## International scientific seminar "Advanced Functional Materials for Digital and Quantum Electronics' 2024"

Thursday, 19 September -- Saturday, 21 September 2024

# BOOK OF ABSTRACTS

MIPT

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The workshop was supported by the project "Advanced functional materials for digital and quantum electronics" (No.075-15-2024-632) - Grant from the Ministry of Science and Higher education of the Russian Federation.

## Thursday, September 19, 2024

## Location: Room 119, Main Building, MIPT

## Session Chair: Prof. Alexander GOLUBOV

08:30-09:15	Registration
09:15-09:30	Opening Ceremony. CMN' review of scientific activity ( <b>Prof. Vasily</b> <b>STOLYAROV</b> , <b>Prof. Alexander GOLUBOV</b> )
09:30-09:45	BIT' review of scientific activity (Prof. Wei JIANG, Yang GAO)
09:45-10:15	<b>Prof. Alexander MELNIKOV</b> <i>Photogalvanic phenomena in superconductors supporting intrinsic diode effect</i>
10:15-10:30	<b>Mark NAUMOV</b> Transport measurements and technology of Sb, Ge doped magnetic topological insulator MnBi <sub>2</sub> Te <sub>4</sub> with superconducting contacts
10:30-11:00	Coffee Break & Take Photos
11:00-11:30	Prof. Peng LIU Constraint-Dependent Physical Quantities in Active Baths
11:30-11:45	<b>Can ZHANG</b> Nanoscale visualization of symmetry-breaking electronic orders and magnetic anisotropy in a kagome magnet YMn <sub>6</sub> Sn <sub>6</sub>
11:45-12:15	<b>Prof. Quanzhen ZHANG</b> Controllable Construction and Electronic Properties Investigation of Two-Dimensional TMDs Heterojunction and Homojunction
12:15-12:30	<b>Dr. Andrey ZHUKOV</b> <i>Quantum error mitigation in the regime of high noise using deep neural network: Trotterized dynamics</i>
12:30-14:00	Lunch at MIPT Cafe

Session Chair: Prof. Alexander MELNIKOV	
14:00-14:30	<b>Prof. Valter POGOSOV</b> <i>Effects of photon statistics in wave mixing on a single qubit</i>
14:30-14:45	Jingyi DUAN Three-Dimensional Multi-Orbital Flat Band Models and Materials
14:45-15:15	<b>Prof. Alexander KORNEEV</b> <i>Cryogenic low-range resistors for advanced superconducting quantum electronics</i>
15:15-15:30	<b>Pavel ABRAMOV</b> Impact of copper ions and aqueous cations on eumelanin properties: insights from infrared spectroscopy
15:30-16:00	Coffee Break
Session Chair: P	rof. Valter POGOSOV
16:00-16:15	<b>Jijian LIU</b> A Universal Strategy for Synthesis of 2D Ternary Transition Metal Phosphorous Chalcogenides
16:15-16:45	<b>Prof. Yangguang JU</b> Exploring Oxygen Instability in Tin Perovskites: Insights and Advances in Sensing Applications
16:45-17:00	Lin JIA Mixing entropy
17:00-17:30	<b>Stepan SOTNICHUK</b> Electrochemical preparation of metallic nanowires for superconducting microelectronics
17:15-20:00	Reception (2 <sup>nd</sup> floor of Concert Hall)

## Friday, September 20, 2024

## Location: Room 119, Main Building, MIPT

## Session Chair: Prof. Irina BOBKOVA

09:00-09:30	<b>Prof.</b> Dmitry USACHOV Surface and bulk electronic structure and magnetism of lanthanide compounds probed with photoemission
09:30-09:45	Lili ZHOU Intertwined quantum confinement effects in charge-density-wave nanostructures
09:45-10:15	<b>Prof. Alexander BARYSHEV</b> Magneto-optical materials for optical applications: Bi:YIG made by metal-organic decomposition and crystallized by laser annealing, and gasogyrochromism in oxidized permalloy
10:15-10:30	<b>Alexander MELENTEV</b> Controlling the dielectric response of SrTiO <sub>3</sub>
10:30-11:00	Coffee Break
11:00-11:30	<b>Prof. Geliang YU</b> Novel physics in twisted systems
11:30-11:45	Victor KOCHETKOV (CRYOSYSTEMS)
11:45-12:00	Artem Ryabokul (AKMETRON)
12:00 -12:15	Mikhail ALEKSEEV (CRYOTRADE ENGINEERING)
12:15-12:30	COLAB.WS
12:30-14:00	Lunch at MIPT Cafe

Session Chair: Prof. Dmitriy USACHOV	
14:00-14:30	<b>Dr. Sergey BAKURSKIY</b> Superconducting Trigger Effect in Multilayer Hybrid Structures
14:30-14:45	<b>Dmitriy KALASHNIKOV</b> <i>Demonstration of a Josephson vortex-based</i> <i>memory cell with microwave energy-efficient readout</i>
14:45-15:15	<b>Dr. Victor SEMIN</b> XPS study of native oxide films formed onto TiNi-based alloy modified by ion-beam treatments
15:15-15:30	Liu YANG A new Mn-Bi-Te ternary antiferromagnetic topological insulator
15:30-16:00	Coffee Break
Session Chair: P	rof. Alexander BARYSHEV
16:00-16:15	<b>Yaoyou CHEN</b> Visualization of Confined Electrons at Grain Boundaries in a Monolayer Charge-Density-Wave Metal
16:15-16:45	<b>Dr. Dmitriy ESTUNIN</b> Recent progress in the study of magnetic topological insulators of the MnBi <sub>2</sub> Te <sub>4</sub> -family by photoemission spectroscopy
16:45-17:00	<b>Mengmeng NIU</b> Defect engineering in monolayer transition metal dichalcogenides
17:00-17:30	<b>Dr. Artem TARASOV</b> Topological phase transitions in MnBi <sub>2</sub> Te <sub>4</sub> : an electronic structure view

## Saturday, September 21, 2024

### Location: Room 119, Main Building, MIPT

## Session Chair: Prof. Alexey ALADYSHKIN

09:00-09:30	<b>Prof. Wei JIANG</b> Enhancement of Intrinsic Spin Hall Effect in Chiral Topological Semimetals
09:30-09:45	<b>Alexander LUKYANOV</b> <i>Predicting local order parameter from disorder</i> <i>distribution</i>
09:45-10:15	<b>Prof. Yu ZHANG</b> <i>Manipulation of strongly correlated electrons in monolayer 1T-NbSe</i> <sub>2</sub>
10:15-10:30	<b>Mu TIAN</b> <i>Two-dimensional Ferrovalley Semi-Half-Metal and Tunable Valley-Unbalanced Quantum Anomalous Hall Effect</i>
10:30-11:00	Coffee Break & Take Photos
11:00-11:30	Prof. Lada YASHINA
11:30-11:45	<b>Zichun LIU</b> 4 inch Gallium Oxide Field-Effect Transistors Array with High-k Ta <sub>2</sub> O <sub>5</sub> as Gate Dielectric by Physical Vapor Deposition
11:45-12:15	<b>Prof. Denis VODOLAZOV</b> Nonlinear kinetic inductance of composite superconductors
12:15-12:30	<b>Vyacheslav NEVEROV</b> <i>Microscopic Insights into Superconducting Transition</i> from Type I to Type II
12:30-14:00	Lunch at MIPT Cafe

Session Chair: Prof. Vasily STOLYAROV	
14:00-14:30	<b>Prof. Yuhui CHEN</b> <i>Realization of a continuous time crystal in an erbium doped solid</i>
14:30-14:45	<b>Peng ZHU</b> Crystal growth of topological insulators with bulk-insulating property
14:45-15:15	<b>Prof. Alexey VAGOV</b> <i>Temporal evolution of topological domain-wall defects in ferromagnetic superconductors</i>
15:15-15:30	Weikang DONG 2D Edge Dependent local exciton on MoS <sub>2</sub>
15:30-16:00	Coffee Break
16:00-16:15	<b>Yujiu JIANG</b> Research on Electrochemical Biosensors Based on Topological Materials
16:15-16:45	Dr. Arkadiy SHANENKO Theory of surface superconductivity

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#### Superconducting Trigger Effect in Multilayer Hybrid Structures

<u>S.V. Bakurskiy</u> \*, A.A. Neilo, N.V. Klenov, I.I. Soloviev, M.Yu. Kupriyanov Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119991, Russia \*Email: <u>r4zz@mail.ru</u>

The proximity effect has been studied in an  $SF_1S_1F_2s$  superconducting spin valve comprising a massive superconducting electrode (S) and a multilayer structure constituted by thin ferromagnetic  $F_{1,2}$  and superconducting  $S_1$  and  $S_2$  layers. Within the framework of the Usadel equations, it has been demonstrated that rotation the mutual orientation of the magnetisation vectors serves to initiate superconductivity in the outer thin s-film [1]. The pair potential in the outer S-film was studied, and regions of parameters with a significant spin-valve effect were identified. The strongest effect was observed in the region of parameters where the  $0-\pi$  transition inside the structure occurs. We discussed the possible applications of such trigger effect such as reconfigurable Josephson junctions and tunable inductance elements.

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The work was supported by Russian Science Foundation (project No. 22-79-10018)

## Magneto-optical materials for optical applications: Bi:YIG made by metal-organic decomposition and crystallized by laser annealing, and gasogyrochromism in oxidized permalloy

P.N. Tananaev, D.P. Kulikova, E.M. Sgibnev, A.V. Shelaev, A.V. Baryshev\* The Federal State Unitary Enterprise Dukhov Automatics Research Institute \*Email: baryand@yandex.ru

This talk presents the results of a study on the synthesis of bismuth-substituted yttrium iron garnets (Bi:YIG), fabricated using a metal-organic decomposition method [1] with subsequent crystallization under laser irradiation [2,3]. The integration of Bi:YIG with silicon-on-insulator technology is investigated through the study of micron- and sub-millimeter-sized Bi:YIG stripes and areas crystallized in air, oxygen, and inert gas atmospheres. The effect of gasogyrochromism is demonstrated, and the applicability of oxidized permalloy nanofilms to hydrogen sensing is discussed.

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[2] A. Shelaev, Y. Sgibnev, S. Efremova, P. Tananaev, A. Baryshev, Optics and Laser Technology 155, 108411, (2022).

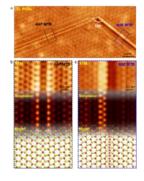
[3] Y. Sgibnev, A. Shelaev, D. Kulikova, A. Salatov, P. Tananaev, G. Yankovskii, A. Baryshev, Crystal Growth and Design 22(2), 1196 (2021).

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## Visualization of Confined Electrons at Grain Boundaries in a Monolayer Charge-Density-Wave Metal

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The properties of atomically thin 2D materials are extremely sensitive to structural imperfections including defects, edges, wrinkles, and grain boundaries. In the past decade, diverse structural imperfections have been widely studied in graphene, which are confirmed to realize rich physical phenomena, such as magnetic moments and topologically protected state. Structural imperfections in transition metal dichalcogenides (TMDs) have been explored to a lesser extent, but are ubiquitous and supposed to generate more plentiful physics. One-dimensional grain boundaries in TMDs are ideal for investigating the collective electron behavior in confined systems. However, clear identification of atomic structures at the grain boundaries, as well as precise characterization of the electronic ground states charge-density-wave in (CDW) metals, have largely been elusive. Here, using molecular beam epitaxy, we successfully synthesize two types of mirror twin boundaries (MTBs) in monolayer NbSe<sub>2</sub>, that is, 4|4P and 4|4E MTBs. With high resolution scanning tunneling microscopy observations, we provide direct experimental evidence for confined electronic states and charge density modulations at MTBs in CDW metals. Our measurements show that both MTBs can introduce local band bending effects and additional resonance peaks. Moreover, the intrinsic CDW signatures of monolayer NbSe<sub>2</sub> are efficiently suppressed as approaching an isolated MTB, but can be either enhanced or suppressed in MTB-constituted confined regions, depending on the electron energies. Such a phenomenon is well explained by the MTB-CDW interference. Our results reveal the significance of MTB-CDW interference in CDW metals, paving the way for the investigation of collective electron behavior in confined systems.



Pic.1 a) Large-scale STM image of monolayer NbSe<sub>2</sub>. There are two types of MTBs, that is, 4|4P and 4|4E, with their intersection angle of 120°. b,c) Zoomed-in STM images of 4|4P and 4|4E MTBs from panel a, as well as the corresponding STM simulations and atomic structures.

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[1] Chen, Y.; Zhang, Y.; Wang, W.; Wang, Y. Adv. Sci. 2023: 2306171.

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#### Realization of a continuous time crystal in an erbium doped solid

Yuhui Chen

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Time crystals are many-body states that spontaneously break translation symmetry in time the way that ordinary crystals do in space. While experiments have demonstrated the existence of discrete or continuous time crystals, these manifestations have typically relied on periodic forces or effective modulation from cavity feedback. The original vision for time crystals was that they would embody self-sustaining motions without any external periodic influence. In this talk, we present both theoretical and experimental evidence indicating that many-body interactions can lead to a phase with spontaneously broken time translation symmetry. By using a continuous-wave laser to drive an erbium-doped crystal, we experimentally revealed a new dynamical phase of intrinsic optical instability, where the transmission through the sample became unstable for intense laser inputs. Furthermore, the erbium ions can spontaneously repeat its pattern in time, forming a phase of continuous time crystal. These states are inherently self-organized, and is self-protected by many-body interactions, showing a coherence time beyond that of individual erbium ions.

## Recent progress in the study of magnetic topological insulators of the MnBi2Te4-family by photoemission spectroscopy

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Representing almost a quarter of the materials known in nature, materials with topologically nontrivial electronic structure naturally attract considerable interest of condensed matter researchers. A special group among them are materials classified as magnetic topological insulators, which are defined by the coexistence of magnetism and the topological electronic structure in one compound [1]. This enables the realization of advanced quantum transport phenomena, including the quantum anomalous Hall effect, and, potential, the realization of Majorana particles, which could lead to the creation of topologically protected qubits for use in quantum computers.

Currently, the most promising in regard to practical application are magnetic topological insulators belonging to the MnBi<sub>2</sub>Te<sub>4</sub>-family [1,2]. The parent material of the family, MnBi<sub>2</sub>Te<sub>4</sub>, has a layered structure consisting of septuple-layer blocks [Te-Bi-Te-Mn-Te-Bi-Te] connected by van der Waals forces. It is characterized by the A-type antiferromagnetic interaction of magnetic moments of Mn atoms, which allows for the  $Z_2$  topological classification of this compound [2]. A distinctive feature of the electronic structure is the presence of topological surface states within a bulk band gap, manifested as a Dirac cone with the band gap at the Dirac point, which is observable at temperatures below the Neel temperature ( $T_N = 25$  K for MnBi<sub>2</sub>Te<sub>4</sub>) [3]. The layered structure of MnBi<sub>2</sub>Te<sub>4</sub> allows the incorporation of blocks exhibiting the same crystal symmetry, such as [Bi<sub>2</sub>Te<sub>3</sub>] block, between [MnBi<sub>2</sub>Te<sub>4</sub>] blocks, thereby modifying the electronic and magnetic properties [4]. Furthermore, element-by-element substitution of Mn, Bi, Te into appropriate elements is an effective method for controlling of the MnBi<sub>2</sub>Te<sub>4</sub>'s physical properties. For instance, Mn can be substituted with Ge, Sn, or Pb; Bi with Sb; and Te with Se [5]. Since the first works devoted to MnBi<sub>2</sub>Te<sub>4</sub>, significant progress has been made in the investigation of the electronic properties of MnBi<sub>2</sub>Te<sub>4</sub> family compounds, with the active use of photoemission methods. However, a number of properties, including the band gap at the Dirac points, the presence and size of which determines the efficiency of quantum transport, have been found to be significantly smaller than predicted by theory [6]. Currently, efforts are being made to optimize the composition of the material with the aim of reducing the number of defects and modifying the transport and electronic properties.

The work was done as part of the SPbU project No. 95442847

#### **Bibliography**

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- [4] Klimovskikh I.I. et al., npj Quantum Mater. 5, 54 (2020)
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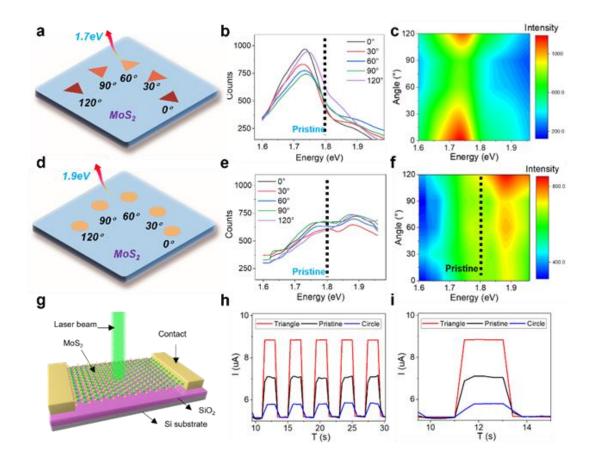
#### 2D Edge Dependent local exciton on MoS2

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Transition metal dichalcogenides (TMDCs) exhibit fascinating physics and have garnered significant attention due to their tunable exciton. Although recent advancements in edge-dependent exciton have been reported, achieving exciton tunning by different Mo/S ratios on edge remains a challenge. In this work, we successfully fabricate different Mo/S ratio edge structures on MoS<sub>2</sub>, including circular (messy Mo/S ratio) and triangular (Mo/S = 4:1, 2:1, 1:1, 1:2, and 1:4) edges, using a Si<sub>3</sub>N<sub>4</sub>-protected focused ion beam (FIB) system. We demonstrate on triangle edge, a local exciton that experiences a redshift from the pristine 1.8 eV to 1.7 eV due to the high-order atomic arrangement, and exciton on the circle edge, present a blue shift to 1.9 eV, attributed to lower connection energy. Specifically, the exciton of triangular edge shows a significant intensity variation dependent on the Mo/S ratio, which the edge of Mo/S = 1: 4 present high intensity than other ratios. Furthermore, we find the triangular edge MoS2 devices exhibit enhanced photocurrent on-off switching behavior using a time-resolved photodetector. These findings open a new way to tunning exciton by designing edge structures, which increases the field of photoelectric device applications.



**Figure.** Edge angle and its PL properties. a) the schematic of triangle edge structure of 0, 30, 60, 90, and 120 degrees on MoS<sub>2</sub>, the color of triangle present the intensity of 1.7 eV. b) the PL intensity of 0, 30, 60, 90, and 120 degrees, the black dashed line shows the pristine signal of 1.8 eV. c) the intensity mapping of 0, 30, 60, 90, and 120 degrees corresponding to b). d) the schematic of circle edge structure of 0, 30, 60, 90, and 120 degrees on MoS<sub>2</sub>, the color of triangle present the intensity of 1.9 eV. e) the PL intensity of 0, 30, 60, 90, and 120 degrees, the black dashed line shows the pristine signal of 1.8 eV. c) the intensity of 0, 30, 60, 90, and 120 degrees, the black dashed line shows the pristine signal of 1.8 eV. e) the PL intensity of 0, 30, 60, 90, and 120 degrees, the black dashed line shows the pristine signal of 1.8 eV. f) the intensity mapping of 0, 30, 60, 90, and 120 degrees corresponding to e). g) the schematic of the device. h) Photocurrent on–off switching behavior in the MoS<sub>2</sub> device triangle-fabricated (red), circle-fabricated (blue), and with pristine (black). i) the photocurrent generation ( $\tau_{rise}$ ) and decay ( $\tau_{decay}$ ) times corresponding to h).

#### Bibliography

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#### Supercurrent Reversal in Zeeman-Spit Josephson Junctions

#### A.A. Golubov Moscow Institute of Physics and Technology, Dolgoprudny, Russia

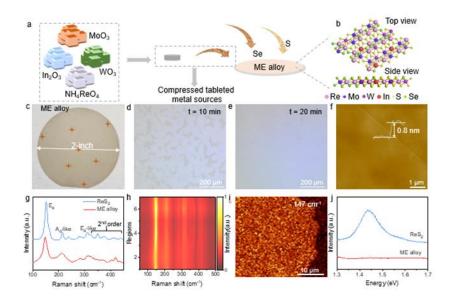
An overview is given of various mechanisms of unconventional current-phase relations (CPR) in Josephson junctions. The results of theoretical study of the CPR in a junction comprising the Zeeman-split superconductors (ZSs) and a normal metal (N) are presented. It is shown that at low temperatures the Josephson current in the ZS/N/ZS junctions exhibits an additional reversal in direction at a certain value of the phase difference. Based on the calculations of the spectral Josephson current, it is shown that the band-splitting due to the Zeeman interaction leads to the level crossing in the spectra of the Andreev bound states and to sign reversal of the Josephson current. Additionally, a method is proposed to electrically control the critical phase difference by tuning the Rashba spin-orbit coupling.

#### Mixing entropy engineering

Lin Jia, Ruichun Luo, Xiaoyu Zheng, Ping Wang, Lu Lv, Longyi Fu, Weikang Dong, Chunyu Zhao, Dian Li, Minghui Li, Jing Li, Yang Yang, Denan Kong, Jijian Liu, Qingmei Hu, Yang Zhao, Yan Xiong, Wu Zhou<sup>\*</sup>, Jiadong Zhou<sup>\*</sup>, Yao Zhou<sup>\*</sup>

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Mixing entropy engineering is a promising strategy to tune the physical and chemical properties of materials. Although high-entropy in van der Waals bulk solids have been reported, entropy engineering in 2D monolayer remains unconquered. In this work, we report the epitaxial growth of 2inch 1T" hexanary medium-entropy alloy monolayers ( $Re_aW_bMo_cIn_dS_xSe_v$ ) via chemical vapor deposition method. The atomic structure and chemical composition are confirmed by X-ray photoelectron spectroscopy, scanning transmission electron microscopy, energy dispersive X-ray spectroscopy and electron energy loss spectroscopy, illustrating the uniform distribution of the six elements. The hexanary medium-entropy alloy field-effect transistors exhibit metallic transport behavior and photodetectors show an ultrawide photo response from visible to near-infrared wavelengths with a responsivity of 110.2 A W<sup>-1</sup> under 520 nm laser illumination. Meanwhile, the hexanary medium-entropy alloy monolayer exhibits excellent electrocatalytic hydrogen production with an overpotential of 176.6 mV in dark. Importantly, an overpotential of 43.7 mV at 10 mA cm<sup>-2</sup> with a lowered Tafel slope of 51.9 mV dec<sup>-1</sup> under 520 nm laser irradiation is obtained due to excellent electrical conductivity. Our work opens a new way to design mixing entropy alloys and realize the application of transition metal dichalcogenides (TMDs) in photo-enhanced electrocatalytic hydrogen production.



#### Enhancement of Intrinsic Spin Hall Effect in Chiral Topological Semimetals

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The spin Hall effect (SHE), which transduces charge current into spin current, is one of the essential cornerstones of spintronics. Here we propose a new intrinsic SHE (ISHE) enhancement mechanism in topological semimetals with high Chern numbers, and present a series of promising material candidates with large intrinsic spin Hall conductivities (ISHC) and spin Hall angles (SHA) for potential spintronic applications. By way of model Hamiltonian calculations and statistical analysis of 260 non-magnetic semimetals with chiral crystal structure, we unravel a positive correlation between the maximum Chern number and the ISHE, i.e., the ISHC and, under specific conditions, the SHA. Such positive correlations in topological gapless systems represent a novel mechanism to enhance ISHE, distinct from the conventional spin-orbit induced anticrossing mechanism in gapped systems. Additionally, our first-principles calculations of 38 chiral topological semimetals from space group 198, which can support zero-dimensional nodes with the highest Chern number (C = 4), reveal multiple realistic materials with large ISHC and even larger SHAs than Pt. Our discovery not only enriches the fundamental understanding of SHE but also provides an ideal material system conducive to efficient charge-to-spin conversion applications.

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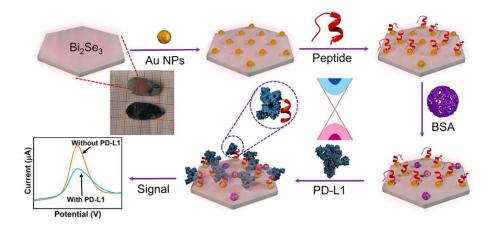
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#### **Research on Electrochemical Biosensors Based on Topological Materials**

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Topological materials are a new class of quantum materials, which have robust surface states with Dirac-like electronic structures. The robust surface state is originated from the intrinsic bulk properties and is immune to the defects and impurities. The use of the topological surface state in the solid-liquid interface for electrochemical detection avoids the interference from defects and impurities. Programmed cell death-1 (PD-L1) is an important immune checkpoint protein. PD-L1 expression has become a predictive biomarker of response to immune checkpoint inhibitors (ICIs) in several types of solid tumors. In this work, we developed a biosensor based on the topological insulator material Bi<sub>2</sub>Se<sub>3</sub> with a targeting peptide on it. the biosensor based on topological insulator material with peptide on it has great potential in the application of detecting various biomarkers of diseases.



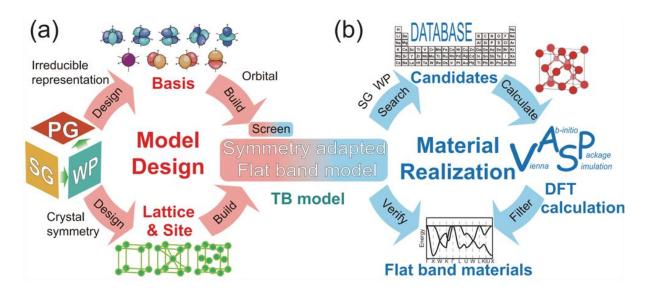
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#### **Three-Dimensional Multi-Orbital Flat Band Models and Materials**

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The study of flat band (FB) models and their physical manifestations serve as a crucial basis for probing exotic quantum phenomena associated with strong correlation. Here we present a systematic theoretical framework that simultaneously enable the construction of multi-orbital FB models and identification of feasible material candidates. This is achieved by integrating group theory and crystallography for the symmetry-adapted tight-binding model, which incorporate lattice, site, and orbital degrees of freedom. We elucidate this framework's practical applicability by uncovering a novel three-dimensional (3D) multi-orbital FB model in the basic face-centered cubic lattice, fundamentally distinct from typically studied single-orbital Lieb and Kagome models. Most importantly, we successfully identify a plethora of high-quality binary material candidates exhibiting ultra-clean 3D FB near the Fermi level. We further show the diversity of orbital bases within the model and expand our analysis to other cubic lattices with varying space groups for the realization of various 3D multi-orbital FB systems. We believe that this research lays a solid foundation for studying the correlated physics of FB systems, especially for multi-orbital systems.



Pic. 1 Theoretical framework for exploring multi-orbital FB systems. The FB searching framework contains two modules. (a) The first module handles the FB model design based on symmetry-adapted TB model designing, building, and screening processes, which consider the lattice, site, and orbital degrees of freedom. SG, PG, and WP represent the space group, point group, and Wyckoff position, respectively. (b) The second module handles the material realization by treating the FB materials searching, calculating, filtering and verification processes. It searches material candidates using the WP and SG information from the model design process, followed by high-throughput DFT calculations, and FB material verification.

#### Exploring Oxygen Instability in Tin Perovskites: Insights and Advances in Sensing Applications

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Metal halide perovskites are highly promising solution-processed semiconductors for photovoltaic and other optoelectronic applications. Among the alternatives to lead (Pb)-based perovskites, tin (Sn)-based perovskites have emerged as strong candidates. However, their susceptibility to oxygen-induced instability presents significant challenges. In our recent study, we investigated the interactions between oxygen and PEA<sub>2</sub>SnI<sub>4</sub> across various oxygen concentrations. By integrating experimental results with theoretical analysis, we clarified the impact of oxygen concentration on the structural stability of PEA<sub>2</sub>SnI<sub>4</sub> and unveiled the interaction mechanisms between the PEA<sub>2</sub>SnI<sub>4</sub> film and oxygen. Furthermore, we developed a halide perovskite-based oxygen optical fiber sensor, combining PEA<sub>2</sub>SnI<sub>4</sub> with a tilted fiber Bragg grating (TFBG), thereby extending the application of tin-based perovskites to trace oxygen detection. We also enhanced the stability of two-dimensional layered Sn-based perovskites through ligand engineering and successfully demonstrated color-stable pure-red PEA<sub>6</sub>SnI<sub>8</sub> derivative single crystals with a heterogeneous structure for the first time, revealing their potential in trace humidity detection applications.

## Demonstration of a Josephson vortex-based memory cell with microwave energy-efficient readout

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The ongoing progress of superconducting logic systems with Josephson junctions as base elements requires the development of compatible cryogenic memory. Long enough junctions subject to magnetic field host quantum phase 2pi-singularities — Josephson vortices. In this talk we consider the realization of the superconducting memory cell whose state is encoded by the number of present Josephson vortices. This cell was formed by integrating the long Josephson junction into a coplanar resonator. By applying a microwave current with an amplitude much less than the critical current, we can read the number of vortices in the junction in an energy-efficient and non-destructive manner. The memory effect arises due to the presence of the natural edge barrier for Josephson vortices. This talk covers such stages of the research as measurement methodology, description of the results and prospects for improving the developed system.

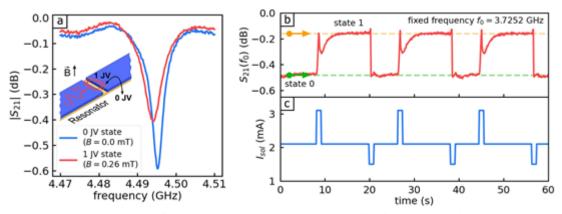


Figure 1. a) resonance modes of the resonator observed as sharp dips in the scattering parameter S21(f) signal at zero-applied magnetic field (blue curve) and at B=0.26 mT (red curve). Inset: a scheme of microwave measurements of JVs; b) experimental demonstration of the switching detection in S21 by applying magnetic field pulses shown in c).

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#### Cryogenic low-range resistors for advanced superconducting quantum electronics

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Cryogenic thin-film resistors are components of various superconducting integrated circuits and devices. In rapid single-flux quantum circuits (RSFQ) and superconducting quantum processors the resistors are used for shunting Josephson junctions and for fabrication of RC filters [1]. In superconducting photon detectors [2], resistors provide impedance matching, which is required for the recovery of superconductivity in the detector with low kinetic inductance after photon absorption. Many applications require resistors as small as a few Ohms. For reproducible fabrication of such resistors, the electrical resistance of the superconductor/normal metal interface is critical [3, 4].

We present a study of thin-film Mo resistors for NbN electronics operating at cryogenic temperatures. The key step is the 0.5–1.5 keV ion cleaning–activation of NbN before Mo deposition, which allows us to obtain a high-quality Mo/NbN interface by removing the NbNOx layer. Using Ar plasma activation, we observed additional contact resistance as low 7–8  $\Omega$  at room temperature, which we attribute not to the resistance of the interface, but to the resistance of the Mo contact pad. To eliminate the contact pad resistance, we put an additional low-resistivity Al layer ('bandage') on top of the contact pads. In this case, the contact resistance is below the accuracy of our measurement, which is about 1  $\Omega$ . Although the NbN/Al and Mo/Al boundaries feature thin oxide layers, it does not affect the interface resistance in all the studied ranges of contact areas from 30 µm × 30 µm to 3 µm × 3 µm. The quality of the interfaces is confirmed by transmission electron microscopy and x-ray reflectometry. We believe that our results are useful for the design of NbN-based superconducting electronics such as photon-number resolving detectors and SNSPD arrays.

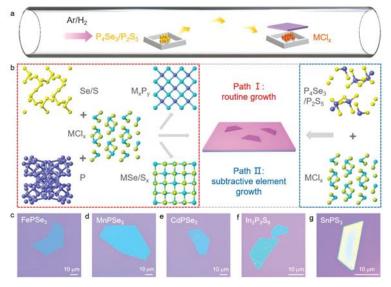
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#### A Universal Strategy for Synthesis of 2D Ternary Transition Metal Phosphorous Chalcogenides Yang Yang<sup>1#</sup>, Jijian Liu<sup>1#</sup>, Chunyu Zhao<sup>1#</sup>, Jiadong Zhou<sup>1\*</sup>

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The 2D ternary transition metal phosphorous chalcogenides (TMPCs) have attracted extensive research interest due to their widely tunable band gap, rich electronic properties, inherent magnetic and ferroelectric properties. However, the synthesis of TMPCs via chemical vapor deposition (CVD) is still challenging since it is difficult to control reactions among multi-precursors. Here, a subtractive element growth mechanism is proposed to controllably synthesize the TMPCs. Based on the growth mechanism, the TMPCs including FePS<sub>3</sub>, FePSe<sub>3</sub>, MnPS<sub>3</sub>, MnPSe<sub>3</sub>, CdPS<sub>3</sub>, CdPSe<sub>3</sub>, In<sub>2</sub>P<sub>3</sub>S<sub>9</sub>, and SnPS<sub>3</sub> are achieved successfully and further confirmed by Raman, second-harmonic generation (SHG), and scanning transmission electron microscopy (STEM). The typical TMPCs–SnPS<sub>3</sub> shows a strong SHG signal at 1064 nm, with an effective nonlinear susceptibility  $\Box^{(2)}$  of 8.41  $\times$  10<sup>-11</sup> m V<sup>-1</sup>, which is about 8 times of that in MoS<sub>2</sub>. And the photodetector based on CdPSe<sub>3</sub> exhibits superior detection performances with responsivity of 582 mAW<sup>-1</sup>, high detectivity of 3.19  $\times$  10<sup>11</sup> Jones, and fast rise time of 611 µs, which is better than most previously reported TMPCs-based photodetectors. These results demonstrate the high quality of TMPCs and promote the exploration of the optical properties of 2D TMPCs for their applications in optoelectronics.



**Figure 1. a)** Schematic of the CVD process via subtractive-element-based growth strategy. **b)** The mechanism of routine and subtractive element growth. **c–g)** Optical images of the synthesized FePSe<sub>3</sub>, MnPSe<sub>3</sub>, CdPSe<sub>3</sub>, In<sub>2</sub>P<sub>3</sub>S<sub>9</sub>, and SnPS<sub>3</sub>.

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#### **Constraint-Dependent Physical Quantities in Active Baths**

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**Abstract:** We have developed a method to measure active depletion forces, directly determining the active depletion force between two colloidal particles through optical tweezer experiments and computer simulations. Our study further explores related phenomena such as active noise, active pressure, and the mean potential energy of colloidal particles in an optical trap, all of which are closely related to the degree of constraint applied to the particles. This work represents a significant extension of physical concepts and relationships from equilibrium thermal baths to nonequilibrium systems. [Phys. Rev. Lett. 124, 158001 (2020).]

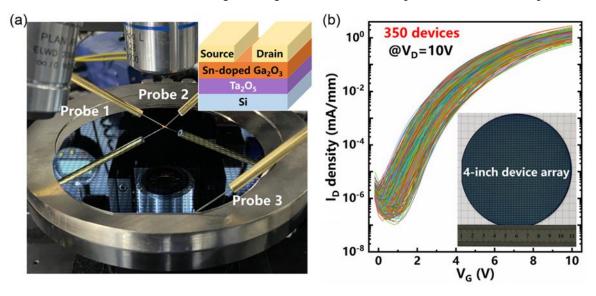
In equilibrium, the entropic force (also known as the depletion force) refers to an effective attractive interaction between large particles suspended in a thermal bath composed of many smaller particles. The origin of this force lies in the fact that the proximity of the large particles reduces their configurational space, thereby increasing the configurational space available to the smaller particles, ultimately leading to an increase in the system's total entropy. In equilibrium thermal baths, the entropic force is independent of external constraints on the particles, meaning that it can be determined either by the radial distribution function of freely moving large particles or by direct measurement through a scheme where the large particles are fixed. Similarly, in equilibrium, the noise experienced by suspended particles is white noise, the pressure exerted on them can be expressed as a state function independent of external constraints, and the energy equipartition relation is also unaffected by the strength of the constraints. This invariance with respect to external constraints is a fundamental result of equilibrium statistical physics. However, it remains unclear whether this invariance holds in nonequilibrium active baths, and even the correct method to measure active depletion forces is not well understood.

We first propose a correct method for measuring active depletion forces and directly determine the active depletion force between two colloidal particles by constraining them with optical tweezers. We find that this depletion force is highly sensitive to the external constraints applied; neither the radial distribution function of free particles nor the fixed particle scheme can provide the correct active depletion force. Subsequently, we extended our research to a series of thermodynamic properties of active matter, measuring the pressure [J. Phys.: Condens. Matter 35, 445102 (2023)], noise characteristics [Soft Matter 16, 4655 (2020)], and potential energy in an optical trap [Chin. Phys. B 29, 058201 (2020)] for colloidal particles in a nonequilibrium active bath. We discovered that these physical quantities or relationships are highly dependent on the external constraints imposed on the inert colloidal particles, in stark contrast to the situation in equilibrium thermal baths. At a microscopic level, this constraint dependence originates from the impact of colloidal particle relaxation dynamics on the distribution of active particles and the intensity of their collisions. These studies demonstrate that the physical concepts in active baths are far more complex than those in thermal baths and cannot be treated using equilibrium methods.

#### 4-inch Gallium Oxide Field-Effect Transistors Array with High-k Ta2O5 as Gate Dielectric by Physical Vapor Deposition

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Field-effect transistors (FETs) with ultra-wide bandgap semiconductor  $Ga_2O_3$  have been fabricated by physical vapor deposition with advantages of low cost, wafer scale, and rapid production. The insulator-like pristine  $Ga_2O_3$  is converted to semiconductor by co-sputtering Sn with post-annealing, which demonstrates a  $5.6 \times 10^7$  times higher on-state current. Importantly, this Sn-doped  $Ga_2O_3$  sample shows a high breakdown voltage near 500 V. Furthermore, a 4 inch array of Sn-doped  $Ga_2O_3$  FETs with high-k  $Ta_2O_5$  gate dielectric has been fabricated on a silicon substrate, successfully showing a large on-current density of  $1.3 \text{ mA mm}^{-1}$ , a high  $I_{ON}/I_{OFF}$  of  $2.5 \times 10^6$ , and a low threshold voltage of 3.9 V, which are extracted from the average 350 devices. This work paves a promising way for  $Ga_2O_3$ -based nanoelectronics to serve medium-high voltage with low cost, rapid, and wafer-scale production.



(a) The photo of the fabricated 4-inch device array during data measurement. (b) Transfer curves of 350 randomly-measured FETs. The inset in (b) shows the 4-inch device array.

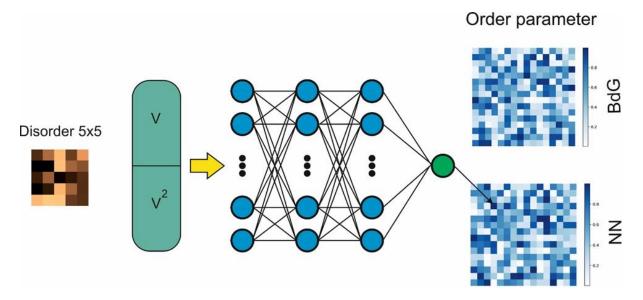
#### Predicting local order parameter from disorder distribution

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Machine Learning (ML) is making significant advancements across various scientific disciplines, transforming research methodologies and data analysis techniques. Since its appearance, ML has evolved into a robust instrument capable of handling vast quantities of data, uncovering patterns, and forecasting outcomes, thereby expediting scientific advancements.

For example, ML techniques have been effectively utilized to replicate the results of Density Functional Theory (DFT) [1]. The deep learning model developed in this context successfully circumvents the direct solution of the Kohn-Sham equations, achieving a speed enhancement by an order of magnitude.

In our research, we designed a machine learning algorithm that predicts the distribution of local order parameter in a superconductor based on a correlated disorder. This ML model aims to enhance both the efficiency and precision of solving the Bogoliubov-de Gennes (BdG) equations, which are an extremely powerful tool for analyzing the local electronic structure in inhomogeneous superconductors including those in an external magnetic field. [2,3].



Pic. 1. Disorder distribution (V) used for training the neural network to predict the distribution of the local order parameter.

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#### Controlling the dielectric response of SrTiO3

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Strontium titanate (SrTiO<sub>3</sub>, STO) is a quantum paraelectric used in novel energy storage, memory and microwave optical devices for its high permittivity and low losses in a broad frequency range from radio to sub-terahertz [1,2]. Real permittivity of pure crystalline SrTiO3 reaches values as high as 24000, and more than 99% of it is contributed by the TO1 phonon soft mode (SM) associated with a potential ferroelectric phase transition [3]. However, in other forms of STO such as thin films or ceramics dielectric response can differ significantly. Sufficiently strained thin films can become ferroelectric. Polycrystalline samples exhibit SM hardening, resulting in a decreased maximal permittivity in a broader temperature range. In order to tailor the dielectric properties of STO to a specific application, we need to understand microscopic mechanisms governing the SM behavior. We will discuss how chemical doping, oxygen vacancies and mechanical strains influence the soft mode dynamics and the crystal structure of STO crystals [4] and thin films [5].

The study was supported by the Ministry of Science and Higher Education of the Russian Federation grant No. 075-15-2024-632.

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#### Photogalvanic phenomena in superconductors supporting intrinsic diode effect

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We suggest a phenomenological theory of photogalvanic phenomena in superconducting materials and structures revealing the diode effect. Starting from a generalized London model including the quadratic nonlinearity in the relation between the supercurrent and superfluid velocity, we show that the electromagnetic wave incident on the superconductor can generate a nontrivial superconducting phase difference between the ends of the sample. Being enclosed in a superconducting loop, such a phase battery should generate a dc supercurrent circulating in the loop. By increasing the electromagnetic wave intensity one can provoke the switching between the loop states with different vorticities.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation (Grant No. 075-15-2024-632).

#### Transport measurements and technology of Sb, Ge doped magnetic topological insulator MnBi2Te4 with superconducting contacts

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 $MnBi_2Te_4$  is an intrinsic magnetic topological insulator with A-type antiferromagnetic order, where the neighboring ferromagnetic Mn layers are coupled in an antiparallel manner

It was reported that Quantum anomalous Hall effect (QAHE) can be observed at 1.4 Kelvin

in five-SL  $MnBi_2Te_4$  [1]. Even more interesting topic is the study of interaction of a magnetic topological insulator with a superconductor. The chiral Majorana fermions [2], cooper-pair splitting [3] have been theoretically predicted in such systems. These types of structures have a potential application in quantum technologies and need to be developed.

The presentation will contain general information about sample manufacturing, ultra-low temperature transport measuring and discussion of transport properties of structures. Devices are flakes of Sb, Ge doped  $MnBi_2Te_4$  with contacts from Nb, Al in SNS junction and Hall geometries.

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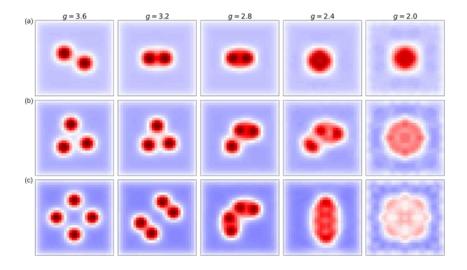
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#### Microscopic Insights into Superconducting Transition from Type I to Type II

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Superconductors, known for their magnetic properties, can be categorized into two primary types based on their response to an externally applied magnetic field. Type I superconductors completely expel the magnetic field, while type II superconductors allow it to penetrate, resulting in a mixed state.



**Fig. 1:** Color density plots of the spatial profile of the induced magnetic field inside the sample calculated for various values of the coupling constant g (columns) and the magnetic field (rows).

Intriguingly, investigations on materials possessing a  $\kappa$  value close to one have uncovered a group of superconductors that do not easily fit into the traditional classifications. Empirical findings have demonstrated the presence of an intermediate mixed state (IMS) within these materials. The magnetic field permeates such superconductors, resulting in diverse spatial arrangements of vortices, including the co-existence of Meissner domains, vortex lattice islands, vortex clusters, and chains. Within this investigation, a convenient microscopic approach based on self-consistent computation of the Bogoliubov-de Gennes and magnetic state equations [1] is employed to reveal various phenomena, such as vortex clustering and the interactions between multiple vortices.

In this study [2], we investigate the transition of the system from type I to type II superconductivity, which involves passing through IMS. Our research reveals that intricate many-body interactions among vortices lead to the emergence of unconventional vortex patterns during this transition (Fig.1).

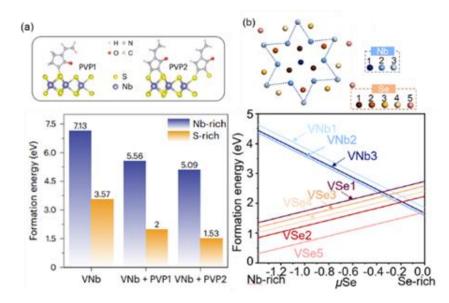
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# Defect engineering in monolayer transition metal dichalcogenides

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Atomically precise defect engineering is an effective method to modulate the physical properties of transition metal dichalcogenides (TMD), making them promising candidates for various applications, including electronics, optoelectronics, and catalysis, etc. However, constructed precise vacancies, especially metal vacancies, are limited. The effect of defects on electron-correlated properties is poorly understood. Recently, precisely fabricating metal and chalcogen vacancies in TMD has been achieved by molecular modification.<sup>[1]</sup> Besides, we investigated the properties of 1T-NbSe<sub>2</sub> charge density wave (CDW) monolayer with various single Se/Nb vacancy using density functional theory calculations.<sup>[2]</sup> We found a unique Se vacancy site, called magic Se vacancy, could precisely erase the Mott electrons. Besides, Mott electrons could be more flexibly manipulated when the magic Se site is substituted with As, Br and K elements. The electronic properties of 1T-NbSe<sub>2</sub> with defects are tuned by the synergistic effect of compressive strain and electron doping. Our findings reveal that defect engineering is an ingenious strategy for atomically manipulating electron-correlated properties and manufacturing electronic patterns, guiding to erase and write in Mott electrons in two-dimensional materials.



Pic.1. (a) Atomic models and formation energies of metal vacancy in pristine and PVP-capped 1H-NbS<sub>2</sub>. (b) Eight types of vacancies in the Charge-Transfer insulator 1T-NbSe<sub>2</sub> supercell were considered.

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# Effects of photon statistics in wave mixing on a single qubit

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We theoretically consider wave mixing under the irradiation of a single qubit by two photon fields. The first signal is a classical monochromatic drive, while the second one is a nonclassical light. Particularly, we address two examples of a nonclassical light: (i) a broadband squeezed light and (ii) a periodically excited quantum superposition of Fock states with 0 and 1 photons. The mixing of classical and nonclassical photon fields gives rise to side peaks due to the elastic multiphoton scattering. We show that side peaks structure is distinct from the situation when two classical fields are mixed. The most striking feature is that some peaks are absent. Thus, the analysis of peak amplitudes can be used to probe photon statistics in the nonclassical mode. A cascade of two-level superconducting artificial atoms -- a source and a probe -- strongly coupled to a semi-infinite waveguide is a promising tool for observing such non-trivial phenomena. The probe atom can scatter an antibunched output from the source, thereby generating the field with specific properties. We experimentally demonstrate wave acting on the probe. We observe unique features in the wave-mixing stationary spectrum that cannot be reproduced by mixing two classical waves on the probe. These features are well described by the theory for a strongly coupled cascaded system of two atoms.

# XPS study of native oxide films formed onto TiNi-based alloy modified by ion-beam treatments

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Implementation of novel titanium alloys in the medical industry is manifested by social needs to heal (or replace) damaged tissues, treat diseases of the musculoskeletal system. Biochemical laboratory (in-vivo, in vitro) tests of the developed medical devices in simulated physiological conditions are required in order to assess their biocompatibility. To date, the corrosion characteristics of TiNi shape memory alloys are widely described [1, 2]. It is shown that the mechanisms of corrosion destruction of these alloys are associated with selective corrosion and anodic oxidation of nickel being toxic for human body. So far, the issue of corrosion performance remains complex and can not be solved without understanding the structure of the protective oxide layer [3, 4]. Surface modification of the TiNi alloys by ion beams is a promising method aiming to form the nanocomposite oxide films with enhanced dielectric properties. The physical reasons responsible for the corrosion resistance of the ion-modified alloys are still unclear. The purpose of this work is to reveal the mechanisms of anodic oxidation of metals (Ti, Ni, Cu, Zr) and determine their chemical state in the oxide layer of the developed Ti-Ni-Cu-Zr alloy modified by ion beams.

The Ti-Ni-Cu-Zr alloy was prepared in a vacuum arc furnace by six-fold remelting of pure components. The nominal chemical composition of the alloy was  $Ti_{35}Ni_{35}Cu_{15}Zr_{15}$  (at. %). Test samples were mechanically grinded (using SiC abrasive) and electrolytically polished in acid mixture (CH<sub>3</sub>COOH + HClO<sub>4</sub>). Then, the samples were modified by niobium ions using Mevva-5.Ru setup: an irradiation dose was  $5 \cdot 10^{16}$  cm<sup>-2</sup>, an accelerating voltage was 30 kV and a residual vacuum was  $5 \cdot 10^{-4}$  Pa. The corrosion rate was estimated in artificial saliva and 0.9 wt. % NaCl using the Tafel extrapolation method in a three-electrode electrochemical cell consisting of a working electrode, an Ag/AgCl reference electrode and a counter graphite electrode. Studies of the chemical state of the elements {Ti, Ni, Cu, Zr, O} were carried out by X-ray photoelectron spectroscopy by means of K-Alpha Nexsa spectrometer (Thermo Scientific, USA) using a monochromatic X-ray source Al Ka ( $\Box$  = 1486.6 eV).

It has been found that after ion implantation the Ti-Ni-Cu-Zr alloy exhibits a significant decrease in the corrosion rate (by ~7 times) in comparison with the reference unirradiated alloy. The high-resolution XPS spectra of the ion-modified alloy possess O1s peak consisting of two lines belonging to the oxidized form ( $O^{2-}$ ) and hydroxyl group (OH<sup>-</sup>). The chemical state of titanium, according to the fitting of the Ti  $2p_{3/2}$  line, corresponds to TiO<sub>2</sub> oxide. The Nb 3d energy band is complex and corresponds to Nb<sup>5+</sup> in the Nb<sub>2</sub>O<sub>5</sub> oxide phase. It is suggested that the low rate of anodic oxidation of the alloy treated by ion beams is associated with depletion of the outer layer in nickel and formation of Nb<sub>2</sub>O<sub>5</sub> dielectric oxide phases onto the surface of the alloy.

This work was supported by the Russian Science Foundation (Grant No. 24-22-00080). **Bibliography** 

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#### Electrochemical preparation of metallic nanowires for superconducting microelectronics

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This work is dedicated to the development of a new approach for creating superconducting microelectronics based on metallic nanowires. This innovative geometry, compared to traditional fabrication methods, allows for significantly reducing the lateral dimensions of the devices, as well as enhancing the performance parameters of future systems with high element density.

Using a template-assisted electrodeposition technique, we have successfully synthesized various types of nanowires using porous templates of anodic aluminium oxide (AAO). The nanowires have a diameter of 30–65 nm and include monometallic Au, ferromagnetic Co, and segmented Au/Ni/Au structures, where a thin layer of ferromagnetic material separates the segments of normal metal. We have paid close attention to studying the influence of the electrodeposition process on the composition, structure, and properties of the nanowires.

To create hybrid systems based on individual nanowires, current-carrying Nb contacts were fabricated using electron lithography and magnetron sputtering techniques. Measurements of the low-temperature transport properties of the SNS systems (Nb/Au/Nb) showed high values for the critical current density, up to  $1.6 \cdot 10^6$  A/cm<sup>2</sup>. Gold nanowires with a diameter of 60 nm have a coarse crystalline structure, whereas those with a diameter smaller than 30 nm are characterized by a polycrystalline structure. The lack of the proximity effect for small-diameter nanowires with weak link lengths larger than 300 nm indicates the important role of grain boundaries in electronic transport. The experimentally observed monotonic decrease in the critical current with increasing temperature and the strength of the external magnetic field was quantitatively described using the Usadel approach for long SN-N-SN junctions with diffuse normal metal regions.

For Nb/Co/Nb hybrid structures with cobalt nanowires ranging in length from 280 to 365 nm, no transition to the superconducting state was observed. The fabricated structures exhibit  $\rho_{Co}(5 \text{ K}) = 4.94 \pm 0.83 \ \mu\Omega \cdot \text{cm}$ , a residual resistivity ratio of 4.5 and low contact resistance values.

For the first time, SNFNS junctions based on individual segmented Au/Ni/Au nanowires were fabricated, and the occurrence of the proximity effect in these structures was demonstrated for Ni layer thicknesses of less than 12 nm at temperatures below 3.5 K. The critical current increases to 50  $\mu$ A when the temperature drops to 13 mK. The results obtained, combined with additional research in an external magnetic field, offer new possibilities for the development of miniature digital components and superconducting devices for quantum and spin-based technologies.

The work was performed under financial support of the Ministry of Science and Higher Education of the Russian Federation (grant number 075-15-2024-632) and the National University of Science and Technology MISIS (grant number K2-2022-029).

#### Theory of surface superconductivity

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In the usual perception, surface superconductivity is associated with the surface nucleation of a superconducting condensate above the upper critical field in type-II superconductors or with a rearrangement of phonon properties and the electron-phonon coupling near surfaces/interfaces. Recently, it has been found that there exists another example when the surface superconducting temperature is significantly increased as compared to the bulk superconductive temperature due to constructive interference of quasiparticles (without magnetic fields and reconstruction of the phonon spectrum). In this talk, we discuss the latter example of the surface (boundary) superconductivity within the attractive Hubbard model for the two variants: the standard one-dimensional tight binding model with the uniform hopping parameter and the Su-Schrieffer-Heeger model. The first variant represents a metallic chain on top of an s-wave bulk superconductor while the second variant represents lowdimensional topological insulator deposited on top of an s-wave superconducting sample. We discuss the corresponding numerical solutions of the Bogoliubov-de Gennes equations and demonstrate that the critical temperature of the superconductivity nucleation near the chain ends (boundaries) can be considerably enhanced as compared to its bulk value. In the first variant we obtain that all the quasiparticle states are delocalized and occupy the entire volume of the sample. Then, the enhancement of the end critical temperature originates from the quantum interference of different quasiparticle states [1,2]. In the Su-Schrieffer-Heeger model, the scenario of the end superconductivity is more complex: in addition to the interference of the delocalized quasiparticles, one finds the contribution of the topological bound end states [3].

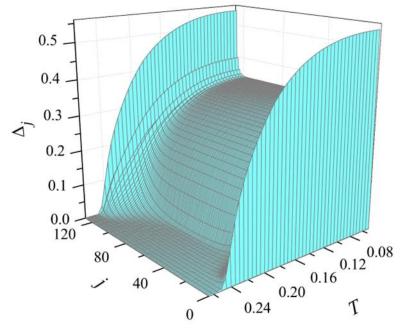


Fig.1 The order parameter as a function of the chain site j and temperature T for the one-dimensional attractive Hubbard model. The results are calculated for the half-feeling case at the coupling g = 2 and the Debye energy 5 (both in units of the hopping parameter). The number of sites N = 128. One can see that the order parameter is zero in the chain center above T=0.2 (also in units of the hopping

parameter) while it survives up to T=0.25 near the chain ends.

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#### Topological phase transitions in MnBi<sub>2</sub>Te<sub>4</sub>: an electronic structure view

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### Abstract

Topological quantum materials, such as MnBi<sub>2</sub>Te<sub>4</sub>, are of great interest in modern physics due to their unique electronic properties, particularly the presence of topological surface states (TSS) that exist at the boundary between topological and trivial materials. These states are protected by time-reversal symmetry, which prevents electron scattering and makes them highly stable against local perturbations, making such materials promising for applications in quantum computing and spintronics [1]. In magnetic topological insulators, where time-reversal symmetry is broken, new quantum phenomena emerge. This opens the possibility for states such as the quantum anomalous Hall effect and magnetic Weyl semimetals, further broadening the technological potential of these materials [2].

This study investigates the topological phase transitions (TPTs) in the antiferromagnetic topological insulator MnBi<sub>2</sub>Te<sub>4</sub> using density functional theory (DFT). It focuses on how variations in spin-orbit coupling (SOC) affect the electronic and spin structures of MnBi<sub>2</sub>Te<sub>4</sub>. At the critical point of the TPT, the bulk band gap and the Dirac point gap in the TSS reach their minimum as the SOC strength decreases. Beyond this point, the bulk band gap increases as the system transitions to a trivial state, accompanied by an inversion of the Bi-pz and Te-pz orbital states and a corresponding inversion of spin polarization in the Dirac cone.

Doping MnBi<sub>2</sub>Te<sub>4</sub> with Sn or Ge produces a similar effect. Changes in the spin-orbit interaction and interlayer coupling caused by doping result in a non-linear dependence of the gap on the concentration of Sn or Ge. Like the SOC variation, the bulk band gap initially decreases and then increases as the system transitions to a trivial state, also accompanied by the Bi-pz and Te-pz orbital state inversion. These findings show that doping can control topological phase transitions similarly to SOC variation, with orbital contributions playing a key role.

Additionally, the study explores how magnetic ordering and SOC tuning can produce different electronic phases. In the ferromagnetic (FM) phase, MnBi<sub>2</sub>Te<sub>4</sub> transitions from a topological insulator (TI) to a Dirac semimetal (DSM), then to a Weyl semimetal (WSM), and finally back to DSM before reaching the trivial insulator (TrivIns) state. In the antiferromagnetic (AFM) phase, the system transitions directly from an AFM TI to a TrivIns state via a single-point transition through the DSM phase.

These findings highlight the potential of MnBi<sub>2</sub>Te<sub>4</sub> for studying exotic quantum phenomena and its promising applications in spintronics and quantum computing.

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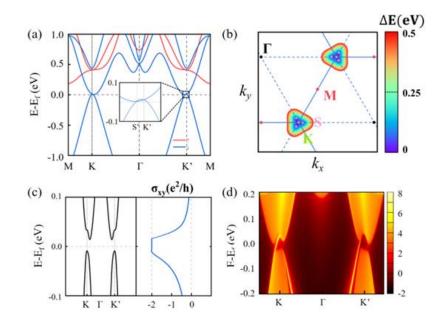
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# Two-dimensional Ferrovalley Semi-Half-Metal and Tunable Valley-Unbalanced Quantum Anomalous Hall Effect

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As a promising competitor for novel quantum devices, magnetic topological materials attract much attention in recent year for its interesting physical properties in magnetism and electron transport. In this work, we find a ferromagnetic topological material with a high Chern number of 2. Based on first principle calculations, we find 1T-CrS<sub>2</sub>F<sub>2</sub> monolayer, which is halogenide of 1T-CrS<sub>2</sub> that has been successfully synthesized is stable at regular situation and possess intrinsic ferromagnetism as well as energy valleys. When spin-orbit coupling(SOC) is considered, the anomalous hall conductance appears as a quantum platform of  $-2 e^2/h$  and two metallic edge states are discovered between valence band and conduction band. However, the presence of space inversion symmetry makes valleys equivalent and restrict further application. So a Janus structure 1T-CrS<sub>2</sub>FCl is constructed to introduce energy valley polarization. After considering SOC in ferromagnetic 1T-CrS<sub>2</sub>FCl, we can destroy the equivalence between energy valleys and apply a perpendicular electric field to tune the band structure. With electric field we can attain tunable QAH conductance. Our research provides are instructive for the discovery of magnetic topological materials and the research of novel spintronic devices.



Pic.1 Electronic properties and topological properties of 1T-CrS<sub>2</sub>F<sub>2</sub>. (a) The spin-polarized band without considering SOC, and the inset shows the quadratic crossover between conduction and valence bands near K'.(b) The triangular warping structure in the ferromagnetic band. (c) Band structure and the quantum anomalous Hall effect of 1T-CrS<sub>2</sub>F<sub>2</sub> with SOC considered. (d) Two metallic edge states between the conduction band and the valence band.

# Surface and bulk electronic structure and magnetism of lanthanide compounds probed with photoemission

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Photoemission spectroscopy is one of the most direct and powerful methods of studying the electronic structure of solids. By measuring the kinetic energy and angular distribution of the electrons photoemitted from a sample, one can obtain detailed information on both the energy and momentum of the electrons propagating inside a crystalline material. This is of high importance for uncovering the relation between electronic, magnetic, and chemical properties of solids. Also, complementary information on the atomic structure can be obtained by analyzing angular distributions of core-level photoelectrons obtained from photoelectron (PED) diffraction measurements.

Here, we use photoemission spectroscopy to study the electronic structure, magnetism and related properties of layered crystals of lanthanide compounds  $LnT_2X_2$ , where Ln is a rare-earth element, T = Rh, Ir or Co, and X = Si or P. Some of these materials exhibit strongly correlated electronic behavior and unusual magnetic properties. Our results demonstrate the capabilities of various photoemission techniques to reveal the features of the electronic and spin structure of quantum materials, including bulk and surface electronic states, spin-orbit interaction effects, electron-boson interactions, changes in the valency of 4f elements, differences in the magnetic properties of the surface layers from the bulk ones, variations of the crystal field near the surface that leads to changes in the direction of 4f magnetic moments[1-4].

The work was supported by the Ministry of Science and Higher Education of the Russian Federation (No. 075-15-2024-632) and by the St Petersburg State University (Grant No. 95442847).

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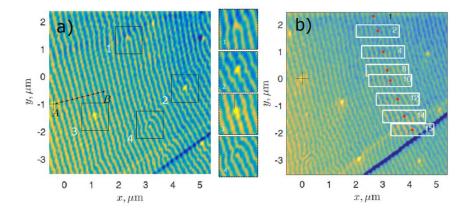
#### Temporal evolution of topological domain-wall defects in ferromagnetic superconductors

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The coexistence of seemingly contradictory phenomena, such as superconductivity and ferromagnetism in EuFe<sub>2</sub>(As<sub>1-x</sub>P<sub>x</sub>)<sub>2</sub>, gives rise to a variety of effects not observed in materials that exhibit either ferromagnetism or superconductivity alone [1]. The interplay between two competing order parameters, characterizing the magnetic and superconducting subsystems, leads to the emergence of complex magnetization patterns, contributing to a highly diverse phase diagram [1,2]. In this unique system, ferromagnetic bulk domain walls are stabilized, and can coexist with vortices and anti-vortices of the superconducting condensate [2]. In our study, we show that the formation of ferromagnetic domain walls in the Meissner state of such a material is accompanied by the temporal evolution of topological Y-shaped defects of the domain wall structure. Through experimental observation of the magnetization pattern on the surface of the bulk sample, we identified the slow motion of the defects along the domain walls. The experimental findings align with the theoretical analysis of emerging patterns, utilizing a model that combines the Ginzburg-Landau theory for the superconducting condensate and the Landau-Lifshitz-Gilbert equations for magnetization.



**Fig. 1:** a) Domain walls in  $EuFe_2(As_{1-x}P_x)_2$  at T=18K; defects in boxes 1-4 are enlarged in the corresponding panels; 2 and 3 are vortex defects, 1 and 4 are topological Y-shaped defects. b) A defect (red spot) moves downwards along the domain wall (time-frame insets are numbered as 1-15).

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#### Nonlinear kinetic inductance of composite superconductors

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Superconductors are characterized by the presence of a kinetic inductance  $L_k$  in addition to the ordinary, geometric inductance  $L_g$ . While  $L_g$  determines the magnetic field energy stored in a superconductor with a current  $E_B \sim L_g I^2/2$ ,  $L_k$  is related to the kinetic energy of superconducting electrons  $E_k \sim L_k I^2/2$ . The dependence of the concentration of superconducting electrons on the temperature T and current I leads to the dependence  $L_k(I,T)$ , which is used in many applications such as electromagnetic radiation detectors, parametric amplifiers, magnetic field/current detectors.

In my talk I present the results of our works devoted to the study of the  $L_k(I,T)$  dependence in two types of composite/hybrid superconductors: superconductor/ferromagnet/normal metal (SFN) [1] and superconductor/normal metal (SN) [2,3]. For the SFN composite in the Fulde-Ferrell state, the unique properties are theoretically predicted: a) the presence of a hysteretic dependence  $L_k(I)$ , leading to the presence of two states with different  $L_k$  values at the same current value; b) strong nonlinearity of  $L_k$  both at the depairing current and at a much lower current; c) divergence of  $L_k$  not only at the critical temperature, but also at the temperature of the transition to the Fulde-Ferrell state.

For the SN composite consisting of a 'dirty' superconductor and a low-resistive normal metal, a range of parameters was found where the  $L_k(I)$  dependence has a strongly nonlinear region at a current significantly lower than the depairing current [2,3], which was confirmed in the experiment [2]. Based on the obtained result, a new type of detector (sensor) of single photons (including the gigahertz range) and magnetic field/current was proposed – a sensor on nonlinear kinetic inductance [3].

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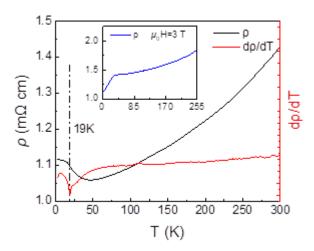
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## A new Mn-Bi-Te ternary antiferromagnetic topological insulator

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MnBi<sub>2</sub>Te<sub>4</sub> antiferromagnetic topological has been attracted people's attention owing to its special surface states meanwhile its intrinsic magnetic<sup>[1-3]</sup>. The gapless surface states of topological material expected to achieve quantum spin hall effect and further to attain lossless energy transport<sup>[4]</sup>. But the temperature required to achieve quantum anomalous hall effect far below room temperature, due to material limitations, therefore, there is an urgent need to develop new topological insulators. In this work, we successfully growth Mn-Bi-Te ternary antiferromagnetic topological insulator by melting method and characterized using scanning transmission electron microscopy (STEM), Single Crystal X-Ray Diffraction (SXRD), physical property measurement system magnetic (PPMS) and Angle-resolved photoemission spectroscopy (ARPES). Novel Mn-Bi-Te ternary material belong to R m space group, antiferromagnetic transition temperature is around 20K. When the magnetic field rises to 0.5T, a magnetic phase transition occurs which from antiferromagnetic to ferromagnetic. A amount of Bi<sub>Te</sub> lead to P-type doped, so after evaporating cesium on the surface of the sample, the Fermi level can be seen to shift upwards through ARPES, thus revealing the surface state of the sample.



Pic.1 Resistance versus temperature curve of Mn-Bi-Te

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# Stability and surface reactivity of topological insulators and related materials

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The unique properties of three-dimensional topological insulators (TIs) offer the possibility of creating entirely new electronic and spintronic devices for future information technologies. In contrast to trivial insulators, the appearance of spin-polarized electronic states inside the bulk band gap at the surface or interface with a trivial insulator is caused by band inversion due to strong spin–orbit coupling. The surface of such materials is highly conductive, and the surface electronic and spin transport. The surface states are protected by the time-reversal symmetry; they are not influenced by any perturbations such as surface defects, non-magnetic impurities or even partial oxidation.

Device applications of these materials require deep knowledge of their stability towards the ambient atmosphere and other media used in material processing. It has been well established that the reactivity of  $Bi_2Se_3$  to oxygen is very low.  $Bi_2Te_3$  and especially  $Sb_2Te_3$  are much more reactive. Therefore, their preparation and processing conditions should be carefully controlled. For mixed crystals with cation substitution, the reactivity can be predicted as an intermediate between the counterparts.

Experimental studies are mainly performed using photoemission methods including synchrotron-based ones. Experiments can be performed in situ or ex situ. The in situ results are obtained at a constant oxygen pressure of 0.01-10 mbar (ultimately till 1 bar). The oxidation kinetics is measured by XPS in course of reaction, i.e. spectra were acquired when spectrometer chamber filled with oxygen to reveal reaction mechanism. Typically, the in situ oxidation results do not indicate the presence of any induction period, and oxidation proceeds faster compared to the ex situ experiments due to additional oxygen activation by photons. For ex situ measurements, where the reaction is considered as "frozen" in UHV, the crystals were cleaved under atmospheric condi- tions and exposed to air at controlled humidity. Therefore, quantitative evaluation of the reactivity is more releable in this case.

# Novel physics in twisted systems.

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Twisted systems, starting with twisted bilayer graphene, have emerged as one of the most fascinating platforms in condensed matter physics with a wide range of potential applications. These systems exhibit an array of novel properties including correlated insulating states, magnetism, and superconductivity. By manipulating the twist angle between the layers, the electronic properties of the system can be precisely tuned. Beyond twisted bilayer graphene, such as graphene/hBN superlattice, twisted monolayer-bilayer graphene, twisted double bilayer graphene and alternating twisted graphene have also demonstrated many unique correlated phase diagrams and band topology. These systems provide a distinctive platform for investigating correlation phenomena and have potential applications in fields such as electronics and quantum computing. Continued research into twisted graphene systems is anticipated to yield many exciting discoveries and advancements.

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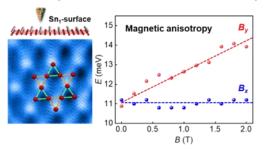
# Nanoscale visualization of symmetry-breaking electronic orders and magnetic anisotropy in a kagome magnet YMn6Sn6

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Kagome lattice hosts a plethora of quantum states arising from the interplay between nontrivial topology and electron correlations. The recently discovered kagome magnet  $RMn_6Sn_6$  (R represents a rare-earth element) is believed to showcase a typical kagome band, with Dirac cones, flat bands, and Van Hove singularities located near the Fermi level. The Mn-Kagome layers dominate the nontrivial topological electronic properties of the crystal, while the R element significantly influences the magnetic structure. Therefore, the  $RMn_6Sn_6$  family possesses numerous novel and tunable quantum properties<sup>[1]</sup>. YMn\_6Sn<sub>6</sub>, as one of its members, exhibits a spiral antiferromagnetic structure along the c-axis at low temperatures due to the non-magnetic  $Y^{[2]}$ . Investigating the kagome lattice electronic states and magnetization responses is crucial for understanding the unconventional electronic behaviors and complex magnetic phenomena arising from its unique geometric structure.

Here, we report the characterization of local electronic states and their magnetization response in YMn<sub>6</sub>Sn<sub>6</sub> via scanning tunneling microscopy measurements under vector magnetic fields<sup>[3]</sup>. Our spectroscopic maps reveal a spontaneously trimerized kagome electronic order in YMn<sub>6</sub>Sn<sub>6</sub>, where the sixfold rotational symmetry is disrupted while translational symmetry is maintained, exhibiting correlation-driven unusual orbital textures. Further application of an external vector magnetic field demonstrates a strong coupling of the YMn<sub>6</sub>Sn<sub>6</sub> kagome band to the field, which exhibits an energy shift discrepancy under different field directions, implying the existence of a magnetization-response anisotropy and anomalous g factors. Our findings establish YMn<sub>6</sub>Sn<sub>6</sub> as an ideal platform for investigating kagome-derived orbital magnetic moment and correlated magnetic topological states.



**Pic. 1** There exists a spontaneously trimerized kagome electronic order in YMn<sub>6</sub>Sn<sub>6</sub>, and it exhibits anisotropic magnetic responses when external vector magnetic fields are applied in different directions.

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# Controllable Construction and Electronic Properties Investigation of Two-Dimensional TMDs Heterojunction and Homojunction

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Two-dimensional (2D) materials have drawn intensive attention since they can be manipulated to form different electronic structures, which gives rise to a variety of strongly correlated physical properties, once the long-range Coulomb interaction exceeds kinetic energy of electrons. Moreover, the construction of low-dimensional homostructures and heterostructures based on 2D transition-metal dichalcogenides (TMDs) has attracted widespread attention recently. Among them, the in-plane one-dimensional (1D) structures that consist of atomically thin TMDs with strongly correlated electrons are especially important, since they hold potential for exploring low dimensional correlated electronic properties.

Here we demonstrate that, using STM manipulation technique, we can precisely construct the 2D TMDs homojunctions and heterojunction based on the 2D atomic crystal thin T-NbSe<sub>2</sub> and H-NbSe<sub>2</sub> films, which provides a dynamic way to modify the correlated electronic states at the junctions. In the homojunction, we confirm the existence of 1D-confined potential at the homojunction of two single-layer 1T-NbSe<sub>2</sub> islands.<sup>[1]</sup> Such potential is structurally sensitive, and shows a non-monotonic function of their interspacing. In the heterojunction, the H-NbSe<sub>2</sub> metallic state penetrates the Mott insulating T-NbSe<sub>2</sub> at the H/T phase interface, with a prominent 2D charge density wave (CDW) proximity effect.<sup>[2]</sup> Moreover, an insulating Mott gap collapse with the disappearance of the upper Hubbard band is detected at the electronic phase transition region.

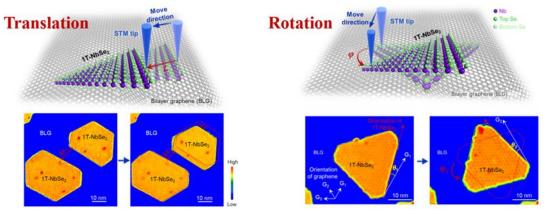


Fig.1 Controllable translation and rotation movement of NbSe<sub>2</sub> islands using STM manipulation technique.

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# Manipulation of strongly correlated electrons in monolayer 1T-NbSe2

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Monolayer transition metal dichalcogenides can host exotic phenomena such as correlated insulating and charge-density-wave (CDW) phases. Such properties are strongly dependent on the precise atomic arrangements. In this work, we firstly provide experimental evidence of the quantum spin liquid (QSL) state in 1T-NbSe<sub>2</sub> via measurements of the Kondo effect in a 1T-1H heterostructure, further supported by measurements for magnetic molecules on 1T-NbSe<sub>2</sub> [1]. And then, we concentrate on the phase transition of correlated insulating states under 1D confinement [2]. We find out that the CDW phase of 1T-NbSe<sub>2</sub> can survive under both tensile and compressive strains. Moreover, significant strain-induced phase transitions are observed, i.e., tensile (compressive) strains can drive 1T-NbSe<sub>2</sub> from an intrinsic correlated insulator into a band insulator (metal). Furthermore, we find that the multiple electronic phases can coexist at the nanoscale [3].

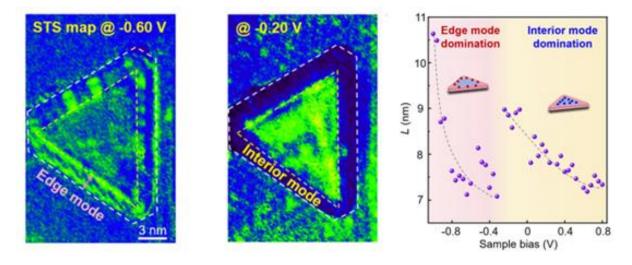
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#### Intertwined quantum confinement effects in charge-density-wave nanostructures

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Charge carriers confined into a geometrical configuration approaching the nanoscale are expected to show remarkable confinement phenomena that depart from the intrinsic ground states. Especially for the many-body interacting systems, understanding the underlying physics of quantum confined behaviors at the atomic scale is critical for the advancement of nanoscience and nanotechnology. Here we report anomalous quantum confinement effects and modulation effects of the substrates in triangular-like nanostructures of monolayer H-NbSe<sub>2</sub> by scanning tunneling microscopy experiments. The monolayer H-NbSe<sub>2</sub> nanostructures on graphene substrates usually generate domain boundaries which disappear when the substrates are H/T-NbSe<sub>2</sub>. Moreover, both H-NbSe<sub>2</sub> and T-NbSe<sub>2</sub> substrates can effectively induce striped charge states in monolayer H-NbSe<sub>2</sub> nanostructures. More importantly, our spectroscopic measurements reveal remarkable electron confinement behaviors in monolayer H-NbSe<sub>2</sub> nanostructure edges or within the nanostructures, dependent on the electron energies, resulting in intertwined quantum confinement effects, which are anomalous quantum confinement effects. Our results provide a fruitful playground for investigating the intertwined quantum confinement effects in charge-density-wave nanostructures under the two-dimensional limit.



Intertwined quantum confinement effects in in charge-density-wave nanostructures.

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#### Crystal growth of topological insulators with bulk-insulating property

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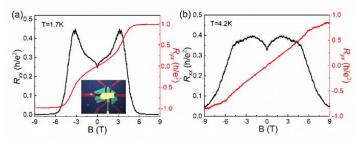
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Topological insulators (TIs) represent a novel quantum state of matter, characterized by an insulating bulk property and a conducting edge or surface state that protected by time-reversal symmetry <sup>[1, 2]</sup>. This topological surface state gives rise to numerous exotic transport phenomena, including Shubnikov-de Haas (SdH) oscillations, anti-weak localization and the quantum Hall effect (QHE) <sup>[3, 4]</sup>, etc. In three-dimensional (3D) TIs, the two half-integer quantized Hall conductances from the top and bottom surfaces collectively contribute to the integer quantized Hall conductance. The Bi<sub>2</sub>Se<sub>3</sub> family, including Bi<sub>2</sub>Se<sub>3</sub>, Bi<sub>2</sub>Te<sub>3</sub>, and Sb<sub>2</sub>Te<sub>3</sub>, is considered an ideal class of 3D TIs <sup>[5]</sup>. However, these materials often have poor bulk insulating property due to the presence of vacancies and anti-site defects. Thus, the bulk-dominated transport induces significant challenge in observing the QHE in 3D TIs <sup>[3, 6, 7]</sup>.

 $Bi_{2-x}Sb_xTe_{3-y}Se_y$  displays an amazing low carrier density, especially for the composition of x=1 and y=2, that is BiSbTeSe\_2. The surface mobility was improved to 4000 cm<sup>2</sup>/Vs through a two-step melting-Bridgman growth<sup>[8]</sup>. On this basis, we further improved the surface mobility to 7000cm<sup>2</sup>/(Vs) in device and realized QHE without gating. Besides, we observed a bulk insulating behavior in Bi<sub>2</sub>Te<sub>3</sub> derived from topological superconductor candidate  $Tl_{0.6}Bi_2Te_3$  through increasing Te content.



Pic. 1 QHE of Sn<sub>0.02</sub>Bi<sub>0.98</sub>SbTeSe<sub>2</sub> device without gating.

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# Quantum error mitigation in the regime of high noise using deep neural network: Trotterized dynamics

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Noisy intermediate-scale quantum (NISQ) devices represent the current edge of quantum computing technology. Particularly, such processors can be useful for solving evolutionary problems. However, the simulation of the dynamics of such systems at long times requires a large number of Trotter decomposition steps of evolution operator. This leads to the fact that a large number of quantum gates are required for simulation, which means that the outcomes from the quantum computer become too noisy. To address these limitations, advanced quantum error mitigation strategies like probabilistic error cancellation and zero noise extrapolation have been developed and are proving critical in enhancing the utility of NISQ machines.

We proposed a learning-based method to mitigate quantum errors using deep neural networks (DNNs). This method focuses on optimizing error reduction in quantum circuits, specifically those employed in Trotterized quantum simulations. The fundamental concept involves training a deep neural network with data from shallower, less noisy circuits, and then applying this model to deeper, noisier circuits. In order to get noisy data for training we artificially increase of the quantum circuits depth by incorporation of fictitious Trotter blocks formally equivalent to identity gates into the circuit. Their role is to increase noise level due to the hardware imperfections while preserving the circuit's general structure and its relevant features.

The main goal of this study is to thoroughly evaluate the performance of our neural network-based approach for quantum error mitigation under various noise conditions. We focus on conducting detailed numerical simulations to differentiate between distinct types of quantum noises, which is particularly crucial for understanding the complex dynamics in superconducting quantum devices. Our study specifically investigates the impact of several noise channels, including depolarizing and inhomogeneous Pauli noises, as well as ZZ crosstalk, which is particularly challenging in fixed-frequency superconducting qubits. The ultimate goal is to demonstrate marked improvements in data quality for all these noise channels. This research aims to establish a robust method that effectively combines machine learning with quantum error mitigation techniques to significantly improve the accuracy and practicality of NISQ devices.