Te quasicrystals exhibit relatively broad quasiperiodic peaks in XRD patterns, indicating low quasiperiodic order. In general, quasicrystals with more constituent elements tend to better stabilize their intrinsic structure. Therefore, multicomponent substitution is expected to improve quasiperiodic order. It may also modify T_c . Expanding the material family is important for understanding superconductivity in quasicrystals.

In this study, we performed ternary substitution at the Ta site to improve structural quality and investigate trends in T_c . Polycrystalline samples were synthesized by reactive sintering. The nominal composition was $(\text{Ta}_{1-x}\text{X}_x)_2\text{Te}$ ($\text{X}=\text{Ti, Cu, Nb, Mo, Ag, In, Sb, Au}$; $x=0.05, 0.10$). Nb-substituted samples with $x = 0.15, 0.20$, and 0.30 were also prepared. The samples were labeled X-n% based on the nominal substitution level. I_2 was added as a reaction promoter. The mixtures were pressed into pellets and heat-treated.

Two heat-treatment methods were employed. Low-temperature sintering was performed in evacuated quartz tubes at 1000 °C. High-temperature sintering was carried out in Mo crucibles, which were arc-melted under an Ar atmosphere, using a two-step heat treatment, with an initial step at 1100 °C followed by heating up to 1400 °C. Low-temperature sintering was used for all elements except Nb and for Nb5%–Nb20%. High-temperature sintering was applied to additional Nb20% and Nb30% samples. Phase identification was performed by powder XRD. Electrical resistivity was measured by a four-probe method from 0.4 to 300 K for single-phase samples.

XRD results showed that Mo- and Au-substituted samples contained impurity phases. Cu-, Ag-, In-, and Sb-substituted samples were single-phase at 5% substitution but contained impurity phases at 10%. Ti-substituted samples remained single-phase up to 10%. Nb-substituted samples remained single-phase up to 15%, while Nb20% contained impurity phases under low-temperature sintering. These results indicate that Ti and Nb substitutions provide relatively wide single-phase regions. High-temperature sintering yielded single-phase samples for Nb20% and Nb30%. These results indicate that high-temperature sintering is effective for stabilizing single-phase samples at higher substitution levels, particularly for high-melting-point elements such as Nb. Furthermore, high-temperature samples exhibited narrower quasiperiodic peaks (smaller FWHM) than binary Ta–Te samples, suggesting improved quasiperiodic order due to Nb substitution and high-temperature sintering.

All samples exhibited superconducting transitions with zero resistance at low temperatures. The highest T_c was 1.35 K for Nb-30%, which is the highest T_c reported for superconducting quasicrystals. The variation of T_c will be discussed in detail together with specific heat measurements.

In conclusion, ternary substitution successfully expanded the material family of Ta–Te quasicrystals. The superconducting transition temperature depends on the substituted element. Nb substitution yielded the highest T_c of 1.35 K. High-temperature sintering enables an expanded single-phase region for high-melting-point elements. It also contributed to improved quasiperiodic order.

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Keywords— quasicrystal, experimental study, layer materials, superconductivity, elemental substitution effect

Atomistic Investigation of Martensitic Transformations in Cu-Based Shape Memory Alloys Using a Machine-Learned Interatomic Potential

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SIMaP, Grenoble INP - UGA, CNRS, Université Grenoble Alpes

Cu-based shape memory alloys are promising candidates for elastocaloric cooling due to their low cost, high thermal conductivity, and large reversible strain. Their functional behavior is governed by the stability of the high-temperature bcc-based phase and its transformation into martensitic structures. However, the atomic-scale relationship between chemical ordering in the bcc phase and subsequent martensitic transformation remains difficult to resolve. In this work, we train a machine-learned interatomic potential for Cu–Zn alloys using first-principles data covering disordered and ordered bcc configurations. We first examine chemical ordering in the bcc phase through atomistic simulations combined with Monte Carlo atom-swap sampling, identifying the evolution from disordered A2-like configurations toward ordered B2-like local environments. We then use large-scale molecular dynamics simulations to investigate temperature-induced and stress-induced martensitic transformations from the bcc-based austenite phase. The simulations capture the transformation into martensitic structures, as well as the reverse transformation upon heating or unloading, consistent with experimental observations. This work provides an atomistic framework for understanding how chemical order and mechanical or thermal driving forces influence martensitic transformation pathways in Cu–Zn shape memory alloys.

Hydrogen Absorption Behavior of Hypermaterials Containing Hydrogen-Affinity Elements

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Abstract

Hypermaterials refer to the substances such as quasicrystals and approximant crystals that can be uniformly described in a high-dimensional space [1]. Compared to conventional crystal structures, hypermaterials contain more interstitial tetragonal sites within their unit cells, and are believed to have the potential to absorb more hydrogen. It is also thought that the hydrogen absorption in hypermaterials can induce unique structural transformations and the formation of new hydrides. Some hypermaterials containing Ti, Zr, and Mg, which exhibit a high chemical affinity for hydrogen, have been reported to show promise for hydrogen storage, including Ti-Zr-Ni and Zn-Mg-Al quasicrystals [2,3]. However, hydrogen absorption behavior in hypermaterials containing other hydrogen-affinity elements is rarely reported. In this study, we aim to investigate the hydrogen absorption behavior and related structural changes in hypermaterials containing the hydrogen affinity elements Ca, Sc, and Pd.

Alloy ingots with the following nominal compositions were prepared by arc melting under an Ar atmosphere using high-purity metal raw materials: $\text{Ag}_{40.5}\text{In}_{45}\text{Ca}_{14.5}$, $\text{Ga}_{50.5}\text{Pd}_{35.5}\text{Tb}_{14}$, $\text{Al}_{70}\text{Pd}_{20}\text{Mn}_{10}$, and $\text{Sc}_{81}\text{Pt}_{19}$. After evacuation, the ingots were sealed in quartz tubes under an argon atmosphere and subjected to a heat treatment to homogenize the structure at specified temperatures, followed by water quenching. The samples were ground in acetone to prepare powder samples for XRD and hydrogen adsorption measurements. The hydrogen absorption behavior was evaluated by measuring the time-dependent change in hydrogen pressure within a sample cell set to an initial hydrogen pressure of 4 MPa at 373 K, using a PCT property measurement system (Suzuki Syokan, Japan). Structural changes before and after hydrogen absorption were evaluated using XRD analysis (SmartLab, Rigaku, Japan).

XRD measurements confirmed that all prepared samples consisted almost entirely of a 1/1 quasicrystal phase after homogenization treatment. Hydrogen absorption measurements revealed the maximum hydrogen absorption capacity ($[\text{H}]/[\text{M}]$) of each alloy to be as follows: less than 0.1 for $\text{Al}_{70}\text{Pd}_{20}\text{Mn}_{10}$, 0.2 for $\text{Ga}_{50.5}\text{Pd}_{35.5}\text{Tb}_{14}$, 0.5 for $\text{Ag}_{40.5}\text{In}_{45}\text{Ca}_{14.5}$, and 2.0 for $\text{Sc}_{81}\text{Pt}_{19}$. No obvious structural changes were observed after hydrogen absorption for $\text{Al}_{70}\text{Pd}_{20}\text{Mn}_{10}$ and $\text{Ga}_{50.5}\text{Pd}_{35.5}\text{Tb}_{14}$. In contrast, the AgIn_4 and CaH_2 phases were identified alongside the original 1/1 quasicrystal phase after hydrogen absorption for $\text{Ag}_{40.5}\text{In}_{45}\text{Ca}_{14.5}$. Furthermore, an amorphous structure was identified after hydrogen absorption for $\text{Sc}_{81}\text{Pt}_{19}$.

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Keywords— hydrogen absorption, 1 / 1 quasicrystal, hydrogen storage material

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Non-Fermi-liquid behavior in a quasicrystal and its 2/1 cubic approximant

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Abstract

We report non-Fermi-liquid behavior at ambient-pressure and zero-magnetic field in a newly identified icosahedral quasicrystal (*i*-QC) and its 2/1 cubic approximant (*c*-AC) in Yb–Pt–Zn system. The results of the crystal structure analysis revealed that the 2/1 and 1/1 *c*-ACs consist of Tsai-type clusters. As in the known Yb₃Zn₁₇ 1/1 *c*-AC [1], either a Yb atom or a Zn tetrahedron is located at the cluster center. Furthermore, Pt was found to partially occupy the edge-center sites of the rhombic triacontahedron. Temperature dependence of electrical resistivity, specific heat coefficient, and uniform magnetic susceptibility of the *i*-QC and 2/1 *c*-AC exhibit pronounced deviations from Landau's Fermi-liquid theory, whereas the 1/1 *c*-AC remains a conventional metal (see Fig. 1). Moreover, both the *i*-QC and the 2/1 *c*-AC show quantum-critical-like divergence of the magnetic susceptibility as the temperature reaches 0 K without external tuning.

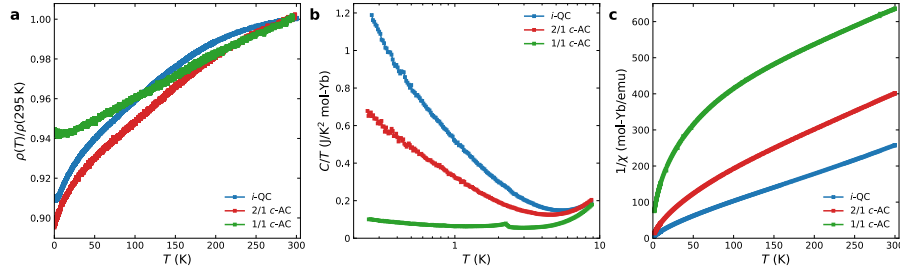


Figure 1: Temperature dependence of (a) the electrical resistivity, (b) the heat capacity, and (c) magnetic susceptibility for the Yb–Pt–Zn *i*-QC and the 2/1 and 1/1 *c*-ACs.

Acknowledgments

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Keywords— Icosahedral quasicrystals, Approximants, Non-Fermi-liquid behavior

Correspondence between exact eigenstates on distinct electron site configurations with identical quasiperiodicity

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Abstract

Quasiperiodicity is a form of long-range structural order that lacks periodicity. This geometric concept is realized in quasicrystals, which exhibit diffraction patterns with sharp Bragg peaks and rotational symmetries forbidden in any periodic crystal. Such a lack of periodicity prevents the application of Bloch's theorem, making the concept of crystal momentum ill-defined. Consequently, standard k -space band descriptions become inapplicable, posing a significant theoretical challenge. To overcome this problem, we introduce the Sutherland-Kalugin-Katz (SKK) states [1], which serve as a natural generalization of Bloch's theorem. While the conventional Bloch's theorem block-diagonalizes the Hamiltonian via translation group representations to label eigenstates by crystal momentum, SKK states generalize this framework to be applicable to quasicrystals, achieving block-diagonalization based on a broader class of geometric properties than translational symmetry. This yields exact eigenstates that are classified by a new set of quantum numbers instead of crystal momentum. However, directly deducing such block-diagonalization conditions from the complex geometry of quasiperiodic systems is highly difficult. To make the problem analytically manageable, we restrict our analysis to tight-binding models and propose a requirement-driven approach using a generalized Fourier transform. In this study, we apply this framework to the Ammann-Beenker (AB) tiling, specifically investigating two distinct electron site configurations: the vertex model and the dual model (Figure 1). Notably, because the coordination number is constant across all sites, the dual model serves as a unique platform where the physical effects induced by quasiperiodicity emerge directly. We first validate our approach by confirming its consistency with the known SKK state that appears as the ground state of the vertex model, which was topologically derived in prior studies [2]. Furthermore, utilizing this SKK state of the vertex model and our derived conditions, we construct a corresponding SKK state for the dual model. We ultimately reveal that this constructed SKK state appears as the ground state of the dual model, thereby establishing a direct connection between exact eigenstates across distinct site configurations with identical quasiperiodicity. This indicates a mathematical correspondence in electronic properties of the vertex and dual models on the AB tiling.

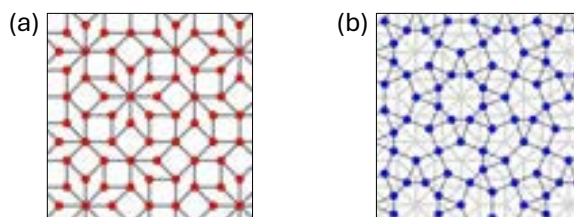


Figure 1: (a) The vertex model, where electron sites (red dots) are positioned at the vertices of the tiling. (b) The dual model, where sites (blue dots) are positioned at the centers of the constituent polygons.

References

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Relaxation of Magnetic Structure in the Regularly Ordered Frustrated Magnet DyRu₂Si₂

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Abstract

In the magnetic materials, strong non-equilibrium phenomena are usually found in the system with strong randomness such as spin glasses, where ferro- and antiferromagnetic interactions randomly coexist and compete. On the other hand, in some regular frustrated magnets without apparent randomness, non-equilibrium phenomena such as long-time relaxation are also observed despite of their uniform and periodic crystal and magnetic structures[1-3]. It is very likely that strong frustration effects also contribute to such non-equilibrium phenomena in the regular frustrated magnets, however, there are few examples and the role of frustration is still unclear.

Among them, we have investigated the frustrated magnet DyRu₂Si₂ with huge and peculiar magnetization hysteresis and found the long-time magnetization relaxations in the field-induced phase, called phase IV, with a regularly ordered magnetic structure[3]. DyRu₂Si₂ has a tetragonal lattice (space group: *I4/mmm*) and exhibits strong magnetic anisotropy along the c-axis. Magnetic frustration arises from the competing long-range oscillating RKKY interactions, through which Dy³⁺ moments interact. Interestingly, the three-days-long relaxations were observed from the initial states of the phase IV prepared in both zero-field-cooled and field-applied (ZFC-FA), and field-applied field-cooled (FA-FC) process. The presence of the long-time relaxation indicates that the phase IV is the non-ergodic phase, like a spin glass phase. It is particularly noted that the overtake of the magnetization relaxation after the FA-FC by that after the ZFC-FA, suggesting that the thermal equilibrium state differs depending on the cooling process.

In the present study, we performed a neutron scattering experiment using a single crystalline sample with the aim of investigating the details of this non-equilibrium phenomena in the phase IV by observing the relaxation of the magnetic scattering pattern and its temperature cooling-process dependency. The experiment was done using a TOF Laue diffractometer, SENJU, at the BL18 in J-PARC/MLF (Tokai, Japan). It was found that the intensities of the magnetic satellite reflections of the phase IV change with time drastically in both the ZFC-FA and FA-FC conditions, indicating that the magnetic structure varies with time corresponding to the previously observed long-time magnetization relaxations. Surprisingly, it was also observed that, while the satellite reflections characterizing the phase IV ($\mathbf{k}_m^{\text{IV}} = (1/9, 2/9, 0)$) have a single peak in the ZFC-FA condition, they split in the FA-FC condition even at the identical temperature and magnetic field. This is the microscopic evidence of the coexistence of the different equilibrium states with different magnetic periodicity, which can be controlled by manipulating the temperature process to reach the phase IV. These highly unconventional features we found in the phase IV should be attributed to the frustrated long-range RKKY interaction.

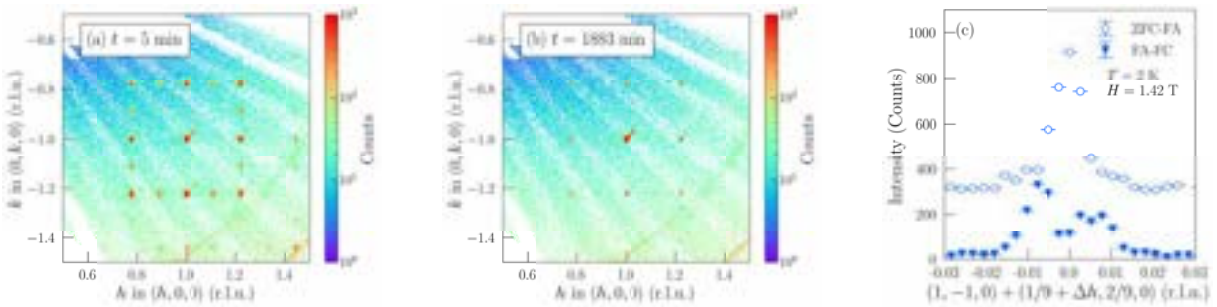


Figure 1: Neutron scattering intensity map in the phase IV prepared in the ZFC-FA condition at the waiting time of (a) $t = 5$ min and (b) $t = 1883$ min after reaching the measurement temperature and magnetic field ($T = 2$ K and $H = 1.42$ T). (c) The $(h, 2/9, 0)$ -line scan profiles at $t = 5$ min prepared in the ZFC-FA and FA-FC conditions. The peak at $\mathbf{k}_m^{\text{IV}} = (1/9, 2/9, 0)$, characterizing the magnetic structure of the phase IV, splits in the FA-FC condition. The data is offset for the clarity.

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