International Research Network

Open space between aperiodic order and physics & chemistry of materials

3-7 October 2021 - Carry le Rouet France

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Program

Sunday 3 October 2021

17h30 – 19h00 On site registration
19 h 00 Welcome Party

Monday 4 October 2021

8h00	Introduction		
8h20	R. Tamura : Magnetism of Tsai-type hypermaterials On line	Invited	30 min.
8h50	V. Baledent : Interplay between electronic and spin configurations under magnetic field in multiferroic materials. The case of GdMn2O5. On site	Invited	30 min.
9h20	K Nawa : Magnetic Properties of the quasicrystal approximant Au65Ga21Tb14. On line	Contributed	20 min.
9h40	F. Labib : Synthesis and Magnetic Properties of In-Pd-RE 1/1 Approximants. On line	Contributed	20 min.
10 h 00	Break		
10 h 30	F. Damay : Unusual Magnetic Orderings from the Interplay of Triangular Topology and Magnetic Anisotropy. On site	Invited	30 min.
11 h 00	K. Deguchi Strongly : correlated electrons in quasicrystals and approximants. On line	Invited	30 min.
11h 30	T. Sugimoto : Quantum Criticality in a Classical-SpinFibonacci Mille-Feuille Model. On line	Contributed	20 min.
11 h 50	T Trevizam Dorini : Two-dimensional oxide quasicrystal approximants with tunable electronic and magnetic properties. On site	Contributed	20 min.
12 h 10	N. Varela - Rosales : Free energy calculations of 2D and 3D model quasicrystals. On site	Contributed	20 min.
12 h 30	Lunch		
14 h00	M. Souliou : Competing orders in superconducting cuprates:insights from lattice dynamics. On site	Invited	30 min.
14 h 30	M. D'Astuto : Bulk charge density wave and electron-phonon coupling in superconducting copper oxychlorides. On site	Contributed	20 min.
14 h 50	M. Mihalkovic : Three families of quasicrystal approximants in Si, G and Sn nanolayer systems. On site	Contributed	20 min.
15 h 10	Poster Clip session - On site	4 mn/poster	
15 h 40	Break		
17h30-19h	On site Poster session and aperitif		

Tuesday 5 October 2021

8 h 00	N. Takemori : Theoretical Investigation on Superconducting Hypermaterials. On line	Invited	30 min.
8 h 30	C. Pay Gomez: Structures of RE-Au-Si (RE=Tb, Ho) Quasicrystal Approximants. On line	Invited	30 min.
9 h 00	G. Rai : Bulk topological signatures of a 1D quasicrystal. On line	Contributed	20 min.
9 h 20	H. Takatura : Cluster covering in a Bergman-type 2/1-1/1-1/1 quasicrystal approximant. On line	Contributed	20 min.
9 h 40	T. Yamada : 2/1 and 1/1 cubic approximants in ternaryR-Cd-Mg (R= Y, Er) systems. On line	Contributed	20 min.
10 h 00	Break		
10 h 30	Y. Katsura : Data curation projects for quasicrystal-related alloys. On line	Invited	30 min.
11 h 00	E. Lorenzo : Interplay between charge density wave and magnetism: what do we know ? On site	Invited	30 min.
11 h 30	A. Benoit-Gonin : Transport properties of pure $AuTe_2$. On site	Contributed	20 min.
11 h 50	S. Kotla : Incommensurately Modulated Rb_2ZnCl_4. On site	Contributed	20 min.
12 h 10	J. Stelhorn : Insights into Aperiodic Structures by Atomic Resolution Holography. On line	Contributed	20 min.
12 h 30	Lunch		
14 h 15	Excursion to Marseille		
19 h 00	Dinner		

Wednesday 6 October 2021

8 h 00	M. Tezuka: Many-body localization in quasiperiodic systems and effect of nonhermitian terms. On line	Invited	30 min.
8 h 30	E. Svanitze : Physical and chemical properties of complex intermetallic compounds. On site	Invited	30 min.
9 h 00	S. Sarkar : An experimental investigationof bulk electronic structure of high-order approximants and quasicrystal. On line	Contributed	20 min.
9 h 20	V. Singh : Thick quasiperiodic Sn layer. On line	Contributed	20 min.
9 h 40	J. Grin : Superconductivity of metastable intermetallic compounds. On line	Contributed	20 min.
10 h 00	Break		
10 h 30	A. Minelli : Evolution of the CDW-type in the monophosphate tungsten bronzes family. On site	Invited	30 min.
11 h 00	M. Groshe : Strong coupling superconductivity in incommensurate host-guest structures. On site	Invited	30 min.
11 h 30	C. Ruano : Complex 2D oxide phases in reduced $SrTiO_3$grown on Pt(111)/Al_2O_3(0001): an experimental and theoretical approach. On site	Contributed	20 min.
11 h 50	P. Kalugin : Flat-branched semi-simplicial complexes: a versatile tool for aperiodic solids. On site	Contributed	20 min.
12 h 10	M. Haller : Triangle-square-rhombus tilings arising from anti-phase domain boundaries in the σ-phase On line	Contributed	20 min.
12 h 30	Lunch		
14 h	S. Francoual : Resonant Elastic X-ray Scattering at beamline P09 at PETRA III at DESY. On line	Invited	30 min.
14 h 30	I. Mandal : Correlated Insulators in Twisted Bilayer Graphene. On site	Invited	30 min.
15 h	S. Schenk : Large unit cell approximant derived from$SrTiO_3$on Pt(111). On line	Contributed	20 min.
15 h 20	P. Bereciartua : MagStREXS: a Crystallographic Software for Magnetic Structure Determination through Resonant X-Ray Magnetic Diffraction. On line	Contributed	20 min.
15 h 40	Break		
20 h 00	Workshop Dinner		

Thursday 7 October 2021

8 h 00	S. Watanabe : Elasticity, crystalline electric field and magnetism in the Yb- and Tb-based quasicrystal and approximant. On line	Invited	30 min.
8 h 30	M. Henriques : Magnetic structure superspace and Jana. On line	Invited	30 min.
9 h 00	U. Lieu : Inverse Design of Two-dimensional Self-assembly of Patchy Particles. On line	Contributed	20 min.
9 h 20	N. Yoshinaga : Bayesian Inference of Phase-Field Crystal Models for Target Crystalline Patterns. On line	Contributed	20 min.
9 h 40	N. Fujita :Pseudo-merohedral twinning of AlCuRu. On line	Contributed	20 min.
10 h	Break		
10 h 30	D. Le Bolloc'h : Deformation of an incommensurate CDW under currents. On site	Invited	30 min.
11 h 00	S. Foerster : Accounting for complexity in periodic systems: A classification scheme for quasicrystal approximants. On line	Invited	30 min.
11 h 30	S. Coates : A 6-fold golden-mean tiling. On line	Contributed	20 min.
11 h 50	R. Lifshitz : Thermodynamic stability of quasicrystals: From fluid dynamics to soft condensed matter. On site	Contributed	20 min.
12 h 10	Closing remarks		20 min.
12 h 30	Lunch		
14 h 00	Departure		

ORAL PRESENTATIONS

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8h00	Introduction		
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15 h 40	Break		
17h30-19h	On site Poster session and aperitif		

Magnetism of Tsai-type hypermaterials

Ryuji Tamura[1], Shintaro Suzuki[1], Asuka Ishikawa[2], Maxim Avdeev[3], Taku J Sato[4]
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[2]*Res. Inst. for Sci. & Tech., Tokyo University of Science, Tokyo, Japan*
[3]*Australian Nuclear Science and Technology Organisation, Australia*
[4]*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Japan*

One of the main goals of our study is to realize a long-range magnetic order in QCs, such as ferromagnetic and antiferromagnetic ones. For this aim, we have searched for the empirical rule to realize long-range magnetic order in Tsai-type 1/1 approximants (ACs) that have been extensively synthesized for the last decade. As a result, the average electron-per-atom ratio (*e/a*) was found to be the most important factor that characterizes the magnetism of the 1/1 ACs [1]. We then applied this empirical rule to synthesize higher-order ACs and successfully obtained the first ferromagnetic 2/1 ACs [2]. By assuming that Tsai-type QCs also follow the same empirical rule obtained for 1/1 ACs, we searched for new QCs whose *e/a* ratio falls in the ferromagnetic region of 1/1 ACs, i.e., *e/a* ~ 1.70. We successfully obtained new Au-based QCs with e/a = 1.70 by use of the rapid-quenching technique. The magnetic susceptibility of both the QCs clearly show the occurrence of a ferromagnetic transition [3]. This is the first observation of a long-range magnetic order in QCs. The detail including neutron diffraction experiments will be reported in the presentation.

Acknowledgement:
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Referrences

[1] S. Suzuki *et al.*, *Mater. Trans.,* **62**, 298 (2021).
[2] K. Inagaki *et al.*, *Phys. Rev.* B **101**, 180405(R) (2020).
[3] R. Tamura *et al.*, *submitted.*

Interplay between electronic and spin configurations under magnetic field in multiferroic materials. The case of GdMn2O5.

Victor Balédent[1], *Antoine* Vaunat[1,2], *Pascale* Foury[1]

[1]*Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405, Orsay, France*

[2]*Université Paris-Saclay, CEA, CNRS, LLB, 91191, Gif-sur-Yvette, France.*

RMn2O5 (R: rare earth) multiferroics present a strong magneto-electric coupling, in particular for the R=Gd composition. This coupling manifests itself in this family at low temperature (~30K) when the electric polarisation develops together with a complex ordering of the spins. We recently exposed the microscopic mechanism responsible for this coupling as the exchange striction mechanism [1,2]. To further challenge our comprehension of the physics at play, we then focused on dynamical manifestation of such coupling. By studying low energy excitations using complementary experimental techniques, we revealed the presence of an electro-active magnon, called electromagnon, and characterised it with unprecedented experimental details [3]. While the interpretation of such electromagnon usually involves phonon or crystal field excitation, our careful measures show no evidence for such component.

Our very recent study of elastic and inelastic properties of GdMn2O5 under magnetic field showed a complex magnetic phase diagramm, with several incommensurate magnetic orders. The interpretation of the effect of magnetic field is not trivial owing the numerous frustrated exchange interactions in this system. We will present an interpretation of the evolution of the phase diagram, in the light of other composition's magnetic structure and numerical simulation.

[1] Physical Review B 95, 184112 (2017)

[2] Physical Review B 97, 085128 (2018)

[3] Accepted in Physical Review (2021)

Magnetic Properties of the quasicrystal approximant $Au_{65}Ga_{21}Tb_{14}$

Kazuhiro Nawa[1], Maxim Avdeev[2], Chin-Wei Wang[3,2],
Hiroyuki Takakura[4] Asuka Ishikawa[5], Ryuji Tamura[6] and Taku J Sato
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[2]*Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Locked Bag 2001, Kirrawee, NSW 2232, Australia*
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[4]*Faculty of Engineering, Hokkaido University, Sapporo, Hokkaido 060-8628, Japan*
[5]*Research Institute for Science and Technology, Tokyo University of Science, Katsushika, Tokyo, Japan*
[6]*Department of Materials Science and Technology, Tokyo University of Science, Katsushika, Tokyo, Japan*

Magnetism in quasicrystals and quasicrystal approximants has attracted interest due to the expectation of nontrivial ground states. Recently, noncollinear magnetic structures were found in a few magnetic quasicrystal approximants from neutron diffraction experiments[1,2]. For instance, in the $Au_{72}Al_{14}Tb_{14}$ 1/1 quasicrystal approximant, magnetic moments are found to be aligned almost tangential to the cluster surface. They follow a threefold symmetry around the [111] axis, leading to the whirling arrangement[1]. The previous study indicates that competing magnetic interactions and formation of the magnetic clusters are key ingredients to stabilize the noncollinear magnetic structure. A variety of noncollinear magnetic structures may be realized by tuning the magnetic interactions and the magnetic anisotropy of the Tb^{3+} ions.

In this study, we report the magnetic properties of the $Au_{65}Ga_{21}Tb_{14}$ 1/1 quasicrystal approximant. The temperature dependence of the magnetic susceptibility and the magnetization curve indicate dominant ferromagnetic interactions. The powder neutron diffraction pattern collected by using ECHIDNA diffractometer, shown in the Figure, indicates the occurrence of the whirling antiferromagnetic order. The magnetic properties similar to those of $Au_{72}Al_{14}Tb_{14}$ suggest the robustness of the easy-axis anisotropy against the chemical substitution of the nonmagnetic atoms.

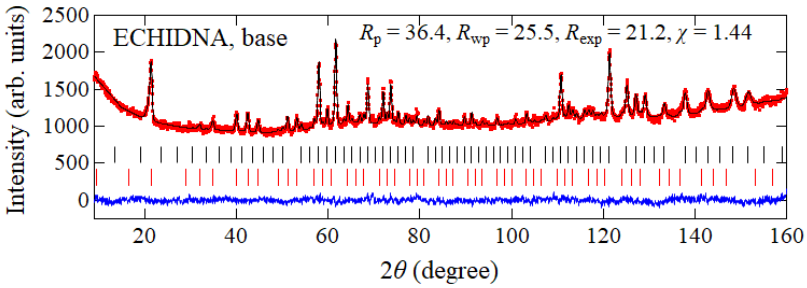

Fig. Powder diffraction pattern collected at 4 K. (λ = 2.4395 Å).

[1] T. J. Sato et al., Phys. Rev. B 100, 054417 (2019).
[2] T. Hiroto et al., Journal of Physics: Condensed Matter 32, 415802 (2020).

Synthesis and Magnetic Properties of In-Pd-RE 1/1 Approximants

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[2]*Research Institute for Science and Technology, Tokyo University of Science, Tokyo, Japan*

Tsai-type quasicrystals (QCs) and their approximant crystals (ACs) have a unique atomic structure, wherein the interplay between localized f-electrons of RE (rare earth) and itinerant electrons in complex atomic environments could result in long-ranged magnetic order. So far, all the magnetic iQCs exhibit spin-glass-like (SG) freezing behavior at low temperatures. Despite the fact that the antiferromagnetic (AFM) ordering is theoretically possible for primitive and body-centered iQCs [1], thus far, there is no experimental evidence of iQCs of such kind. The ACs, on the other hand, exhibit ferromagnetic (FM), AFM or SG-like behavior at low temperatures [2]. Lately FM and AFM 2/1 AC [3,4] have been discovered proving that AFM ordering can still survive in the higher-order 2/1 AC, which has all the building blocks for creating an iQC.

In order to fully clarify the magnetic properties of the Tsai-type iQCs and ACs and to develop a comprehensive guideline for tailoring the magnetic properties of aperiodic compounds, it is necessary to examine various alloy systems (in terms of their formation and magnetic behavior). This is, indeed, a focus of a great deal of recent work. This study, therefore, aims at contributing to such growing area of research by exploring formation conditions and magnetism of the In-Pd-RE 1/1 ACs. To the best of our knowledge, the stability and magnetic behavior of the In-Pd-RE 1/1 ACs have rarely been investigated by previous studies. Besides, the 1/1 ACs in the In-Pd-RE systems have relatively low e/a ratio (by assuming valence electron numbers of 0, 3 and 3 for Pd, In and RE, respectively), which is believed to be a factor in favor of long-range magnetic order occurrence [2]. These compounds appear inside a very narrow compositional area in the ternary phase diagram with e/a close to 2.0 and are stable after annealing at 773 K for 150h. The stability of the synthesized 1/1 ACs with respect to the composition and annealing temperature varies with the constituent RE element.

Investigating the magnetic properties of these compounds is underway at this moment, however, based on the preliminary results, they are likely to exhibit spin-glass-like magnetic behavior at low temperature.

References:

[1] R. Lifshitz, Mater. Sci. Eng. A. 294–296 (2000) 508–511.
[2] S. Suzuki *et al.* Mater. Trans. 62 (2021) 298–306.
[3] Y.G. So *et al.* J. Phys. Conf. Ser. 1458 (2020) 1–5.
[4] K. Inagaki *et al.* Phys. Rev. B. 101 (2020) 1–5.

Unusual Magnetic Orderings from the Interplay of Triangular Topology and Magnetic Anisotropy

Françoise Damay[1]

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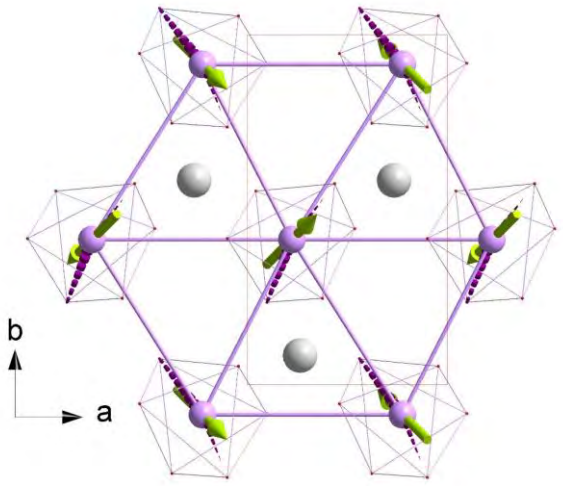
Stackings of perfect triangular planes of magnetic ions offer a vast playground when looking for complex magnetic orderings, as geometrically induced frustration of antiferromagnetic exchanges leads to non-collinear magnetic structures ; moreover, in the case of strong easy-axis magnetic anisotropy, magneto-elastic effects are often at play to lift the degeneracy of the magnetic ground state and allow the system to order. Several examples will be given, in which magnetic exchanges and/or magnetic anisotropy are tuned, to achieve specific physical properties such as multiferroicity, or to investigate more theoretical aspects of condensed matter, such as multi-axis antiferromagnets. Those examples also illustrate the invaluable technique that is neutron scattering, both elastic and inelastic, especially when combined with the modelling tools that are available today.



Zig-zag non-collinear non-coplanar AFM ordering in $BiMnTeO_6$
Shubnikov group P_a2_1/c (#BNS 14.80)

Strongly correlated electrons in quasicrystals and approximants

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Quasicrystals possess long-range, quasi-periodic structures with diffraction symmetries forbidden to crystals. The Au-Al-Yb quasicrystal with Tsai-type cluster exhibits novel quantum critical behavior as observed in Yb-based heavy fermion materials with intermediate Yb valence, while the Au-Al-Yb approximant shows heavy Fermi liquid behavior [1]. Quantum critical phenomenon of the Au-Al-Yb quasicrystal is remarkably robust against hydrostatic pressure, related to the critical state unique to the quasicrystal. By contrast, the Au-Al-Yb approximant shows heavy fermion behavior, very sensitive to hydrostatic pressure and quantum criticality of the approximant is induced by pressure [2]. Therefore, the quantum critical state of the Au-Al-Yb quasicrystal might correspond to an electronic state unique to the quasicrystals. Interestingly, quantum criticality of the Au-Al-Yb quasicrystal seems to be closely related to heavy fermion crystalline compound and the icosahedral Yb quasicrystals and approximants shed a new light on strongly correlated electrons in quasicrystals. Studying the magnetism of icosahedral Yb quasicrystals and approximants by substitution of Yb ligands, we have found that the Au-Al-Yb system is located near the border of the valence change [3,4]. Furthermore, we have found superconductivity of Au-Ge-Yb approximants with Tsai-type cluster for the first time [5] and we have confirmed the emergence of bulk superconductivity of Al-Zn-Mg quasicrystal [6]. We will discuss the variation of magnetism and mean Yb-valence by the chemical pressure effect and itinerant-electron concentration control in the Au-Al-Yb approximant, supporting that the valence fluctuation plays a crucial role in the quantum criticality of quasicrystal.

[1] K. Deguchi, S. Matsukawa, N. K. Sato, T. Hattori, K. Ishida, H. Takakura, and T. Ishimasa, Nature Materials **11**, 1013 (2012).
[2] S. Matsukawa, K. Deguchi, K. Imura, T. Ishimasa, and N. K. Sato, J. Phys. Soc. Jpn. **85**, 063706 (2016).
[3] M. Hayashi, K. Deguchi, S. Matsukawa, K. Imura, and N.K. Sato, J. Phys. Soc. Jpn. **86**, 043702 (2017).
[4] K. Imura, H. Yamaoka, S. Yokota, K. Sakamoto, Y. Yamamoto, T. Kawai, K. Namba, S. Hirokawa, K. Deguchi, N. Hiraoka, H. Ishii, J. Mizuki, T. Ishimasa and N. K. Sato, Sci. Rep. **10**, 17116 (2020).
[5] K. Deguchi, M. Nakayama, S. Matsukawa, K. Imura, K. Tanaka, T. Ishimasa, and N. K. Sato, J. Phys. Soc. Jpn. **84**, 023705 (2015).
[6] K. Kamiya, T. Takeuchi, N. Kabeya, N. Wada, T. Ishimasa, A. Ochiai, K. Deguchi, K. Imura, and N.K. Sato, Nature Communications **9**, 154 (2018).

Quantum Criticality in a Classical-Spin Fibonacci Mille-Feuille Model

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Recent experimental studies have reported striking discoveries in quasicrystals, e.g. quantum criticality [1] and superconductivity [2]. In particular, it is intriguing that the quantum criticality is robust against the pressure in not approximants but quasicrystals. Thus, the quantum criticality is expected to reflect a distinct characteristic inherent in quasicrystals. Although recent theoretical works have proposed a possible scenario [3], its mechanism has almost not been clarified so far.

Here we consider a toy model of classical spins to discuss an interplay between a global structure of quasicrystals and critical behaviors. In this model, we introduce a mille-feuille structure composing of several sorts of layers where the number of neighboring sites are different. Moreover, as a characteristic of quasicrystals, we arrange the layers in a Fibonacci sequence as follows: (i) the number of neighboring sites z_i for ith layer is given by one of two fixed values z_L and z_S, and (ii) the numbers is arranged in a Fibonacci sequence, $\{z_i\} = \{z_L, z_S, z_L, z_L, z_S, \cdots\}$. If we consider a uniform ferromagnetic interaction J as intra-layer interactions without inter-layer interactions, corresponding to decoupled ferromagnetic layers, the critical points appear at $k_B T_c = z_L J$ and $z_S J$ at the mean-field level. On the other hand, we can expect that a finite inter-layer interaction modifies the critical points and induces a cooperative phenomenon of two different criticalities.

In real quasicrystals, the local environments are distributed, so that if the local environments dominate the criticality, there should be a cooperative phenomenon similar to our model. Therefore, our model can give an intuitive picture of the cooperative phenomenon if the system contains several criticalities in nature.

References

[1] K. Deguchi *et al.*, Nat. Mater. **11**, 1013 (2012).

[2] K. Kamiya *et al.*, Nat. Commun. **9**, 154 (2018).

[3] S. Watanabe *et al.*, Jpn. J. Appl. Phys. **56**, 05FA01 (2017); Solid State Commun. **306** 113774 (2019); JPS Conf. Proc. **30** 011027 (2020).

Two-dimensional oxide quasicrystal approximants with tunable electronic and magnetic properties

T. T. Dorini,[1,2] F. Brix,[1,2] C. Chatelier,[1,2] A. Kokalj [2,3] and É. Gaudry [1,2]

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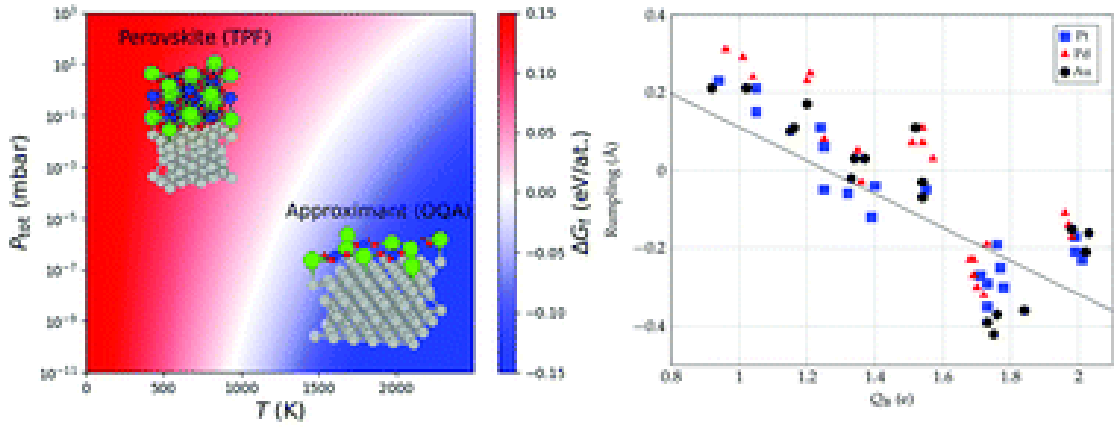
Recently, the discovery of the quasiperiodic order in ultra-thin perovskite films reinvigorated the field of 2-dimensional oxides on metals, and raised the question of the reasons behind the emergence of the quasiperiodic order in these systems. The effect of size-mismatch between the two separate systems has been widely reported as a key factor governing the formation of new oxide structures on metals. Herein, we show that electronic effects can play an important role as well. To this end, the structural, thermodynamic, electronic and magnetic properties of freestanding two-dimensional oxide quasicrystalline approximants and their characteristics when deposited over metallic substrates are systematically investigated to unveil the structure–property relationships within the series (Fig. 1b). Our thermodynamic approach (Fig. 1a) suggests that the formation of these aperiodic systems is likely for a wide range of compositions. In addition, the magnetic properties and work functions of the thin films can be controlled by tuning their chemical composition. This work provides well-founded general insights into the driving forces behind the emergence of the quasiperiodic order in ternary oxides grown on elemental metals and offers guidelines for the discovery of new oxide quasicrystalline ultra-thin films with interesting physical properties [1].



(a) (b)

Figure 1: (a) Gibbs free energy (ΔG_f), as a function of the temperature and O2 partial pressure, for the formation of the BaTiO3 oxide quasicrystal approximant on Pt(111). (b) Plot of the film rumpling (R) of ABO3/Pt(111) quasicrystalline approximants as a function of the Bader charge carried by B-type atoms (QB ; note that positive QB values correspond to cations).

[1] T. T. Dorini et al., ***Nanoscale***, 2021,**13**, 10771-10779

Free energy calculations of 2D and 3D model quasicrystals

Nydia Roxana Varela-Rosales[1], Kwanghwi Je[2], Michael Engel[1]
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Quasicrystals have by now been established as thermodynamic phases that form robustly in particle simulations of certain model systems. Estimating the thermodynamic stability of these quasicrystals, in particular relative to their approximant competitor phases, requires calculating free energies to sufficiently high precision. Standard numerical methods, like the Frenkel-Ladd method, consider entropic contributions from phonons but struggles with the effect of phason modes at elevated temperatures and other anharmonic effects, which are known to be critical in quasicrystals [1]. In this work, we advance free energy calculations of quasicrystals in two directions. First, we evaluate the effect of a periodic substrate potential on the stability of a dodecagonal quasicrystal in two dimensions. These simulations are inspired by experiments on thin-film (Ba,Sc)TiO_3 quasicrystals and their approximants on a Pt substrate [2]. We find that the periodic substrate enhances the stability of the dodecagonal quasicrystal and its approximants at elevated temperatures, this behaviour allows describing the role of the substrate in the stabilization of oxide quasicrystals in the experiments from ref. [2]. We also observe the spontaneous formation of modulated phases and a new hexagonal labyrinth-like quasicrystalline phase in simulation that has not been seen before for this system. Second, we investigate the stability of an icosahedral quasicrystal [3] as a function of phason strain and tile decoration density. We find that the icosahedral quasicrystal is metastable relative to its 1/1 approximant and spontaneously transforms into the 1/1 approximant by a continuous build-up of phason strain. The transformation is a highly complex, collective reorganization process involving all particles in the system. Our simulation results are assisted by novel bond-orientational order parameters that we developed to detect, quantify, and classify crystallographic order in particle simulation data.

[1] A. Kiselev, M. Engel, H.-R. Trebin, *Phys. Rev. Lett.* **109**, 225502 (2012).
[2] S. Förster, S., Schenk et al. *Physica Status Solidi B* **257**, 1900624 (2020).
[3] M. Engel, P.F. Damasceno, C.L. Phillips, et al. *Nature Materials* **14**, 109 (2015).

Competing orders in superconducting cuprates: insights from lattice dynamics

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Charge density waves (CDW) have now been ubiquitously observed as a competitor to high temperature superconductivity (SC) in the cuprates. In the well-studied $YBa_2Cu_3O_{6+x}$ cuprate family, short-range quasi-2D CDW modulations appear in the CuO_2 planes with onset temperatures far exceeding the superconducting T_c. While the 2D CDW order is not soft-phonon-driven, large renormalizations of the low energy phonons are observed around the CDW ordering wavevector both in the charge-ordered state and below T_c. Recent high-resolution inelastic x-ray scattering (IXS) experiments demonstrated the in-plane isotropy of the phonon anomalies, whereas first principle calculations indicated the relevant symmetry of the anomalous phonons. In the first part of this talk, an overview of the low energy phonon anomalies associated with the CDW order in $YBa_2Cu_3O_{6+x}$ will be presented and their origin will be discussed.

The second part of the talk will be focused on the tuning of the interplay between the CDW instability and SC by external pressure. More specifically, the results of IXS and x-ray diffraction experiments in hydrostatically and uniaxially pressurized $YBa_2Cu_3O_{6+x}$ will be presented. The very different response of the two electronic orders obtained under hydrostatic and uniaxial compression will be discussed with respect to the pressure dependence of T_c and the modification of the crystal structure.

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Bulk charge density wave and electron-phonon coupling in superconducting copper oxychlorides

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Charge density waves (CDWs) were theoretically predicted in cuprates not long after the discovery of high-temperature superconductivity [1–3], and are now reported in nearly all cuprate superconductors [4], although their microscopic origin and relation with the superconductivity remain enigmatic. Studying the excitations associated with the CDW opens new routes towards a better description of this phenomenon, enabling to define the pertinent interactions and reveal its interplay with other degrees of freedom. Recently, such excitations were unveiled in Bismuth-based materials [5–7], calling for additional studies to provide a holistic picture of the CDW phenomenology in cuprate superconductors. Here, we focus on the copper oxychloride family, in which a surface CDW was detected more than fifteen years ago [8], with no evidence regarding its bulk behavior. Using resonant inelastic X-ray scattering (RIXS), we unambiguously reveal a bulk CDW in this material. Combining RIXS with non-resonant IXS, we also focus on the lattice excitations, and evidence electron-phonon anomalies occurring in the presence of dispersive CDW excitations.

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Three families of quasicrystal approximants in Si, Ge and Sn nanolayer systems

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We employed ab–initio molecular dynamics within replica-exchange framework, and structural modelling, to search for ground states of thin, free–standing layers of tin, germanium and silicon.

Ground-state Si/Ge monolayers are "dumbbell"-silicene/germanene in orthorhombic 10–atom periodic cell. Analogical stanene structure is unstable and decomposes into a state mixing covalent clusters with stable metallic bilayer. At finite temperature, and/or increased layer thickness, tin exhibits also hexagonal phase related to metallic γ-Sn. In the projection along layer normal, the two bilayer phases can be associated with tilings of squares and triangles, that can mix into a metallic *dodecagonal quasicrystal* bilayer phase.

In case of Si or Ge and up to 3 monolayer (ML) width, the dominant structures are (stacked) puckered honeycomb layers of (111)-terminated diamond structure, with adatoms saturating dangling bonds on the surface. Adatoms arrangements can be described as tilings of three tiles, that at certain layer width admit *hexagonal quasicrystal* ordering.

For layer thickness 3–10 ML (diamond), Si ground state is so called 7x7 DAS reconstruction, while for Ge and Sn energy minimizing layers are surface-reconstructed clathrates – approximants of *dodecagonal* or *decagonal* quasicrystals.

Tuesday 5 October 2021

8 h 00	N. Takemori : Theoretical Investigation on Superconducting Hypermaterials. On line	Invited	30 min.
8 h 30	C. Pay Gomez: Structures of RE-Au-Si (RE=Tb, Ho) Quasicrystal Approximants. On line	Invited	30 min.
9 h 00	G. Rai : Bulk topological signatures of a 1D quasicrystal. On line	Contributed	20 min.
9 h 20	H. Takatura : Cluster covering in a Bergman-type 2/1-1/1-1/1 quasicrystal approximant. On line	Contributed	20 min.
9 h 40	T. Yamada : 2/1 and 1/1 cubic approximants in ternaryR-Cd-Mg (R= Y, Er) systems. On line	Contributed	20 min.
10 h 00	Break		
10 h 30	Y. Katsura : Data curation projects for quasicrystal-related alloys. On line	Invited	30 min.
11 h 00	E. Lorenzo : Interplay between charge density wave and magnetism: what do we know ? On site	Invited	30 min.
11 h 30	A. Benoit-Gonin : Transport properties of pure $AuTe_2$. On site	Contributed	20 min.
11 h 50	S. Kotla : Incommensurately Modulated Rb_2ZnCl_4. On site	Contributed	20 min.
12 h 10	J. Stelhorn : Insights into Aperiodic Structures by Atomic Resolution Holography. On line	Contributed	20 min.
12 h 30	Lunch		
14 h 15	Excursion to Marseille		
19 h 00	Dinner		

Theoretical Investigation on Superconducting Hypermaterials

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In this talk, we review our theoretical investigations on correlation effects in the quasiperiodic system especially the superconductivity [1,2]. We found unconventional weak-coupling superconductivity formed by the Cooper pairs deviating from those of Bardeen-Cooper-Schrieffer superconductivity in periodic systems [1]. This deviation can be seen in the real-space distribution of the superconducting order parameter, jump of specific heat, and current-voltage characteristic curve due to the absence of Fermi surface (Figure) [2]. These results indicate that superconductivity in quasiperiodic systems is qualitatively different from that in periodic and random systems. In particular, the results are consistent with the superconductivity recently discovered in an Al-Mg-Zn quasicrystal [3] and provide a clue to understanding its mechanism and property.

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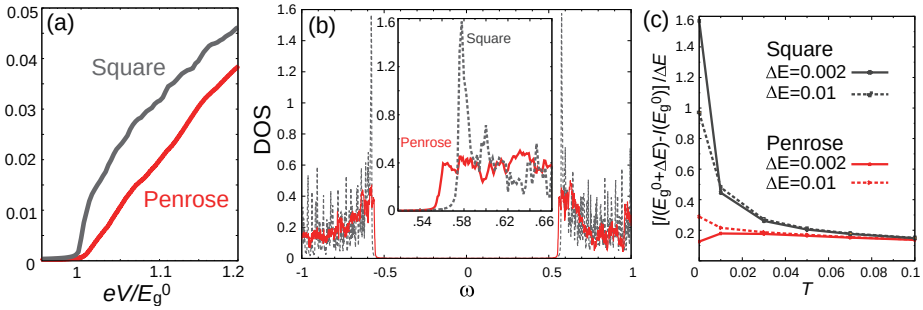

Figure: (a) Current as a function of voltage and (b) the site-averaged density of states at zero temperature obtained for the Penrose tiling and for a square lattice at quarter-filling for U=-3. (c) The temperature dependence of the slope at the threshold voltage for the Penrose and square lattices.

Structures of RE-Au-Si (RE=Tb, Ho) Quasicrystal Approximants

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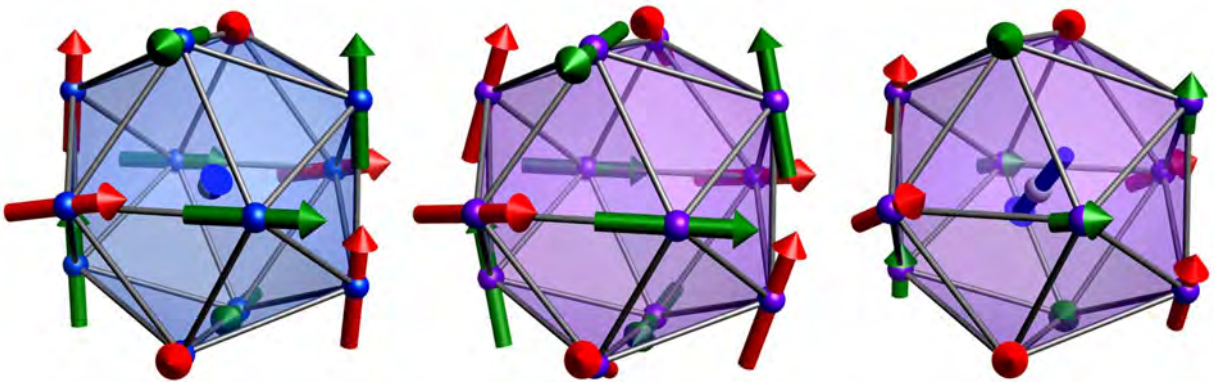
In the following work we will discuss the magnetic structures of three different RE-Au-Si (RE =Ho, Tb) quasicrystal approximants. The structural difference between these approximants lies in the partial replacement of the typical tetrahedron at the core of the Tsai-type cluster by single RE-atoms. This replacement affects the magnetic structures and bulk magnetic properties of the materials in different ways and differs from one approximant to the other depending on the choice of RE-element. The results of refinements on the nuclear and magnetic structures will be discussed in detail along with the effect of the tetrahedron by single RE-atom replacement.



Refined magnetic moments and their arrangements on the atomic clusters of the investigated RE-Au-Si 1/1 APs

Bulk topological signatures of a 1D quasicrystal

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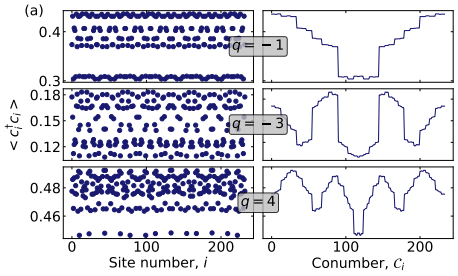
Quasicrystals have recently been shown to exhibit rich, non-trivial topological phases. For example, the widely studied Fibonacci chain has an infinite number of spectral gaps, each labelled by a unique integer. These topological gap labels have previously been measured in experiment by monitoring how the energies of edge states evolve as a function of an external tuning parameter ϕ which controls the phason flips of the system. Given the principle of bulk-edge correspondence, we ask whether the gap labels can also be physically realized in 1) bulk quantities, 2) without tuning the phason ϕ. We find that the gap labels can be observed experimentally be measuring position-dependant quantities such as the charge density or entanglement entropy and mapping them to perpendicular space. The number of times these quantities oscillate in perpendicular space is directly related to the gap labels of the Fibonacci chain. We will present two distinct interpretations of this effect by going to the weak and strong modulation limit. This effect is robust to moderate amounts of disorder and the introduction of local interactions.

arXiv:2106.12654



Cluster covering in a Bergman-type 2/1-1/1-1/1 quasicrystal approxiamnt

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Icosahedral quasicrystal (iQC) in the Al-Zn-Mg system has attracted much attention in recent years due to the first QC that shows superconductivity [1]. However, its atomic structure is still far from complete understanding. To elucidate atomic structure of QCs, it is useful to investigate approximant crystals (ACs) whose local structure is thought to be similar to that of corresponding QC. In the case of Al-Zn-Mg iQC, two cubic ACs denoted as 1/1 and 2/1 are known so far [2,3]. Those structures are characterized by a concentric shell structure of atoms, so-called "cluster", known as Bergman-type.

Recently, we found a new AC, that should be denoted as 2/1-1/1-1/1, belonging to the orthorhombic system in the course of our efforts to synthesize high quality single grains with the aim of clarifying the structure of Al-Zn-Mg iQC. The AC structure determined by means of single crystal X-ray diffraction, similarly to the other ACs, is characterized by Bergmann-type clusters, but can be better understood by considering an even larger rhombohedral trihedral (RTH) shell. Unlike the other ACs, the cluster network observed is not consisting of a combination of *b*- and *c*-linkages [4], but only *b*-linkages, where *b*- and *c*- linkages run along a two-fold and a three-fold direction of the cluster, respectively. Moreover, the AC cannot be described by canonical cell tiling [5], and has a large interstitial structure in between the clusters.

We show that the present AC can be regarded as a covering structure by RTH clusters if incomplete clusters as well are taken into account, and by allowing *a*-linkages along the 5-fold direction and *b*'-linkages that is $1/\tau$ times shorter than *b*-linkage. The present result is consistent with the observation in Zn-Mg-Tm iQC [6], where the structure was recently analyzed, and suggests a covering model for iQCs.

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2/1 and 1/1 cubic approximants in ternary R -Cd-Mg (R = Y, Er) systems

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The atomic structure of three cubic approximants (cAPs), $Y_{12.7}Cd_{61.8}Mg_{25.5}$ (2/1 cAP with space group $Pa\bar{3}$, a = 25.0654(1) Å) and $Er_{12.5}Cd_{72.0}Mg_{15.5}$ (2/1 cAP with $Pa\bar{3}$, a = 24.9658(1) Å), and $Y_{14.5}Cd_{66.1}Mg_{19.4}$ (1/1 cAP with $Im\bar{3}$, a = 15.4577(1) Å), were investigated by means of X-ray structure analysis. The two 2/1 cAPs were found to be isostructural to the binary 2/1 cAP, $YbCd_{5.8}$, which is composed of two building units, i.e., Tsai-type rhombic triacontahedron (RTH) cluster and double-Friauf polyhedron (DFP) [1]. While, the 1/1 cAP was found to be isostructural to the binary 1/1 cAP, $YbCd_6$, which is composed solely of the RTH cluster [2]. The refined structure models of the three cAPs exhibit substitutional disorder due to the Mg content that enters into the Cd sites of the parent binary cAPs. In addition, in the 2/1 cAPs, Y3(Er3) site on the 3rd icosahedron shell of the RTH cluster and two positions inside DFP, Y5(Er5) sites, are partially mixed with Mg. Besides, characteristic positional disorder owing to orientational disorder at the 1st shell of the RTH cluster is observed in all the three cAPs. A close relationship between the occupational disorder of the Y3(Er3) and Y5(Er5) sites in the 2/1 cAPs and the elemental distribution in their 1st coordination shells is revealed.

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Data curation projects for quasicrystal-related alloys

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Quasicrystals are the playgrounds for solid state physics without translation symmetry. Thus, discovery of a quasicrystal deepens the knowledge of solid state physics, especially when they exhibit exotic physical properties. Although over a hundred quasicrystal alloys have been discovered so far, there should be more quasicrystals and their approximant phases, which have not been discovered through the past experiments. The difference of the physical properties of these phases with the normal crystalline alloys have not been statistically investigated.

In our project, we attempted to collect the reported experimental data on these alloys in digital form, by manual data curation from literature. We have digitized the ternary phase diagrams, alloy compositions in the text, and the temperature dependences of electrical resistivity. We developed a number of original web systems to accelerate the manual data curation processes. Our original web system named Starrydata [1] was used to manage and organize the physical property data series extracted from literature.

In our 'Phase diagram' dataset, we succeeded to collect 357 phase diagrams from 198 publications. These included compositions of 613 phases in 65 combinations of the elements were collected. Our 'Composition' dataset included 857 compositions of quasicrystals and their approximants in 263 combinations of the elements, reported in the text and the tables, often without ternary phase diagrams. Our 'Physical Property' dataset included 338 curves of electrical resistivity, extracted from 206 figures.

The 'Phase diagram' and 'Composition' datasets were used to compare with the results of the machine-learning predictions of the compositions of the new quasicrystals and their approximants[2]. These will be also used to increase the prediction accuracy. The 'Physical Property' dataset was analyzed to find the difference in the distributions of electrical resistivities with the crystalline phases.

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Interplay between charge density wave and magnetism: what do we know ?

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Charge Density Wave (CDW) compounds are a class of materials within the family of aperiodic systems. The static modulation of the conduction electrons is a Fermi-surface driven phenomenon that is accompanied by a periodic lattice distortion at wavevector $2k_F$. Conceptually, the CDW instability was predicted by Peierls in 1955 but it was not until the mid 70s that Monceau measured the conductivity of the low dimensionality metal $NbSe_3$ that displays the CDW phase transition. Following this seminal work it is now well established that the CDW is a very common phase of matter observed in a large variety of materials. The discovery of a CDW coexisting with superconductivity in the high TC cuprates has sparkled a renew in this activity.

Recent studies have focused on the physics of CDW in rare earth (RE) compounds and how this wave influences crystal lattice distortions and magnetic ordering. A few years ago, scientists discovered that a CDW can precede and co-exist with the anti-ferromagnetic order.

In this paper I will present a review of magnetic compounds displaying CDW state and I will finally focus on the family $RETe_3$ where an interaction between the CDW and the RE anti-ferromagnetic ordering has been clearly established.

Transport properties of pure $AuTe_2$

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$AuTe_2$, or calaverite, is a well known aperiodic crystal. This compound present a modulated incommensurate structure as well as a known modulation vector [1].

Calaverite being electrically conductive, and a known superconductor when submitted to high pressure [2] or doped by Pd or Pt atoms [3], makes it a good candidate to study the potential relation between aperiodicity and transport properties.

In the past months we have been able to conduct transport (both electrical and thermal) measurements on pure crystals of $AuTe_2$ which were lab-grown in both Grenoble at Institut Neel and in Caen at CRISMAT. This study was motivated by the fact that we needed a good basis of pure $AuTe_2$'s transport properties, especially our newly grown crystals before going further, and the fact that literature lacked on this particular matter.

These experiments were realized in a cryostat from *Quantum Design* and contacts were done on the surface of the $AuTe_2$ crystals using silver paste. Temperatures were ranging from 2 to 400 Kelvin and the field used was up to 14 Teslas. I also had the chance to be part of a inelastic neutron scattering experiment at the Laue-Langevin Institute in Grenoble where we investigated some phonon branches of $AuTe_2$, particularly in the direction of the modulation.

We will present the results of our detailed thermal and electronic transport experiments and discuss the peculiarities of $AuTe_2$ in this context.

The next steps in our study will be to investigate the possibility of an anisotropic character on our pure $AuTe_2$ crystals as well as doing new syntheses with Ag doped $AuTe_2$.

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Incommensurately Modulated Rb_2ZnCl_4

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Rubidium Zinc Chloride (Rb_2ZnCl_4) is isostructural to β-K_2SO_4 and shows ferroelectric behavior below 192K [1]. It belongs to A_2BX_4 crystal family and exhibits successive phase transitions which are characteristic of this family. At high temperature it has an orthorhombic structure with *Pmcn* as its space group with some disorder associated with $ZnCl_4$ tetrahedra, then an incommensurate modulation develops along c-axis at 303K with the wavevector q = (1/3 – δ) c*, where 'δ' is the parameter which shows the incommensurability and it decreases with decreasing temperature. At around T_c = 192K, 'δ' becomes zero and thus Rb_2ZnCl_4 goes from an incommensurately modulated structure to a commensurately modulated structure [2]. Finally, Rb_2ZnCl_4 undergoes an additional phase transition around 75K [3] with a probable monoclinic distortion and additional satellites in *a*b** plane.

In the incommensurate phase the modulation wave function goes from a harmonic sinusoidal function to a highly anharmonic function as it approaches lock-in phase transition at T_c. The modulation function in the incommensurate phase of Rb_2ZnCl_4 is not only given by displacive modulation but also by the modulations of atomic displacement parameters (ADPs) and anharmonic ADPs [4-5]. In the low temperature phase (T<75K), the additional modulation arises in the *ab* plane with the wavevector q = 0.5a*+0.5b*. The detailed structural analysis in each phase, especially near the lock-in transition along with the lattice dynamics studies help us to understand the relation between aperiodic order and physical properties.

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Insights into Aperiodic Structures by Atomic Resolution Holography

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The atomic-resolution holography (ARH) technique offers the possibility to experimentally determine the atomic-scale local structure of crystals. This method can selectively investigate specific elements and their 3D local atomic environment in a comparably wide range (up to around 2 nm), without the need of *a priori* structural information. For these reasons, we are exploring its application to aperiodic systems, for which it may provide a new approach to visualize the structure.

The general usefulness of ARH for the investigation of quasicrystalline systems was noted already some time ago, [1] but it was not yet established widely due to difficulties concerning the experimental implementation and the data analysis. The strong advances of the ARH technique in recent years [2-4] now allow us to use the technique also for more complex systems, like quasicrystals. The interpretation of the images observed by ARH for such systems is challenging, but can be understood in a framework based on the projection of the average structure. [5]

The results of ARH can support the characterization of aperiodic systems, and elucidate details of their complex structure, like atomic disorder. In this presentation, we will report on the recent progress of ARH for quasicrystalline systems both by X-ray fluorescence holography and by neutron holography approaches, and present results for approximant and quasicrystalline systems of decagonal and icosahedral symmetry.

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Wednesday 6 October 2021

8 h 00	M. Tezuka: Many-body localization in quasiperiodic systems and effect of nonhermitian terms. On line	Invited	30 min.
8 h 30	E. Svanitze : Physical and chemical properties of complex intermetallic compounds. On site	Invited	30 min.
9 h 00	S. Sarkar : An experimental investigationof bulk electronic structure of high-order approximants and quasicrystal. On line	Contributed	20 min.
9 h 20	V. Singh : Thick quasiperiodic Sn layer. On line	Contributed	20 min.
9 h 40	J. Grin : Superconductivity of metastable intermetallic compounds. On line	Contributed	20 min.
10 h 00	Break		
10 h 30	A. Minelli : Evolution of the CDW-type in the monophosphate tungsten bronzes family. On site	Invited	30 min.
11 h 00	M. Groshe : Strong coupling superconductivity in incommensurate host-guest structures. On site	Invited	30 min.
11 h 30	C. Ruano : Complex 2D oxide phases in reduced $SrTiO_3$grown on Pt(111)/Al_2O_3(0001): an experimental and theoretical approach. On site	Contributed	20 min.
11 h 50	P. Kalugin : Flat-branched semi-simplicial complexes: a versatile tool for aperiodic solids. On site	Contributed	20 min.
12 h 10	M. Haller : Triangle-square-rhombus tilings arising from anti-phase domain boundaries in the σ-phase On line	Contributed	20 min.
12 h 30	Lunch		
14 h	S. Francoual : Resonant Elastic X-ray Scattering at beamline P09 at PETRA III at DESY. On line	Invited	30 min.
14 h 30	I. Mandal : Correlated Insulators in Twisted Bilayer Graphene. On site	Invited	30 min.
15 h	S. Schenk : Large unit cell approximant derived from$SrTiO_3$on Pt(111). On line	Contributed	20 min.
15 h 20	P. Bereciartua : MagStREXS: a Crystallographic Software for Magnetic Structure Determination through Resonant X-Ray Magnetic Diffraction. On line	Contributed	20 min.
15 h 40	Break		
20 h 00	Workshop Dinner		

Many-body localization in quasiperiodic systems and effect of nonhermitian terms

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Many-body localization (MBL) is the localization of all eigenfunctions of a quantum many-body Hamiltonian. This phenomenon has been extensively studied for several models, such as quantum spin chains under a random magnetic field and interacting particles on tight-binding chains with an inhomogeneous site potential. Despite the intensive theoretical studies in the field, both analytical and numerical approaches have faced many difficulties in investigating MBL. One recent progress has been made in the case of a system without spatial extension, namely the Sachdev-Ye-Kitaev (SYK) model with deformation [1], where the location of the transition and the behavior of various quantities near the transition has been analytically obtained and numerically verified [2].

On the other hand, the Aubry-Andrɛ́-Harper (cosine) type of lattice modulations in one spatial dimension offer a unique possibility of studying the localization where, in the absence of the interaction between the particles, all the single-particle eigenstates localize simultaneously as a function of the strength of the modulation. The stability of the delocalized superfluids in the presence of such a lattice modulation has been studied in [3]. In this work, we extend [3] to the case with nonhermitian terms in the Hamiltonian and discuss the phase diagram as well as the characterizing features of the MBL transition.

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Physical and chemical properties of complex intermetallic compounds

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Crystallographic features play an important role in the physical and chemical properties of a given solid-state material. In particular, crystallographically complex systems exhibit a wide range of properties – from unconventional superconductivity to peculiar magnetic orders. In this talk, I will highlight some of the new complex lanthanide- and actinide-based compounds that have been discovered as part of our recent investigations [1] – [4]. A comprehensive characterization of their properties has revealed a deep interrelation between their physical and chemical features. Notably, these compounds host a large number of atoms per unit cell (111-212) and a highly coordinated environment of lanthanide/actinide atoms (14-20). The $R/A_4Be_{33}Pt_{16}$ (R = Y, La - Nd, Sm – Lu, A = Th or U) compounds crystallize in noncentrosymmetric I43d cubic space groups. While the superconducting temperatures of these materials are rather modest, their noncentrosymmetry opens a possibility of time-reversal symmetry breaking. Additionally, we have shown that it is possible to tune the ground states of these compounds by means of chemical substitution – an enhancement of superconductivity or a suppression of the magnetic order can be achieved. By studying these systems, it is possible to expand the understanding of crystal chemistry of solid-state materials, while simultaneously providing an insight into which crystallographic parameters impact the physical properties of a given solid-state material.

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[2] A. Amon *et al.*, "$Y_4Be_{33}Pt_{16}$ - a noncentrosymmetric cage superconductor with multi-centre bonding in the framework", *Dalton Trans* 48, 9362 (2020)

[3] P. Kozelj *et al.*, "A noncentrosymmetric cage superconductor $Th_4Be_{33}Pt_{16}$", *Sci. Rep.* under review (2021)

[4] E. Svanidze *et al.*, "Crystal structure and physical properties of novel complex noncentrosymmetric compounds $R_4Be_{33}Pt_{16}$ (R = Y, La-Nd, Sm-Lu)" *Phys. Rev. Mat.* accepted (2021)

An experimental investigation of bulk electronic structure of high-order approximants and quasicrystal

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Approximants, the crystalline analogue of quasicrystals, are assumed to represent the quasicrystal phase in the electronic structure calculations and has been very successful to predict the existence of the pseudogap at the Fermi level of the related quasicrystal which is generally considered to stabilize it [1]. The Hume-Rothery mechanism predicts the pseudogap to be deeper in the parent quasicrystals than the approximants due to stronger interaction between the quasi-Brillouin zone and Fermi surface in the former. However, experimental endeavour to explore the bulk electronic structures of approximants, especially of high-order ones is very limited. In this present work, using hard x-ray photoelectron spectroscopy we have investigated the bulk electronic structures of two high-order quaternary approximants of F-type icosahedral (*i*)-Al-Pd-TM quasicrystal: Al-Pd-Cr-Fe and Al-Pd-Mo-Fe, having similar electron to atom (*e/a*) ratio as *i*-Al-Pd-Mn quasicrystal[2]. Both the approximants show a well-formed pseudogap at the Fermi level. Moreover, the pseudogap turns out to be deeper in the approximants compared to *i*-Al-Pd-Mn, and this is supported by specific heat data. Modifications in the line shape of Al 2*s* core-level main peak as well as the plasmon loss peaks provide evidence for enhanced hybridization of Al *sp* and transition metal *d* states in the approximants than *i*-Al-Pd-Mn, which could be one of the possible reasons for their larger pseudogap. The absence of magnetic exchange splitting in the Fe 2*p* core-level spectra establishes the nonmagnetic nature of the approximants.

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Thick quasiperiodic Sn layer

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Among inorganic materials, QCs exist mostly as ternary systems and these phases are stabilized due to existence of pseudogap at the Fermi level [1]. However, elemental quasicrystal in bulk form has not been discovered so far, which would be important for understanding the physical properties of QCs independent of their chemical complexity. In the present work, we have established the thickest (4 nm) quasiperiodic Sn layer reported until date using scanning tunneling microscopy (STM) and other related techniques including density functional theory calculations [3]. For submonolayer coverages, Sn forms pentagonal tiles (P-tiles) and its congregation. The unique motifs made up of P-tiles and hexagonal tile such as *crown* (half circular congregation of P-tiles), *wheel* (full circular congregation of P-tiles) and *triplet* (formed with three P-tiles) are observed. These motifs are different from the motifs observed on the substrate indicating different quasiperiodic arrangement of Sn. Also, the low energy electron diffraction patterns are distinct from the substrate and supports the STM results. Interestingly, thicker Sn layer indicates 3-dimensional quasiperiodic growth with formation of domes and retain its quasiperiodicity up to maximum thickness with motifs similar to the first layer. We propose Sn grows as a novel form of clathrate quasicrystal from our density functional theory calculations. The motifs observed by STM corroborates with clathrate model. The bulk clathrate exhibits gap opening near Fermi energy, while the free slab form exhibits a pronounced pseudogap, which explains the pseudogap observed in photoemission. Finally, our results indicates that Sn might be a suitable candidate for a bulk elemental quasicrystal.

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Superconductivity of metastable intermetallic compounds

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Metastable intermetallic compounds can be typically accessed either by application of high-pressure and/or high-temperature synthesis [1,2] or via redox preparation routes [3]. Recently, the superconductivity was found for the trigermanides [4] and trisilicides [5] of the earth-alkali and non-magnetic rare-earth metals [6] and also for the silicon-containing clathrate of Sr [1] and Ba [3]. For these both groups of compounds the characteristic feature is the covalent bonding in the triel-based frameworks and strongly polar (ionic) interactions between the metal species and the framework. For the other family of metastable superconductors – the compounds of bismuth with transition metals - polarity of the bonding is low [2,7]. Nevertheless, the polarity of atomic interactions transition metal-bismuth is often going in parallel with the low-temperature superconductivity. This correlation starts recently found even for the elemental bismuth (non-polar covalent boning, T_C = 0.00053 K and continues for the binary compounds of transition metals: $CoBi_3$ (0.48 K), $Cu_{11}Bi_7$ (1.36 K), $RhBi_4$ (2.82 K), Rh_3Bi_{14} (3.15 K). The transition temperatures for the interactions with the low polarity of the bonding are markedly lower. From this point of view is understandable, why no superconducting transition is reported for $FeBi_2$: due to the close to zero charge transfer, the T_C (if any) may be very low and comparable with that of elemental bismuth [8].

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Evolution of the CDW-type in the monophosphate tungsten bronzes family

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Charge density wave (CDW) systems are of fundamental and enduring importance because of the competition between incipient CDW formation and superconductivity, and also the possible application of CDW ground states in driving low thermal conductivity for efficient thermoelectric processes [1]. A CDW is a periodic modulation of the carrier density coupled to the crystal lattice and it normally coexists with a periodic lattice distortion.

An interesting example is the monophosphate tungsten bronzes family $(PO_2)_4(WO_3)_{2m}$, which presents a variety of CDW phases (since m denotes the thickness of the perovskite-like WO_6 - octahedra block) [2]. Three members will be used to explain the family behaviour and the evolution of the CDW-type. The first member, m=2, has a quasi-1D instability given by the WO_3-octahedra zig-zag chain and a thorough study of this system will be presented. The other two members (m=6 & 8) have both a quasi-2D electronic instabilities, with a weak and strong interaction between electrons and phonons, respectively.

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[2] P. Roussel *et al.*, Acta Cryst. B 57 (2001) 603-632

Strong coupling superconductivity in incommensurate host-guest structures

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Many complex materials display an interesting interplay between structural and electronic instabilities, which can be studied effectively under applied pressure. If a continuous structural phase transition is suppressed to low temperatures, as in the quasi-skutterudite system $(Sr/Ca)_3(Ir/Rh)_4Sn_{13}$ [1], low-energy vibrational excitations can arise that boost superconductivity and cause a linearly temperature dependent electrical resistivity, similar to the phenomenology near *magnetic* quantum phase transitions in Kondo lattice systems or iron-based superconductors.

The key role of low-lying modes, whether magnetic or vibrational, invites a closer examination of aperiodic host-guest structures. Because of their incommensurate structure, the possibility of a zero-energy sliding or phason mode is built in, without need for fine-tuning. The high-pressure host-guest structure of elemental bismuth indeed displays the hall-marks of enhanced spectral weight at low energies, with a strongly enhanced electron-phonon coupling constant and a steep, linearly temperature dependent electrical resistivity in the normal state [2]. We expand on this study by investigating superconducting and normal states in high pressure antimony and review numerical studies of electron-phonon coupling and strong coupling superconductivity in the aperiodic high pressure structures of potassium and sodium.

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Complex 2D oxide phases in reduced $SrTiO_3$ grown on $Pt(111)/Al_2O_3(0001)$: an experimental and theoretical approach.

[1]C.Ruano M,[1]T. T. Dorini, [1]F. Brix, [1]L. Pasquier, [1]S. Andrieu, [1]K. Dumesnil, [1]J. Ledieu, [1]O. Copie, [1]E. Gaudry, [1]V. Fournée and [1]M. Sicot

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Two dimensional oxide quasicrystals (OQCs) were recently discovered by annealing $BaTiO_3$ perovskite thin films epitaxially grown by magnetron sputtering on a single-crystalline Pt(111) substrate [1]. A similar OQC has been obtained in $SrTiO_3$ grown by molecular beam epitaxy (MBE) on Pt(111). In addition, Schenk *et al.* have shown that this OQC coexists with an approximant phase characterized by a monoclinic unit cell [2]. Here, we use a different approach in which the (111)-oriented single crystal is replaced by a 10 nm thick Pt(111) buffer layer grown by MBE on $Al_2O_3(0001)$ substrate. An ultra-thin film of $SrTiO_3$ was subsequently deposited by pulsed-laser deposition and annealed. The formation of a large square approximant with a lattice parameter approximately equal to 44.4 Å is evidenced by low-energy electron diffraction and scanning tunneling microscopy. High-resolution images allowed us to precisely determine the complex tiling consisting in 72 elements. Other complex hexagonal 2D phases have been observed depending on the preparation conditions. The structural and electronic properties of the phases were investigated by means of density functional theory (DFT). Simulated microscopy images were also obtained from a model identifying the bright protrusions as Sr atoms, providing an excellent agreement with the experimental observations. Charge transfer is found to occurs at the interface, from most electropositive elements (Sr, Ti) to most electronegative ones (Pt and O), influencing the rumpling and the adhesion energy of the oxide films.

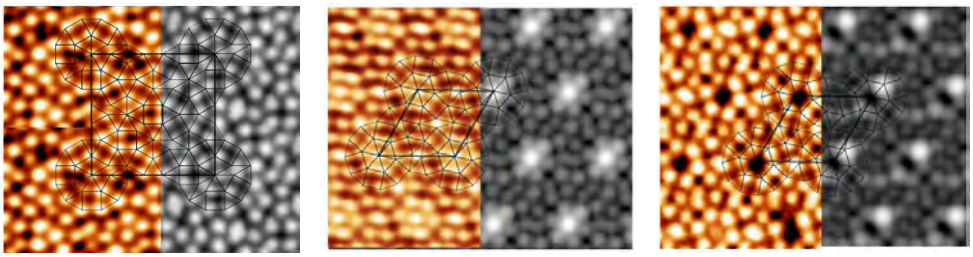

Figure1. Comparison between the experimental (orange) and calculated (gray) STM images for the square approximant (left) and the large hexagonal phase (middle and right). The ideal unit cells decorated with square, triangle and rhombus tiling elements are highlighted as well.

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[2] S. Shenck *et al.*, J. Phys.: Condens. Matter 29, 134002 (2017)

Flat-branched semisimplicial complexes: a versatile tool for aperiodic solids

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We introduce flat-branched semisimplicial (FBS) complexes as a universal language to describe aperiodic structures of finite local complexity. An FBS-complex naturally represents the set of local atomic arrangements occurring in the structure. It includes both metric and combinatorial data; the flexibility of the latter allows for incorporation of structural constraints on a longer range. An FBS-complex can embody "local rules" of any kind, whether or not they impose a perfect long-range order. We propose an algorithm for exploration of local rules in terms of an FBS-complex directly from the phased diffraction data [1]. The FBS complex describing a structure entirely determines the density of atomic species, and yields experimentally verifiable constraints on their contribution to the structure factors [2].

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Triangle-square-rhombus tilings arising from anti-phase domain boundaries in the σ-phase

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Dodecagonal oxide quasicrystals are the first natural realization of an aperiodic triangle-square-rhombus tiling described by Niizeki and Gähler [1-3]. Aiming on a fundamental understanding why these aperiodic structures spontaneously form on hexagonal substrates, a systematic screening of various substrate/overlayer combinations has been performed in recent years. In two-dimensional films derived from $BaTiO_3$ or $SrTiO_3$ on Pt(111), Pd(111) and Ru(0001), a multitude of approximants has been observed as a result of stoichiometry variations and the exact heat treatment [4-6]. We report here on a mechanism to compensate for stoichiometry variations, based on the formation of anti-phase domain boundaries. With their help, the vertex density in periodic structures is tuned over a wide range. Our examples are based on the σ-phase approximant. It is a pure triangle-square tiling with one vertex configuration only (white in Fig.1). In two-dimensional layers derived from $BaTiO_3$ and $SrTiO_3$ on Pd(111), anti-phase domain boundaries between σ-phase patches generate rhombuses in the tiling. Thus, a new vertex configuration appears (black in Fig. 1). Compared to the σ-phase, the vertex density in these tiling motifs can be increased beyond that of the Niizeki-Gähler tiling.

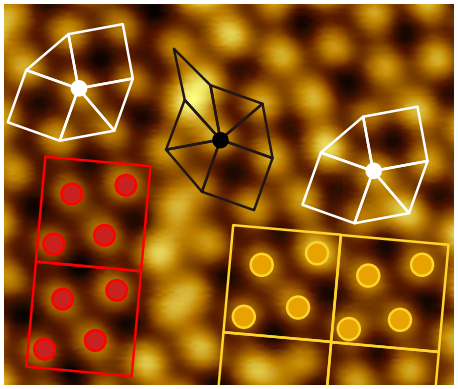

Fig. 1: Scanning tunneling microscope image of a $BaTiO_3$ 2D-film on Pd(111) with the unit cells of two domains of the σ-phase in red and yellow. The anti-phase domain boundary results in the formation of rhombuses and a new vertex configuration (black).

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Resonant Elastic X-ray Scattering at beamline P09 at PETRA III at DESY

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Resonant X-ray elastic scattering (REXS) is a unique element, site and valence specific probe to study the charge, spin and orbital degrees of freedom in solids. This technique, which combines x-ray diffraction with x-ray absorption spectroscopy, is a powerful probe, accessible at modern X-ray light sources. In Europe, beamline P09 at the PETRA III 3rd generation synchrotron source at DESY is a-state-of-the-art REXS instrument [1] much unique in the variety of low temperature and high magnetic fields sample environments available to investigate strongly correlated electron systems and magnetic materials in the hard X-ray range [2] and by the full polarization analysis capabilities allowing it to disentangle between different order parameters. In this talk, I will introduce the REXS technique and P09 beamline and focus more particularly on our efforts in the last 3 years towards enabling magnetic X-ray scattering in the tender X-ray range, magnetic scattering at high pressure and low temperature, full magnetic structure determination from REXS with the computing crystallographic software MagStREXS. Examples of scientific problems in the field of quantum matter that these implementations are allowing to address will be presented [3][4].

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Correlated Insulators in Twisted Bilayer Graphene

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Recently, moiré superlattices in 2d van der Waals heterostructures have been found to exhibit properties analogous to the high-T_c cuprates, namely, Mott insulating states and unconventional superconductivity. Examples include magic-angle twisted bilayer graphene and transition metal dichalcogenides. These being (chemically) simpler / cleaner systems compared to the transition metal oxide superconductors, have emerged as new experimental systems for studying strongly correlated phases, allowing higher degrees of experimental control. Experiments on twisted graphene bilayers, where the top layer is rotated with respect to the one below, have displayed insulating behavior when the moiré bands are partially filled. I will elaborate on our recent calculations to find the static charge configurations in these phases, and to estimate the excitation gaps.

Large unit cell approximant derived from $SrTiO_3$ on Pt(111)

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The discovery of two-dimensional oxide quasicrystals (OQC) draws attention to aperiodic structure formation from perovskite materials on Pt(111) [1,2]. On the atomic level, the OQC represents an aperiodic self-similar tiling consisting of equilateral triangles, squares and rhombuses first described by Nizeeki and Gähler.

On this poster, we present low-temperature scanning tunneling microscopy (STM) and surface x-ray diffraction (SXRD) investigations of the largest unit cell approximant known so far in 2D systems. Its unit cell covers an area of approximately 44 Å×44 Å and has p2gg symmetry. STM measurements show 48 atoms in the unit cell forming the vertices of 48 triangles, 18 squares and 6 rhombuses. The structure has been solved utilizing over 300 independent reflexes measured by SXRD with an R-factor better than 0.20. Figure 1 shows the SXRD diffraction image of the structure superposed with the grid of reflexes from the approximant and the OQC. From this analysis a profound understanding of the decoration of all tiles with Sr, Ti, and O ions is derived, which also solves the structure of the parent OQC. Note that modified inflation/deflation rules with four inequivalent tiling elements are necessary for a proper description of the Niizeki-Gähler tiling.

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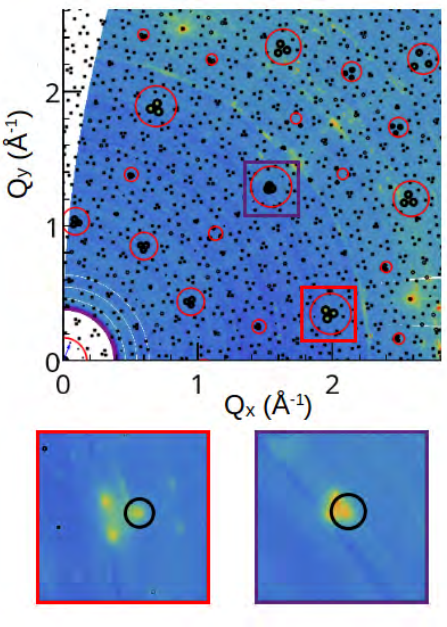

Figure 1: Surface X-ray diffraction data of the QC approximant (top image): Red circles mark position and intensity of the OQC diffraction spots; black cicles indicate the approximant Bragg peaks, which occur in six different domains due to rotational and mirror symmetries. The red and purple boxes correspond to the zoomed images below, where the spots of an individual domain are marked.

MagStREXS: a Crystallographic Software for Magnetic Structure Determination through Resonant X-Ray Magnetic Diffraction Data

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Strongly correlated electron systems have been a very active research field during the last decades because of the wide range of different phenomena found in these materials. In particular, competing interactions within these compounds can lead to exotic long-range magnetic orderings, both periodic and aperiodic.

Resonant Elastic X-ray Scattering (REXS) is a unique element, site, and valence specific probe to study charge, spin and orbital properties in solids and thin films [1,2], and has been successful in unraveling different degrees of freedom and characterizing magnetic structures. Regarding magnetic structure determination, different types of data can be collected during a REXS experiment, but the analysis of these data is highly complex, and no software has been developed to facilitate it.

MagStREXS is a crystallographic software dedicated to the determination of **Mag**netic **St**ructures through **R**esonant **E**lastic **X**-ray **S**cattering and the preparation of magnetic diffraction experiments, being developed since mid-2017 at beamline P09 [5] at PETRA III (DESY).

Hereby, we will present an overview of MagStREXS, its current status and some of the magnetic structures which have already been solved with it in the field of highly correlated systems.

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Thursday 7 October 2021

8 h 00	S. Watanabe : Elasticity, crystalline electric field and magnetism in the Yb- and Tb-based quasicrystal and approximant. On line	Invited	30 min.
8 h 30	M. Henriques : Magnetic structure superspace and Jana. On line	Invited	30 min.
9 h 00	U. Lieu : Inverse Design of Two-dimensional Self-assembly of Patchy Particles. On line	Contributed	20 min.
9 h 20	N. Yoshinaga : Bayesian Inference of Phase-Field Crystal Models for Target Crystalline Patterns. On line	Contributed	20 min.
9 h 40	N. Fujita :Pseudo-merohedral twinning of AlCuRu. On line	Contributed	20 min.
10 h	Break		
10 h 30	D. Le Bolloc'h : Deformation of an incommensurate CDW under currents. On site	Invited	30 min.
11 h 00	S. Foerster : Accounting for complexity in periodic systems: A classification scheme for quasicrystal approximants. On line	Invited	30 min.
11 h 30	S. Coates : A 6-fold golden-mean tiling. On line	Contributed	20 min.
11 h 50	R. Lifshitz : Thermodynamic stability of quasicrystals: From fluid dynamics to soft condensed matter. On site	Contributed	20 min.
12 h 10	Closing remarks		20 min.
12 h 30	Lunch		
14 h 00	Departure		

Elasticity, crystalline electric field, and magnetism in the Yb- and Tb-based quasicrystal and approximant

Shinji Watanabe

Kyushu Institute of Technology, Kitakyushu, Japan

Quantum critical phenomena discovered in quasicrystal (QC) $Au_{51}Al_{34}Yb_{15}$ have attracted great interest in condensed matter physics [1]. The criticality and its robustness against pressure as well as the emergense of the same criticality in the pressure-tuned approximant crystal (AC) were explained by the theory of critical Yb-valence fluctuations (CVF) [2,3]. Recent observation of a sharp change in the Yb valence in the QC $(Au_{1-y}Cu_y)_{51}(Al_{1-x}Ga_x)_{34}Yb_{15}$ at $x = 0$ and $y = 0$ has evidenced the quantum valence criticality in $Au_{51}Al_{34}Yb_{15}$ [4].

The elastic property of the quantum critical QC $Au_{51}Al_{34}Yb_{15}$ has been analyzed theoretically on the basis of the AC [5]. First the effective model for the 4f and 5d states at Yb and the 3p states at Al has been constructed by considering the crystal symmetry accurately. Then the Coulomb repulsion between the 4f and 5d states at Yb is clarifed to be the origin of the quantum valence criticality. At low temperatures well below the first excited energy of the crystalline electric field (CEF), anomalous temperature dependence of the elastic constant is shown to emerge. Below 5 K, remarkable softening in the bulk modulus and longitudinal mode is shown to be caused by the enhanced CVF.

Recently, the CEF Hamiltonian in the rare-earth based QC and AC has been formulated theoretically [6]. By applying this formulation to the quantum critical QC $Au_{51}Al_{34}Yb_{15}$, the CEF has been analyzed with consideration for the effect of Al/Au mixed sites [6]. The ratio of the valences of the ligand ions of Au and Al is shown to play a key role in characterizing the CEF ground state.

Very recently, the CEF in the Au-SM-Tb QC and AC has been analyzed theoretically [7]. By constructing the effective model for the CEF ground state, the magnetic properties have been clarified in the Au-SM-Tb AC and QC [7,8].

In the presentation, I will report these newly clarified theoretical results and will discuss the possible relevance to current and future experiments.

This presentation is based on the work done in collaboration with K. Miyake and M. Kawamoto.

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[7] S. Watanabe, submitted.
[8] S. Watanabe, submitted.

Modulations in magnetic materials

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Modulated magnetic structures are constantly discovered in a variety of materials. Commensurate and incommensurate magnetic structures can be described using the superspace approach [1]: the magnetization density can be generalized to higher-dimensional spaces to recover the translation symmetry. Within this formalism, the underlying spin arrangement can be described by a periodic modulation function of the magnetization density.

The symmetry of modulated magnetic structures can be unambiguously described using magnetic space and superspace groups. The symmetry relations provide a robust description of the symmetry modes for the spin configuration and its constraints consistent with the parent paramagnetic phase and the magnetic propagation vector.

Here we will review the fundamental concepts of superspace formalism and magnetic symmetry. In particular, the magnetic option implemented in Jana2020 is capable of handling different sets of diffraction data to consistently solve and describe commensurate and incommensurate magnetic structures based on symmetry considerations [2]. Several examples of incommensurate magnetic ordering models in magnetic materials containing f-elements will be presented.

In rare-earth-based intermetallic compounds, the oscillatory character of the RKKY (Ruderman-Kittel-Kasuya-Yosida) exchange causes competing interactions which often frustrate magnetic moments. It is the case of the compounds belonging to the families $R_3Ru_4Al_{12}$ (R is a rare-earth element), $R_2Co_3Al_9$ and RFe_5Al_7 [3]. They display multiple spontaneous and induced phase transitions and complex magnetic structures that provide an opportunity to study the interplay among magnetic frustration, exchange interactions, and magnetic anisotropy.

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Inverse Design of Two-dimensional Self-assembly of Patchy Particles

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Patchy particles are the particles with anisotropic surface patterns or patches on specific positions on the surface. The interaction of such particles is not only dependent on the distance, but also on their mutual orientations. Therefore, the patchy particles are capable of organising themselves into complex structures, which are important for the generation of novel materials. Even for the case of spherical particle, there are countless ways designing patchy particle. If one tries the self-assembly of any possible particle design, it consumes exhausting time and cost due to uncountable design of the patchy particle.

This can be solved by applying inverse design, i.e., from a desired target structure, a class of computational iteration techniques is used to tune the design of particle until the particles can self-assemble into the desired target. We have developed and applied our inversed design optimisation scheme for some two-dimensional structures. Among many candidate patchy particles, it suggests some types of patchy particle can create a square lattice or kagome lattice. In particular, we have found the 5-fold symmetry patchy particle can self-assemble into dodecagonal quasicrystal (see Figure). We have also analysed the kinetics and posible mechanisms of the formation of the dodecagonal quasicrystal.

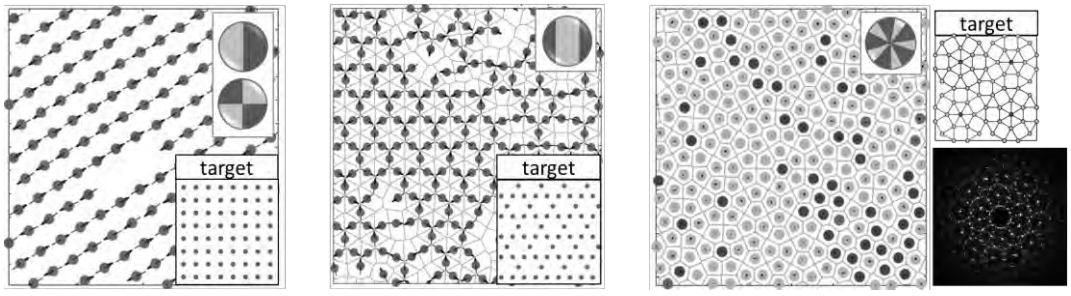

Figure: The generated structure from the optimisation scheme and the estimated patchiness in comparison with the target (inset). The target is square lattice (left), kagome lattice (middle), and dodecagonal quasicrystal (right, with Fourier transform). Voronoi tessellation is included. The arrows on the particle are local orientational field.

Bayesian Inference of Phase-Field Crystal Models for Target Crystalline Patterns

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Partial differential equations (PDE) have been widely used to reproduce patterns in nature. Despite a number of PDE models have been proposed, they rely on pre-request knowledge of physical laws and symmetries, and it requires significant efforts to develop a model reproducing a desired pattern. The challenge is quantitative and physically interpretable modelling of a complex phenomenon, which demands both developing a model and parameter estimation. The identification of a model equation is a recent key topic of machine leaning and data science.

We propose an inverse problem of phase-field crystal models for structural pattern formation [1]. From one snapshot of a target pattern, we successfully estimate the best model and its parameters using Bayesian model selection. We show the order parameters extracting symmetries of a pattern together with Bayesian modelling successfully estimate parameters as well as the best model to make the target pattern. We apply our method to nontrivial patterns, such as 2D quasicrystals (QC), a double gyroid, and also Frank Kasper A15, which is known as an approximant of 3D dodecagonal QC. Using the estimated parameters, we successfully reproduce 3D DDQC using the continuum model, which has been reproduced only by particle models.

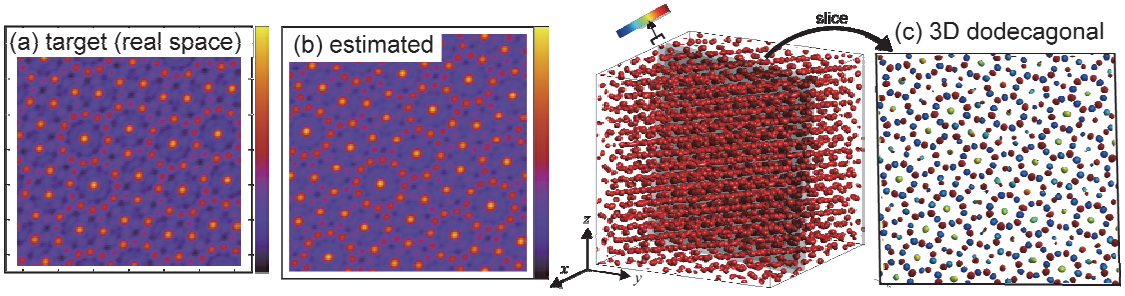

Figure: (a,b) The density field of the target and estimated structures for 2D DDQC. (c) 3D DDQC generated by the phase-field crystal model.

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Pseudo-merohedral twinning of α-AlCuRu

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α-AlCuRu [1] is referred to as the 1/1 cubic approximant to the F-type icosahedral phase, i-AlCuRu [2]. Two decades have passed since it was determined to be a cubic crystal with a CsCl-type arrangement of two Mackay-cluster-like motifs [3]. The latter represents the same structure type and space group ($Pm\bar{3}$) as those reported for α-AlMnSi [4]. However, there is a concern that this structure might not be the ultimate structure solution of α-AlCuRu. In particular, its incompatibility with a recently proposed geometrical framework for describing the atomic structure of icosahedral approximants in Al based alloys [5] motivated us to examine the structure with fresh eyes.

A few years ago, we started to re-examine the structure of α-AlCuRu by synthesizing high-quality mm-sized grains through long-time annealing (up to 30 days) under Ar atmosphere at slightly below the maximum temperature of its satability. Although our single-crystal X-ray as well as electron diffraction data are consistent with the reported cubic structure, dark field electron microscopy images indicate mesoscopic texture patterns showing many single domains of roughly about 100nm in diameter. The diffraction peaks from neighbouring domains fully overlap, such that these domains appears to present pseudo-merohedral twins with symmetry breaking in each twin individual. High-resolution transmission electron microscopy images show that the domain (or twin) boundaries are parallel to two kinds of crystallographic planes: {100} and {110}. We use the STEM-HAADF technique to study atomic details of the twin boundaries. Interestingly, a pair of twin boundaries meeting at a linear intersection can fuse into a single twin boundary. Thus, the texture patterns are characterized by the fusing and splitting of twin boundaries. A tentative use of the Bragg coherent X-ray diffraction imaging technique for studying the mesoscopic domain structures will also be presented.

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Deformation of an incommensurate CDW under currents

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1. *Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, 91405 Orsay.*

Some crystals display incommensurate Charge Density Waves (CDW). Under applied currents, these systems may show a singularity of their resistivity curve involving the CDW itself. This effect, called sliding CDW, is probably related to the appearance of solitons under external fields. However, the origin of these topological singularities, the overall behavior of the CDW at the sample scale is not well understood.

We have studied a model CDW system using x-ray scanning diffraction and phase reconstruction techniques allowing to follow the global deformation of the CDW under applied currents. We observe that the periodic modulation continuously deforms, bends, from one edge of the sample to the other over several tens of micrometers. This effect is surprising given that the CDW period is about ten of Angtroms. This macroscopic deformation of the incommensurate modulation under currents can be explained by considering surface pinning.

From a theoretical point of view, the sliding phenomenon has been always understood by considering an empirical bulk pinning parameter. By considering the incommensuarte modulation as a charged objet, pinned at each surface, the overall deformation can be described without considering bulk pinning, in agreement with the observation.

Accounting for complexity in periodic systems: A classification scheme for quasicrystal approximants

Stefan Förster, Maniraj, Loi Vinh Tran, Friederike Wührl, Oliver Krahn, Sebastian Schenk, Martin Haller, and Wolf Widdra

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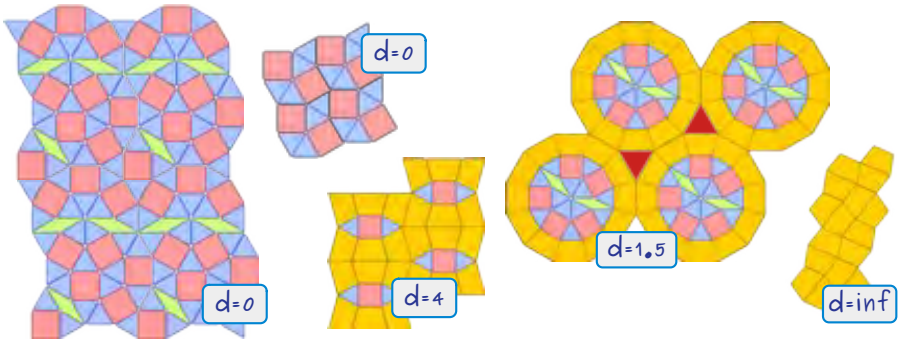
In the last decade a variety of two-dimensional (2D) periodic structures have been reported that relate to 2D quasicrystals (QC) [1-4]. Among these structures, there are QC approximants, but also structures that exhibit only weak relations with a parent QC. However, many of these structures include 2D patches, which originate from the QC.
In the following, we will introduce a classification scheme for QC approximants, which reflects the varying proximity to the parent QC and which will be discussed for the case of dodecagonal oxide quasicrystals. For $BaTiO_3$-derived structures on Pt(111) and Ru(0001) as well as for $SrTiO_3$-derived structures on Pt(111). Structures are covered that periodically repeat QC patches in which the sequence of tiles is flipped, or which consist of tiles of the QC but include vertex configurations that are not allowed for the QC. In addition, we introduce pseudo-approximants as structures that host tiles in the unit cell, which are not present in the QC. We distinguish indexable and non-indexable structures and introduce a deviation factor **d** as a measure for the deviation of the unit cell from a patch of the QC. We apply this classification scheme to all 2D structures related to the oxide quasicrystal and to the prototypical 1D aperiodic example of the Fibonacci sequence. The signatures of all classes of approximants are discussed not only in parallel space, but also in the reciprocal space and the internal space.



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A 6-fold golden-mean tiling

Sam Coates[1], Ron Lifshitz[2], Akihisa Koga[3], Hem Raj Sharma[4], Ronan McGrath[4], Ryuji Tamura[1]

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Aperiodic tilings are of great importance for modelling and investigating quasicrystalline systems. Single-length tilings with rotational symmetries incommensurate with periodicity have, understandably, largely dominated these investigations. However, there is great scope for expanding families of aperiodic tilings both in terms of multiple length-scales, and, rotational symmetries commensurate with periodicity, while still retaining links to physical quasicrystals.

Here, we present a multiple length-scale, 6-fold golden mean aperiodic tiling which is a 'special' case from a family of 3-fold tilings. We introduce its formalism in terms of the dual grid method, substitution rules, and higher-dimensional projection. If time permits, we may discuss a Monte Carlo spin model which demonstrates a rich magnetic phase diagram, and, likewise the tiling's behavior in the tight-binding model.

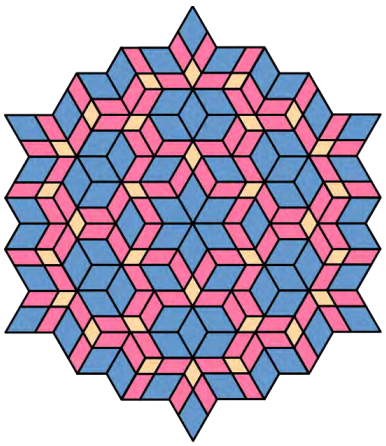

Figure 1: A simplified version of the 6-fold tiling

Thermodynamic stability of quasicrystals: From fluid dynamics to soft condensed matter

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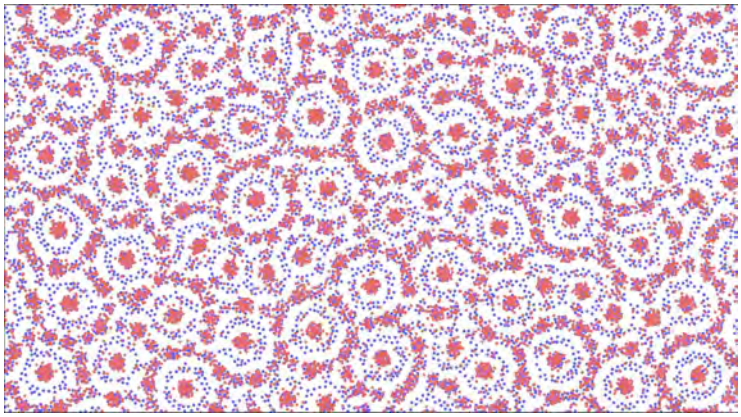
As early as 1985, Landau free-energy models and density-functional mean-field theories were introduced in an attempt to explain the stability of quasicrystals, with only partial success if any. It is only in recent years, that great progress has been made in understanding the thermodynamic stability of quasicrystals in such simple isotropic classical field-theories. Much of this has happened thanks to insight from the experimental observation of quasicrystalline order in diverse systems ranging from fluid dynamics to soft condensed matter. The key to unlocking the stability puzzle was in the realization that more than a single length scale was required, but more importantly in figuring out how to introduce these multiple scales into the models, and identifying the remaining requirements. We and others have since managed to produce Landau and other mean-field theories with a wide range of quasicrystals as their minimum free-energy states, and have also confirmed some of these theories using molecular dynamics simulations with appropriately designed interparticle potentials. I shall give a quick overview of the quasicrystals that can be stabilized in these theories—in systems of one or two types of particles, in two and in three dimensions—and attempt to identify a trend that might be emerging in going from Landau theories to more realistic density-functional mean-field theories. It remains an open question whether this trend may eventually lead to understanding the stability of quasicrystals in complex metallic alloys.



Formation of a binary dodecagonal quasicrystal. [Reches, Savitz & Lifshitz, In preparation].

This research is supported by Grant No. 1667/16 from the Israel Science Foundation.

Posters

Resonant „forbidden” reflections in aperiodic crystals

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Nils Blanc[2], *Stephen* P. Collins[3], *Gareth* Nisbet[3],
Surya Rohith Kotla[4], *Sander* Van Smaalen[4], Peter Gille[5],
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Some symmetries in crystal structures are responsible for systematic extinctions of reflections (for instance, in FCC crystals, it is well known that reflections are allowed only if h, k and l are of the same parity). Nevertheless, in the case of glide plane and screw axes symmetries, the forbidden reflections can be observed at an X-ray absorption edge of the material, thanks to the anisotropy of the tensor of scattering, which encodes the local electronic anisotropy of the resonant atoms [1,2]. Such resonant “forbidden” reflections are well known for periodic crystals.
In this contribution, we present the first experimental demonstration (to our knowledge) of such reflections in aperiodic crystals. We present results on crystals from two classes of aperiodic crystals: d-AlCoNi, a decagonal quasicrystal, and Rb_2ZnCl_4, an incommensurately modulated crystal. In the former case, the forbidden reflections are mostly due to the intrinsic symmetry of the quasicrystal. In the latter case, however, the intensity of forbidden reflections can be related to atomic displacements with respect to the symmetric (commensurate) structure [3], similarly to the case of a few periodic crystals [4–9].

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Complex magnetism in Co-Te systems

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There is great interest in designing and finding new materials with multiferroic properties, or in a broader sense, with magnetic and dielectric ordering close to room temperature [1]. Complex crystal structures with several independent sites for magnetic cations, as well as complex magnetic structures, have been found to favor concomitant dielectric and magnetic coupled states [2]. On the other hand, the complex metal oxides related to corundum have attracted the interest of the scientific community due to their dielectric and magnetic properties, specifically Co_3TeO_6 which shows a monoclinic space group C2/c and displays an incommensurate, multi-propagation vector and temperature-dependent [3]. It is the interest of this work to show a study on two monocrystalline compounds, a new phase b-Co3TeO6, $Pna2_1$ space group with a=5.3465(13) Å, b=8.874(2) Å, c=9.445(2) Å as lattice parameters that has two transition temperatures T_1=20 K and T_2=36 K. As well as the study of $Co_6Te_3O_{12}Cl_2$ $P4_2/mbc$ a=b=8,3871(7) Å, c=18,5634(19) Å. Physical, neutron and X-ray measurements were obtained on single crystal samples that were synthesized using the chemical vapor transport technique. In this work I will show our experimental study of magneto electrical coupling combining neutron and laboratory X-ray diffraction.

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Dynamical Properties of the Incommensurately Modulated Rb_2ZnCl_4 Phase

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Aperiodic crystals structure are generally well described, but their dynamics are more debated. In particular, phason modes have been experimentally observed in few incommensurately modulated phase and quasicrystals.

The Rb_2ZnCl_4 phase displays several transitions. Above T_i=303K the HT phase is described as a crystal structure of space group Pmcn where $ZnCl_4$ tetrahedrons have disordered orientations. From T_i=303K, down to T_C=195K, the orientation of the $ZnCl_4$ tetrahedrons gets incommensurately modulated along the c axis with an increasing anharmonicity. Below T_C, the modulation gets locked-in, the c cell parameter is then tripled. We probed the dynamics of this material through inelastic neutron scattering with the IN6-SHARP, IN5, IN12, IN22 and THALES instruments of the ILL, and with the 1T spectrometer of the LLB for temperatures between 140K and 350K.

At 140K, all the TA phonons have consistent integrated intensities whether they are associated to superstructure or substructure reflections. As temperature increases towards T_C, the integrated intensity of superstructure related TA phonons decreases. At the same time, a large quasi-elastic signal localized around the superstructure reflections appears and increases in intensity with temperature. At T_C, the superstructure reflections are splitted along the c* axis into satellite reflections up to the 5th order. The quasi-elastic signal continues to grow with increasing temperatures in the incommensurate phase while the relative intensity of the TA phonon associated to satellite reflections continues to decrease. This quasi-elastic signal width increases with distance to the satellite and might be interpreted as a diffusive phason mode. Above T_i, the satellites reflections transform into large diffuse elastic spots. At 350K the localized quasi-elastic signal dominates, but a weak and large mode is found to disperse like a TA phonon around the diffuse elastic spots, indicating some remaining long-range correlated excitation despite the prevailing disorder of the $ZnCl_4$ tetrahedrons int the HT phase.

Are incommensurate systems model compounds for disorder revealing low-temperature glass-like behavior ?

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Despite long and continuous efforts during the past century, the physics of glasses and generally non-crystalline (amorphous) materials still stands as one of the most challenging topics in solid state physics. One of the reasons lies in the difficulty to apply theoretical concepts developed for crystalline materials to the non-crystalline counterparts. Glasses lack the translational symmetry of crystals and concomitant periodicity which is the basis of the modern (and highly successful) solid state theory. Although being solids, glasses have the atomic structure without long range order, very close to that observed in the supercooled liquids.

Glasses and liquids have many other features in common as well. A prominent and universal one is the anomalous low temperature (T) specific heat (C_p) which strongly deviates from the $C_p(T) \propto T^3$ dependence coming from gapless acoustic vibrations. Two ubiquitous features are observed in the –*a priori* flat– $C_p(T)/T^3$ plot : i) a broad maximum, so-called Boson Peak (BP), at $\sim$10 K and ii) an upturn below 1 K. These two features are generally considered independently.

As the precise origins of these thermodynamic features are still unknown, it seems reasonable to address these topical problems by studying the simplest, model systems that systematically show them both. The amorphous state can be viewed as a multiple incommensurate modulation of a crystal with the modulation wavevectors spanning the 3D reciprocal space, we believe that our approach may be relevant in the understanding of these two long standing problems in glasses. In this work we present the crystalline systems with incommensurably modulated superstructure as one such model and investigate experimentally and theoretically their low temperature specific heat.

Monte Carlo Study of the Magnetic Properties of Pseudo-Tsai Clusters

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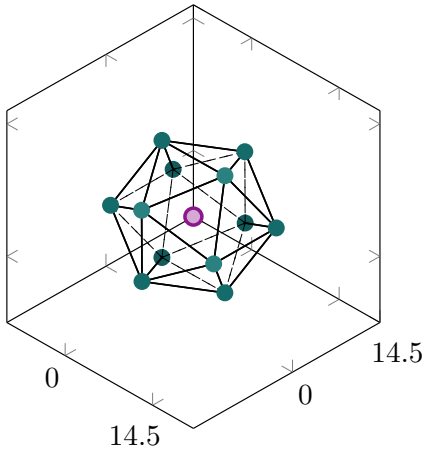
Due to the complex geometries of quasicrystal approximants, sophisticated numerical methods are needed to investigate thermodynamic properties of magnetic models on such lattices. This poster presents an overrelaxed heat bath Monte Carlo algorithm, which we then use to study magnetic models. Results are presented on the novel pseudo-Tsai clusters which have an additional magnetic site in the cluster center. A sketch of the geometry is given in the figure below; an icosahedral shell with magnetic sites at the vertices (in green) and an additional central site at the center (illustrated in purple, with lighter color in the middle). We show that the cluster center moment is more susceptible to thermal fluctuations.



Two-dimensional metal structures revealed by evolutionary computations: $Pb/Al_{13}Co_4(100)$ as a case study

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We have combined extensive Density Functional Theory calculations with an evolutionary algorithm to investigate possible structural models for two-dimensional (2D) Pb films supported on the $Al_{13}Co_4(100)$ quasicrystal approximant. The minimization of the total energy with the constraint of maximizing the atomic density in the layer leads to 2D atomic arrangement with pentagonal motifs, reflecting the symmetry of the substrate. Our findings show that the 2D Pb structure can be interpreted as a stable structure, with 16 Pb atoms in the surface cell, in good agreement with the measured coverage and scanning tunnelling microscopy images. Alternatively, a metastable 15-atom 2D film also fits with the experimental observations. This study opens a route towards the prediction of supported complex 2D films [1].

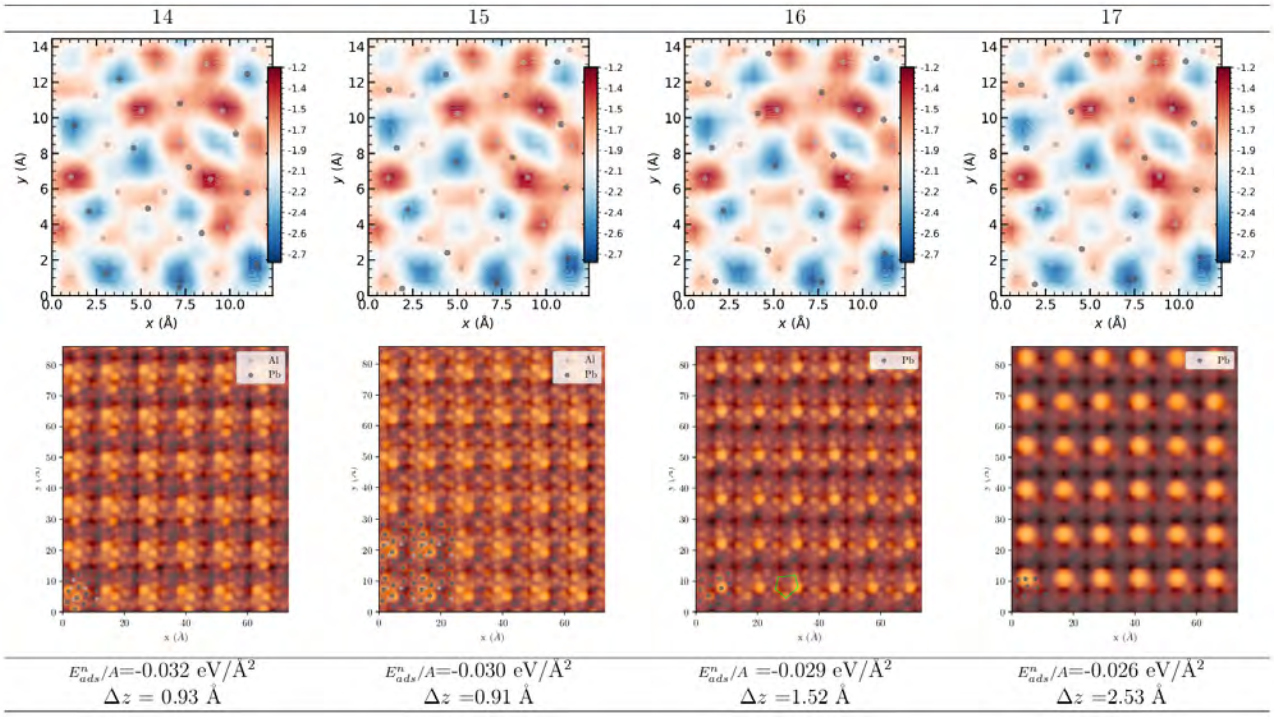

Fig.1 : Adsorption energies, structures and simulated STM (scanning tunneling microscopy) images for 2D Pb-films with different atomic densities on Al13Co4(100).

[1] F. Brix and E. Gaudry , Two-dimensional metal structures revealed by evolutionary computations: $Pb/Al_{13}Co_4(100)$ as a case study, submitted

Beyond the constraints of chemistry: Crystal structure discovery in particle simulation data

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Do we know all conceivable crystal structures? This question appears naive at first, because crystallography is a mature field. But the list of reported inorganic crystal structures is not necessarily representative of all kinds of order that are possible on other scales. Atomic crystal structures are affected by the discreteness of the periodic table and the resulting constraints on chemical bonding. Molecular crystals, metal organic frameworks, nanoparticle superlattices, and other soft-matter assemblies are free from these chemical constraints and can exhibit entirely new types of crystallographic order distinct from those found with atoms. A universal list of all plausible crystal structures in systems of particles ranging from the angstrom to the micrometer scale would benefit the search for—and design of—new materials.

Here, we perform a data-driven simulation strategy to systematically crystallize one-component systems of particles interacting with isotropic multiwell pair potentials resembling Friedel oscillations and encoding and generalizing quantum mechanical interactions [1]. We investigate two tunable families of pairwise interaction potentials. Our simulations self-assemble a multitude of crystal structures ranging from basic lattices to complex networks. The goal is to discover crystal structures on the computer *de novo*, a strategy which has so far not been attempted on such a diverse set of systems. We perform a semi-automatic crystal structure analysis of simulation data. Our analysis reveals sixteen structures that have natural analogues spanning all coordination numbers found in inorganic chemistry. Fifteen more are hitherto unknown and occupy the space between covalent and metallic coordination environments. We describe the numerical search, the analysis technique, phase diagrams, and details of the known and previously unknown crystal structures. The discovered crystal structures constitute novel targets for self-assembly and expand our understanding of what a crystal structure can look like.

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