

EVENT PROGRAM

CONDUCTED BY NEBRASKA EPSCoR WITH FUNDING FROM
NATIONAL SCIENCE FOUNDATION AWARD OIA-2044049



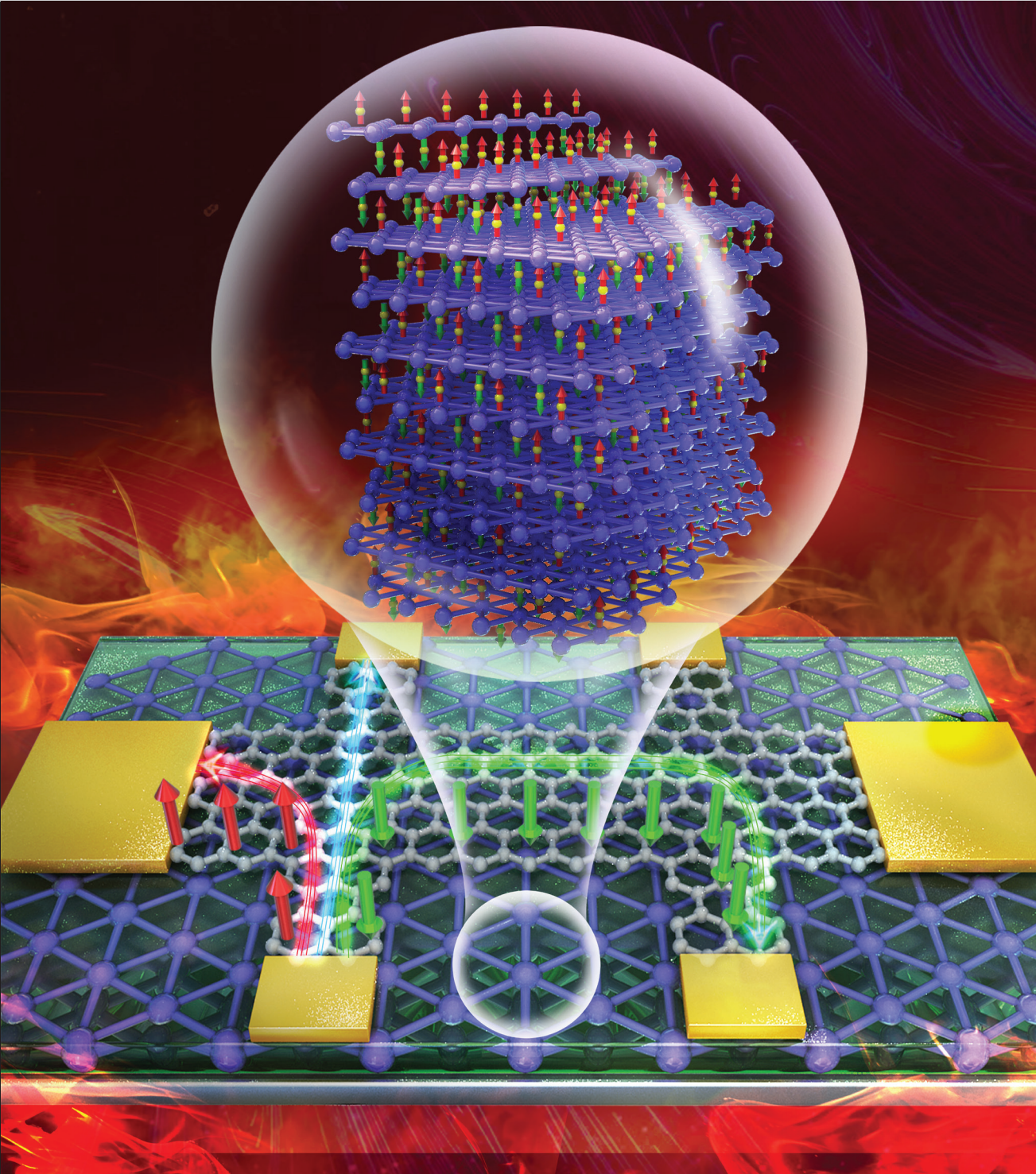
equate.unl.edu | epscor.nebraska.edu

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2023 Nebraska Research & Innovation Conference

TOPOLOGY AND VALLEY-DRIVEN QUANTUM PHENOMENA

MARCH 17 | LINCOLN, NEBRASKA





Message from the Nebraska EPSCoR Director

Welcome to the 2023 Nebraska Research & Innovation Conference (NRIC)! Thank you to our speakers for sharing their time and expertise with us.

Today's event extends an annual series of conferences and symposia that Nebraska EPSCoR has been organizing to advance research activities in this state. This year's conference connects thematically with Emergent Quantum Materials and Technologies (EQUATE), our five-year project funded by the National Science Foundation.

In EQUATE's Year 2, this symposium was coordinated with leadership by the project's FRG1 team, led by Dr. Xia Hong. We thank her for her efforts and excellent connections in gathering this excellent slate of speakers and topics.

Please enjoy this event's knowledge transfer and networking opportunities. We are dividing our poster presentations into two sessions, allowing participants to present their work at one session and enjoy colleagues' presentations in the other session.

Best,

Matthew T. Andrews, Ph.D.
Director, Nebraska EPSCoR
Principal Investigator, Emergent Quantum Materials and Technologies (EQUATE)

Notes:

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EQUATE Leaders

Scientific Director -- Christian Binek, Ph.D. & Associate Scientific Director--Rebecca Lai, Ph.D. (UNL)
FRG1 -- Xia Hong, Ph.D. (University of Nebraska-Lincoln)
FRG2 -- Abdelghani Laraoui, Ph.D. (UNL)
FRG3 -- Jonathan Wrubel, Ph.D. (Creighton University)

Learn More

Emergent Quantum Materials and Technologies:
equate.unl.edu

Nebraska EPSCoR Staff

Carole Allen Communications Specialist
Aaron An, Accountant
Jodi Sangster, PhD, Outreach Coordinator
Nancy Simnitt, Executive Assistant

COVER ART: IMAGE ACKNOWLEDGEMENT

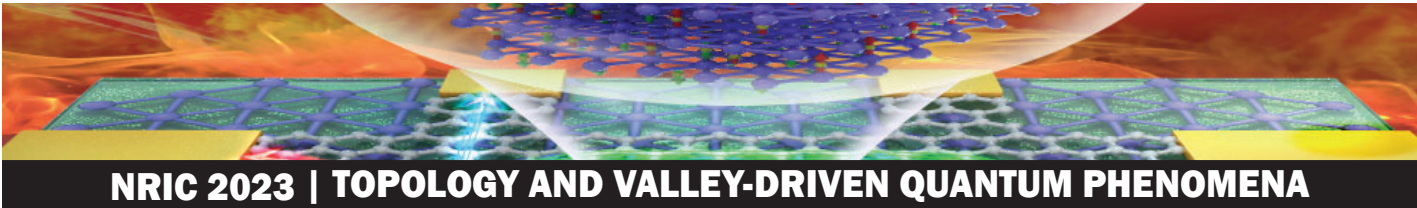
Graphene on Chromia: A System for Beyond-Room-Temperature Spintronics. Keke He, Bilal Barut, Shenchu Yin, Michael D. Randle, Ripudaman Dixit, Nargess Arabchigavkani, Jubin Nathawat, Ather Mahmood, Will Echtenkamp, Christian Binek, Peter A. Dowben, Jonathan P. Bird. (Volume34, Issue12, March 24, 2022, 2105023).

<https://onlinelibrary.wiley.com/share/FH6IDH4TBA6SJ3WGUSGF?target=10.1002/adma.202105023>

AGENDA — FRIDAY, MARCH 17
WiFi Network: HiltonHonorsMeeting (no password needed)

- 7:30 - 8:00 AM Conference Check-In: Materials Pick-Up, Poster Setup & Continental Breakfast
- 8:30 - 8:45 Event Welcome and Introductions — Regents A ballroom
Matthew T. Andrews, Ph.D. - Nebraska EPSCoR Director
- 8:15 - 9:45 **SESSION 1: Magnetism in 2D van der Waals Heterostructures**
Session Host: Xia Hong, Ph.D.
- 8:15 - 9:00 a.m. -- Xiaodong Xu, University of Washington
Interaction induced magnetism in 2D semiconductor moiré superlattices
- 9:00 - 9:45 a.m. -- Branislav Nikolic, University of Delaware
Spin-Orbit Torque and Spin Pumping in van der Waals Heterostructures of Magnetic Two-Dimensional Materials
- 9:45 - 11:00 **MORNING POSTER SESSION & REFRESHMENTS**, Regents B ballroom — *ODD-numbered poster presentations*
- 11:00 - 12:30 **SESSION 2: Topological Semimetals - Regents A ballroom**
Session Host: Xiaoshan Xu, Ph.D.
- 11:00 - 11:45 a.m. -- Liuyan Zhao, University of Michigan
Dual magnetism and magnetic fluctuations in a magnetic Weyl semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$
- 11:45 a.m. - 12:30 p.m. -- Mingzhong Wu, Colorado State University
Harnessing Spin in α -Sn
- 12:30 - 1:30 PM **LUNCH** — Atrium
- 1:30 - 2:15 **SESSION 3: Synergy Between Topology and Spin Current** — Regents A ballroom
Session Host: Evgeny Tsymbal, Ph.D.
- 1:30 - 2:15 p.m. -- Alexey Kovalev, University of Nebraska-Lincoln
Spin currents and topology in magnetic heterostructures
- 2:15 - 3:30 **AFTERNOON POSTER SESSION & REFRESHMENTS**, Regents B ballroom — *EVEN-numbered poster presentations*
- 3:30 - 5:00 **SESSION 4: Novel Topological Materials** — Regents A ballroom
Session Host: Yinsheng Guo, Ph.D.
- 3:30 - 4:15 p.m. -- Seongshik (Sean) Oh, Rutgers - the State University of New Jersey
Hybrid topological superconductors: Toward an optimal platform for topological quantum computation
- 4:15 - 5:00 p.m. -- Suyang Xu, Harvard University
Observation of the Layer Hall Effect in Topological Axion Antiferromagnet MnBi_2Te_4
- 5:00 PM **CONFERENCE ENDS - THANK YOU FOR COMING!**

On Twitter, follow @NebraskaEPSCoR and include #NRIC23 and #NebEQUATE in your tweets related to this event.



NRIC 2023 | TOPOLOGY AND VALLEY-DRIVEN QUANTUM PHENOMENA

Friday, March 17

MATERIALS PICK-UP & CONTINENTAL BREAKFAST

EMBASSY SUITES HOTEL, LINCOLN NE

7:30 - 8:00 A.M.

EVENT WELCOME & INTRODUCTIONS

MATTHEW T. ANDREWS, Ph.D.
Director, Nebraska EPSCoR

8:00 - 8:15 A.M.

ALL GUEST SPEAKER SESSIONS TAKE PLACE IN REGENTS BALLROOM A.

SESSION 1: Magnetism in 2D van der Waals Heterostructures | Host: Xia Hong, Ph.D.

Interaction induced magnetism in 2D semiconductor moiré superlattices

XIAODONG XU, Ph.D.
UNIVERSITY OF WASHINGTON

8:15 - 9:00 A.M.

Many-body interactions between carriers lie at the heart of correlated physics. The ability to tune such interactions would open the possibility to access and control complex electronic phase diagrams on demand.

Recently, moiré superlattices formed by two-dimensional materials have emerged as a promising platform for quantum engineering such phenomena. In this talk, I will present a systematic study of the emergent magnetic interactions (both antiferromagnetic and ferromagnetic) in strongly correlated transition metal dichalcogenides moiré superlattices. I will show that the combination of doping, electric field, and optical excitation provide dynamic controls of the rich many-body Hamiltonian of moiré quantum matter.

Spin-Orbit Torque and Spin Pumping in van der Waals Heterostructures of Magnetic Two-Dimensional Materials

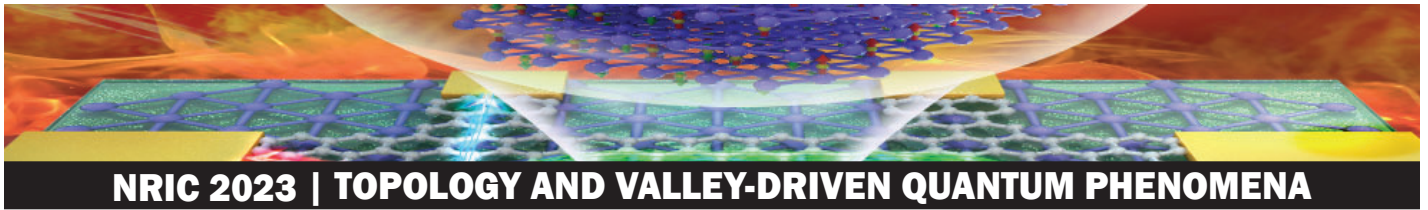
BRANISLAV NIKOLIC, Ph.D. | UNIVERSITY OF DELAWARE
9:00 - 9:45 A.M.

The bilayer heterostructures composed of an ultrathin ferromagnetic metal (FM) and a nonmagnetic material hosting strong spin-orbit coupling (SOC) are a principal resource for spin-orbit torque (SOT) and spin-to-charge conversion effects in next generation spintronics. The key to understand these effects is current-driven nonequilibrium spin density.

For example, it generates SOT when it is noncollinear to the direction of local magnetization and it can arise due to variety of microscopic mechanisms, including the spin Hall effect, spin-orbit proximity effect and different interfacial scattering mechanisms. The recently discovered two-dimensional (2D) magnetic materials offer new avenue for highly efficient and gate- or disorder-tunable SOT in van der Waals (vdW) heterostructures composed of few monolayers of atomically thin materials where the spin Hall effect from the bulk is absent.

Using first-principles quantum transport calculations, which combine nonequilibrium Green functions with noncollinear density functional theory, we predicted that injecting unpolarized charge current parallel to the interface of bilayer-CrI₃/monolayer-TaSe₂ vdW heterostructure will induce SOT-driven dynamics of magnetization on the first monolayer of CrI₃ that is in direct contact with metallic transition metal dichalcogenide (TMD) TaSe₂ and SO-proximitized by it. By combining calculated complex angular dependence of SOT with the Landau-Lifshitz-Gilbert equation for classical dynamics of magnetization, we find that this can reverse the direction of magnetization on the first monolayer to become parallel to that of the second monolayer, thereby converting bilayer CrI₃ from antiferromagnet to ferromagnet as the signature of nonequilibrium phase transition. Such transition can be detected by passing vertical current, and it is of potentially great interest to magnetic memory applications since it does not require any external magnetic field. Another vdW heterostructure exhibiting SOT is doubly proximitized graphene, which is neither magnetic nor hosts SOC in its isolated form, but proximity induced magnetic moments will exhibit SOT in Cr₂Ge₂Te₆/graphene/WS₂ vdW heterostructure which can be tuned by two orders of magnitude via the gate voltage.

Finally, we predict that SO-proximitized 2D magnets, pushed out of equilibrium by microwave absorption which leads to steadily precessing magnetization, will pump spin and charge currents exhibiting high harmonics of the microwave frequency with cutoff order ~20, in contrast to two decades old "standard model" of spin pumping at a single frequency.



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MORNING POSTER SESSION & REFRESHMENTS

REGENTS B BALLROOM

9:45 - 11:00 A.M.

SESSION 2: Topological Semimetals Host: Xiaoshan Xu, Ph.D.

Dual magnetism and magnetic fluctuations in a magnetic Weyl semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$

LIUYAN ZHAO, Ph.D., UNIVERSITY OF MICHIGAN

11:00 - 11:45 A.M.

ABSTRACT: $\text{Co}_3\text{Sn}_2\text{S}_2$ has drawn much attention from multiple aspects, including a magnetic Weyl semimetal candidate, a quantum anomalous Hall effect testbed, and a non-Bravais Kagome-lattice magnet. All these interesting phenomena critically require a comprehensive understanding on the magnetic structure of $\text{Co}_3\text{Sn}_2\text{S}_2$, which is, however, heatedly debated in literature and remains elusive. Here, we report our experimental efforts using femto-second laser based optical techniques to address the magnetism and fluctuations in this system. Using electric quadrupole second harmonic generation (EQ SHG), we show the presence of two magnetic phases – one onset at $T_{C,1} \sim 175\text{K}$ for the Ising-type ferromagnetic order for the out-of-plane spin component, and the other onset at $T_{C,2} \sim 125\text{K}$ for the XY-type antiferromagnetic order for the in-plane spin component. Using magneto-optical spectroscopy, together with anomalous Hall effect measurement, we show significant fluctuations at $T_{C,1} \sim 175\text{K}$ which disappears at lower temperatures.

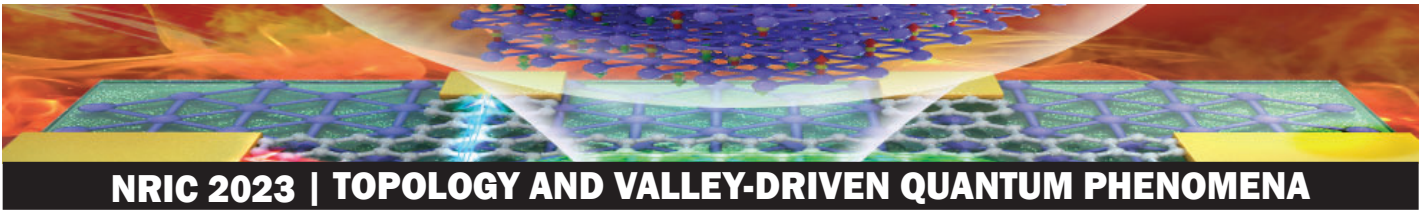
Harnessing Spin in α -Sn

MINGZHONG WU, Ph.D., COLORADO STATE UNIVERSITY

11:45 A.M. - 12:30 P.M.

ABSTRACT: Dirac semimetals are a recently discovered topological phase of quantum matter. α -Sn is unique among the Dirac semimetals because it is a single-element material and is therefore relatively easy to grow. Further, it can be transformed into other topological phases, such as a topological insulator or a Weyl semimetal, under strains or external fields. I will discuss our recent experimental work on α -Sn thin films along four directions:

- (1) Growth of α -Sn thin films by a CMOS-compatible sputtering technique.
- (2) Large damping enhancement in a ferromagnetic thin film due to the presence of topological surface states in an adjacent α -Sn thin film.
- (3) Current-induced magnetization switching via topological surface states in an α -Sn/Ag/CoFeB trilayer.
- (4) Spin-momentum-locking driven large magnetoresistance in α -Sn thin films that scales linearly with both magnetic and electric fields. These results indicate that topological Dirac semimetal α -Sn holds exciting promise of application in next-generation electronics and quantum technologies.



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LUNCH

EMBASSY SUITES HOTEL, ATRIUM

12:30 - 1:30 P.M.

SESSION 3:

Synergy Between Topology and Spin Current

Host: Evgeny Tsymbal, Ph.D.

Spin currents and topology in magnetic heterostructures

ALEXEY KOVALEV, PH.D.

UNIVERSITY OF NEBRASKA-LINCOLN

1:30 - 2:15 P.M.

An ability to control spin currents is important for probing many spin-related phenomena in the field of spintronics, and for designing logic and memory devices with low dissipation. Spin-orbit torque is an important example in which spin current is used to control magnetization dynamics. In this talk, I will discuss the interplay between topology and spin flows that can arise in various types of magnetic systems, e.g., in magnetic insulators, magnetic multilayers, and van der Waals magnets. In particular, I will discuss spin Hall effect of magnons and its possible observation with NV centers, I will discuss spin superfluid transport in van der Waals magnets, and I will discuss absorption of spin currents at interfaces concentrating on interplay between intrinsic and extrinsic contributions and interfacial effects which can have implications for spin-orbit torques.

AFTERNOON POSTER SESSION & REFRESHMENTS

REGENTS B BALLROOM

2:15 - 3:30 P.M.

SESSION 4: Novel Topological Materials

Host: Yinsheng Guo, Ph.D.

Hybrid topological superconductors: Toward an optimal platform for topological quantum computation

SEONGSHIK (SEAN) OH, PH.D.

RUTGERS - THE STATE UNIVERSITY OF NEW JERSEY

3:30 - 4:15 P.M.

Topology has emerged as a new paradigm of classifying electronic materials over the past decade, and a series of topological materials including topological insulators (TIs) and topological semimetals (TSMs) have been predicted and subsequently identified experimentally. On the other hand, another group of topological materials, the topological superconductors (TSCs), have not enjoyed as much progress due to various materials challenges. Unlike TIs and TSMs, whose topological characters can be reasonably well identified from band structure calculations, there does not exist such a general formalism for identifying a TSC. As a work-around, it was shown in 2008 by Fu and Kane that proximity effect between an s-wave superconductor and a TI can be used to implement TSC that can host the Majorana zero mode, which is the building block for topological quantum computation. Despite the conceptual simplicity of this proximity-based approach, its implementation—typically based on elemental superconductors such as Al, Pb, and Nb—suffers from undesirable interfacial problems with the chalcogenide TIs, and this has been a major roadblock to the proximity-based TSC. However, over the past decade, my group has demonstrated that with well-manuevered thin film engineering, it is possible to get around many of the seemingly intractable materials problems in a variety of topological quantum matters. Here, I will present our ongoing endeavors, at the forefront of thin film engineering, to overcome these obstacles to a proximity-based TSC, with a few surprises found along the way.

Observation of the Layer Hall Effect in Topological Axion Antiferromagnet MnBi_2Te_4

SUYANG XU, PH.D. | HARVARD UNIVERSITY

4:15 - 5:00 P.M.

While ferromagnets have been known and exploited for millennia, antiferromagnets were only discovered in the 1930s. The elusive nature indicates antiferromagnets' unique properties:

- At large scale, due to the absence of global magnetization, antiferromagnets may appear to behave like any non-magnetic material;
- At the microscopic level, however, the opposite alignment of spins forms a rich internal structure.

In topological antiferromagnets, such an internal structure leads to a new possibility, where topology and Berry phase can acquire distinct spatial textures. We study this exciting possibility in an antiferromagnetic Axion insulator, even-layered MnBi_2Te_4 flakes. We report the observation of a new type of Hall effect, the layer Hall effect, where electrons from the top and bottom layers spontaneously deflect in opposite directions.

POSTERS

Emergent Ferroic Materials and Phenomena, Posters 1 - 17

Adam Erickson, Qihan Zhang, Suvechhya Lamichhane, Sy-Hwang Liou, Jingshen Chen, Abdelghani Laraoui

POSTER #1

Studying the creation and motion of skyrmions in broken inversion symmetry CoPt gradient single-crystal thin films

Magnetic skyrmions are nanoscale spin textures characterized by a topological charge, and are proposed for the next generation of ultra-dense magnetic memories. Skyrmions can occur as two-dimensional ground states in magnetic systems where strong spin orbit coupling and broken inversion symmetry lead to Dzyaloshinskii-Moriya interaction (DMI). In this work, we use magnetic force microscopy (MFM) and nitrogen vacancy (NV) magnetic scanning microscopy to investigate the effect of broken inversion symmetry in $\text{Co}_x\text{Pt}_{1-x}$ gradient single-crystal films, where stoichiometric coefficient x is engineered to vary continuously from the top surface to the bottom interface. We study the size and type of skyrmions as a function of the $\text{Co}_x\text{Pt}_{1-x}$ film thickness, gradient sign, and applied magnetic field. Furthermore, we study the effect of a direct current via spin-orbit torque mechanisms on the skyrmion creation and motion in $\text{Co}_x\text{Pt}_{1-x}$ thin films.

Sema Guvenç Kilic, Ufuk Kilic, Mathias Schubert, Eva Schubert, Christos Argyropoulos

POSTER #2

Nonreciprocal topological edge states unveiled by all-dielectric metasurface platform

During the last decade, two-dimensional photonic topological insulators (2D-PTIs) have gained great interest due to their potential use in quantum information technologies, waveguide systems, and next-generation photonic integrated circuits. In this research, we propose a planar checkerboard metasurface platform made of all-dielectric, silicon, materials such that the detrimental effects of Ohmic losses can be mitigated. We systematically optimize the unit cell size of our proposed metasurface design so as to operate as a bandpass filter (with a bandwidth of $\sim 130\text{THz}$) in the technologically important optical frequency regime ($\sim 370\text{THz}$ to 500THz). Particularly, the integration of the lattice mismatch in the periodic arrangement of our checkerboard structure results in an ultra-narrowband leak mode (full-width half maxima of $\sim 1\text{GHz}$) within the main bandwidth of the bandpass filter. Based on our energy dispersion band diagram calculations with the incorporation of Kerr effect nonlinearity, we found that this leak mode exhibits topological edge state characteristics. The spectral location of the leak mode observed in transmission/reflection spectra is in excellent agreement with the corresponding eigenfrequency value of the topological edge mode in the energy dispersion band diagram. Based on our other systematic forward and backward light propagations through our proposed metasurface design, we also show that the topological edge state exhibits nonreciprocal behavior. Finally, we introduced a dielectric defect in the shape of a pillar and investigated its effect on the topological edge state. Depending on the size of this defect, we theoretically show a nonreciprocal topological edge mode with extreme spectral tunability. We envision that the modulation and control of light using such metasurface design can provide a substantial boost to the developing field of quantum optics and photonics.

Kai Huang, Ding-Fu Shao, Edward Schwartz, Alexey Kovalev, and Evgeny Y. Tsymlal

POSTER #3

Magnetic antiskyrmions in 2D van der Waals magnets engineered by layer stacking

Skyrmions and antiskyrmions are swirling magnetic textures with nontrivial topologies in magnetic materials. Unlike the widely investigated skyrmions, antiskyrmions are rarely found due to the requirement of the anisotropic Dzyaloshinskii-Moriya interaction (DMI). Here we propose to exploit the recently demonstrated van der Waals (vdW) assembly of two-dimensional (2D) materials that are non-polar in the bulk form to break inversion symmetry and create conditions for the emergence of anisotropic DMI in 2D magnets. We demonstrate, based on symmetry analyses and first-principles calculations, that this strategy is a promising platform to realize antiskyrmions. The polar layer stacking of two centrosymmetric magnetic monolayers, such as CrI_3 , can efficiently lower the symmetry, resulting in anisotropic DMI that supports antiskyrmions. The DMI is reversible by switching the ferroelectric polarization inherited from the polar layer stacking, offering the ability to control antiskyrmions by an electric field. Moreover, we find that the magnetic anisotropy and DMI of CrI_3 can be efficiently changed by Mn doping, creating a possibility to control the size of antiskyrmions. Our work opens a new direction to generate and control magnetic antiskyrmions.

Bharat Giri, Xiaoshan Xu

POSTER #4

Anomalous Hall effect in Platinum/Nickel-Cobaltite bilayer

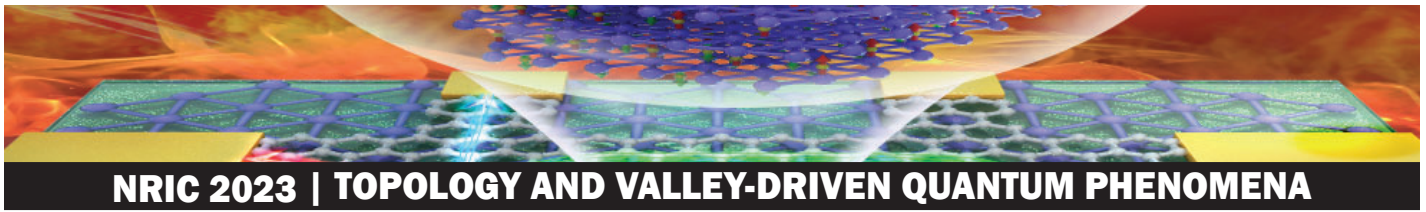
Spin structure of materials plays important roles in their transport properties. In order to study whether the spin interaction at the interface between ferrimagnetic NiCo_2O_4 (NCO) and strongly spin-orbit coupled metal/platinum (Pt) generates novel spin structure, we prepared Pt/NCO bilayer structures on MgAl_2O_4 (001) substrates using pulsed laser deposition (PLD) and studied the spin transport properties at various temperature with different NCO thickness. In addition to the anomalous Hall effect expected from NCO, we observed asymmetric topological-Hall-like effects (humps). The magnitude of the humps and the magnetic field where the humps appear change dramatically with temperature, which is correlated with the coercive field of NCO. These results suggest complex spin interactions at the NCO/Pt interface which may give rise to topological spin texture.

Ahsan Ullah, Balamurugan Balasubramanian, Bibek Tiwari, Bharat Giri, David J. Sellmyer, Ralph Skomski, Xiaoshan Xu

POSTER #5

Berry Curvature in Magnetic Nanoparticles

Berry curvature in ferromagnetic nanoparticles is investigated by analytical calculations and micromagnetic simulations. We estimate the Berry curvature in small nanoparticles due to magnetic states with stray-field effects near corners and edges, such as the flower state and magnetization curling state as the size of the



particle increases. Our results show as the size increases the nonuniformity in $M(r, H)$ also increases which increases skyrmion density. We determine the skyrmion density as a function of particle size and applied magnetic field. The micromagnetic simulation was also performed on either size coherent radii to study the Berry curvature and skyrmion number. Our simulation results agree with analytical calculations for both flower state and flux closure states. The nanoparticles of our focus are those whose radius R is smaller than the coherence radius R_{coh} , a size above at which the reverse magnetic field causes magnetization curling, and vortex. Direct imaging of a single magnetic domain state has been studied. We showed that in a circular dot of Co with a suitable size, a magnetic vortex state with perpendicular (turned-up) magnetization at the core is realized. The existence of the perpendicular magnetization spot has been confirmed by magnetic force microscopy (MFM) for Co.

Yifei Hao, Xuegang Chen, Myung-Geun Han, Yuewen Fang, Le Zhang, Hanghui Chen, Yimei Zhu, Xia Hong

Interface Charge Engineering in Ferroelectric-Gated Mott Transistors

POSTER #6

Epitaxial complex oxide heterostructures composed of ferroelectric gates and correlated channels are promising material platforms for developing high performance, energy efficient electronic devices. In this study, working with a ferroelectric $\text{Pb}(\text{Zr,Ti})\text{O}_3$ (PZT) gate, we present a systematic study of the ferroelectric field effect in rare earth nickelates $\text{Sm}_{0.5}\text{Nd}_{0.5}\text{NiO}_3$ (SNNNO), NdNiO_3 (NNO), and LaNiO_3 (LNO) to identify the optimal channel materials for constructing nonvolatile Mott transistors. For single layer nickelate channels, the resistance switching ratio $\Delta R/R_{\text{on}}$ peaks near the electrical dead layer thickness, then decreases abruptly due to strong depolarization. The highest room temperature $\Delta R/R_{\text{on}}$ of $\sim 200\%$ is observed in 1 nm NNO and LNO channels due to their small electrical dead layer thickness. We also show that inserting a $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ (LSMO) buffer layer can lead to over two orders of magnitude increase in $\Delta R/R_{\text{on}}$ for devices with the same channel thickness, which is attributed to the tailored carrier density profile due to the interfacial charge-transfer between nickelate and LSMO. A record high $\Delta R/R_{\text{on}}$ of 9,000% is observed in the 1.2 nm LNO/0.4 nm LSMO bilayer channel at 300 K. Our study addresses one of the key material challenges that limit the application potential of epitaxial ferroelectric-gated Mott transistors.

Gauthami Viswan, Kun Wang, Po-Shen Lu, Daniel Sando, Robert Streubel, Xia Hong, Valanoor Nagarajan, Archit Dhingra and Peter A. Dowben

Magneto-capacitance at the Ni/BilnO₃ Schottky Interface

POSTER #7

X-ray photoelectron spectroscopy (XPS) reveals the formation of an intermetallic Ni-Bi alloy at the Ni/BilnO₃ interface, grown on (Ba,Sr)RuO₃/SrTiO₃ single-crystals, and a shift in the Bi 4f and In 3d core levels to higher binding energies with increasing Ni thickness. The latter infers a band bending in BilnO₃ with a corresponding p-type Schottky barrier formation. The current-voltage characteristics of the Ni/BilnO₃/(Ba,Sr)RuO₃/SrTiO₃ heterostructure show a remarkable dependence of resistance and capacitance on the applied magnetic field and voltage cycling. These changes indicate a voltage-controlled band bending and a spin-polarized charge accumulation in the vicinity of the Ni/BilnO₃ interface yielding a magneto-capacitance effect without the need for multiferroic properties.

Detian Yang, Arjun Subedi, Yaohua Liu, Chao Liu, Valeria Laiter, Haile Ambaye, Peter A. Dowben, Xiaoshan Xu

POSTER #8

Intrinsic Exchange Bias from Interfacial Reconstruction in Epitaxial Ni_xCo_yFe_{3-x-y}O₄(111)/ α -Al₂O₃(0001) Thin Films

Intrinsic exchange bias up to 12.6 kOe is observed in the epitaxial thin film family of spinel oxides Ni_xCo_yFe_{3-x-y}O₄(111)/ α -Al₂O₃(0001) (0 ≤ x+y ≤ 3) with Co doping ratio in the range 0.15 ≤ y ≤ 2. An interfacial layer of rock-salt structure emerges between Ni_xCo_yFe_{3-x-y}O₄ thin films and α -Al₂O₃ substrates and is proposed as the antiferromagnetic layer unidirectionally coupled with ferrimagnetic Ni_xCo_yFe_{3-x-y}O₄. In NiCo₂O₄(111)/ α -Al₂O₃(0001) films, reflection high energy electron diffraction, x-ray photoelectron spectroscopy, x-ray reflection and polarized neutron reflection corroborate that the interfacial layer is antiferromagnetic Ni_xCo_{1-x}O (0.32 ≤ x ≤ 0.49) of rock-salt structure; the interfacial layer and exchange bias can be adjusted by growth oxygen pressure revealing the key role of oxygen in such interfacial reconstruction mechanism. This work establishes a family of intrinsic exchange bias materials with great tunability by stoichiometry and growth parameters and emphasizes the strategy of interface engineering in manipulating material functionalities.

Bo Zhang, Shuo Sun, Yinglu Jia, Jun Dai, Dhanusha T.N. Rathnayake, Xi Huang, Jade Casasent, Gopi Adhikari, Temban Acha Billy, Yongfeng Lu, Xiao Cheng Zeng, Yinsheng Guo

Simple Visualization of Universal Ferroelastic Domain Walls in Lead Halide Perovskites

POSTER #9

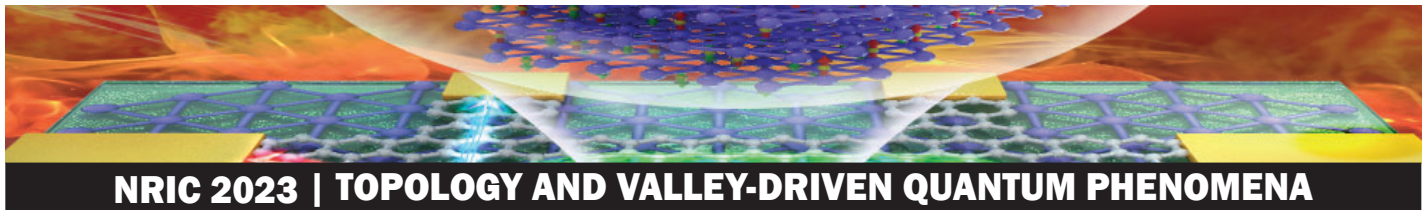
Domain features and domain walls in lead halide perovskites (LHPs) have attracted broad interest due to their potential impact on optoelectronic properties of this unique class of solution-processable semiconductors. Using nonpolarized light and simple imaging configurations, ferroelastic twin domains and their switchings through multiple consecutive phase transitions are directly visualized. This direct optical contrast originates from finite optical reflections at the wall interface between two compositionally identical, orientationally different, optically anisotropic domains inside the material bulk. The findings show these domain walls serve as internal reflectors and steer energy transport inside halide perovskites optically. First-principles calculations show universal low domain-wall energies and modest energy barriers of domain switching, confirming their prevalent appearance, stable presence, and facile moving observed in the experiments. The generality of ferroelasticity in halide perovskites stems from their soft bonding characteristics. This work shows the feasibility of using LHP twin domain walls as optical guides of internal photoexcitations, capable of nonvolatile on-off switching and tunable positioning endowed by their universal ferroelasticity.

Syed Q. A. Shah, Muhammet Annaorazov, Gaurab Rimal, Jian Wang, Mario F. Borunda, Jinke Tang, and Andrew J. Yost

POSTER #10

Controlling the Magneto-Optical Response in Ultrathin Films of EuO_{1-x} via Interface Engineering with Ferroelectric BaTi₂O₇

Utilizing pulsed laser deposition, a film of EuO_{1-x} was deposited onto a Si(001) substrate with MgO buffer and compared to the same heterostructure with an additional BaTi₂O₇ thin film on top of the EuO_{1-x} surface. X-ray diffraction (XRD) indicates the films crystallize into a preferred EuO(111) orientation; it also reveals the clear presence of EuSi₂, which suggests Si or Eu diffuses across the MgO buffer layer. EuO_{1-x} films exhibit a ferromagnetic (FM) signature and temperature-



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dependent exchange bias, indicated by MOKE measurements, suggesting the presence of a magnetic order well above the EuO Curie temperature with possible origins in charge carrier density near the interface. In comparison, an antiferromagnetic character persists well above the EuO Curie temperature of 69 K and the enhanced Curie temperature of 150 K for BaTi_2O_5 films grown on the EuO_{1-x} films. The antiferromagnetic behavior is not seen in thicker EuO_{1-x} thin films when integrated with other ferroelectric (FE) phases of the BaO-TiO_2 system, suggesting an origin in the perturbed charge population at the $\text{BaTi}_2\text{O}_5/\text{EuO}_{1-x}$ interface.

Syed Q. A. Shah, Ather Mahmood, Arun Parthasarathy, and Christian Binek

An investigation of the magnetoelectric monopole response in Chromia

POSTER #11

Powder samples have been suggested as a pathway to fabricate isotropic magnetoelectric (ME) materials which effectively only have a pseudoscalar or monopole ME response. We demonstrate that random distribution of ME grains alone does not warrant isotropic ME response because the activation of a non-vanishing ME response requires a ME field cooling protocol which tends to induce preferred axes. We investigate the evolution of ME susceptibility in powder chromia samples for various ME field cooling protocols both theoretically and experimentally. In particular, we work out the theoretical expressions for ME susceptibility for powder Chromia in the framework of statistical mechanics where Boltzmann factors weigh the orientation of the Néel vector relative to the local orientation of the c-axis of a grain. Previous approximations oversimplified the thermodynamic nature of the annealing process giving rise to misleading conclusions on the role of the magnitude of the applied product of electric and magnetic fields on the ME response. In accordance with our refined thermodynamic theory, a strong dependence of the functional form of α vs. T of Chromia powders on the ME field cooling protocol is observed. It shows on one hand that Chromia powder is not generically an isotropic ME effective medium as sometimes misleadingly stated, but, on the other hand, provides a pathway to realize the elusive isotropic ME response.

Rupak Timalisina, Haohan Wang, Adam Erickson, Bharat Giri, Xiaoshan Xu, and Abdelghani Laraoui

Study of spin waves in rare-earth garnet TmIG thin films

POSTER #12

Spin waves (magnons) are collective dynamic excitations of electronic spin systems in ferromagnetic/ferrimagnetic metals and insulators. Spin waves have wavelengths varying from a few nanometers to hundreds of micrometers and frequencies up to a few Terahertz, making them promising candidates in spintronics with a Joule-heat-free spin transport. In this work we use broadband ferromagnetic resonance (FMR) spectroscopy and nitrogen vacancy (NV) magnetometry to study the spinwave properties in ferrimagnetic insulator Thulium iron garnet (TmIG) thin films (thickness of 2 -35 nm) grown on gadolinium-gallium-garnet (GGG) and substituted-GGG (sGGG) substrates. FMR measurements reveal the FMR frequency dependence with applied magnetic field and damping $\sim 10^{-3}$. NV magnetometry allows measuring the surface propagating spin waves at the sub-micrometer scale, seen by the amplification of the local microwave magnetic field due to the coupling of NV spins with the stray-field produced by the spin waves. We discuss the effects of thickness and substrate (sGGGs vs GGG) on the spin waves properties and outline future experiments on NV-magnon coupling in TmIG nanostructures, relevant for quantum magnonics.

Amir Tarkian, Bryce Herrington, Ruthi Zielinski, Nhat Nguyen, Esha Mishra, Thilini Ekanayaka,1 WaiKiat Chin, and Robert Streubel

Strain-induced magnetic properties of amorphous iron-germanium films

POSTER #13

The magnetic properties of amorphous iron germanium films grown by co-evaporation are quantified using magnetometry. Combining surface-sensitive magneto-optical Kerr effect magnetometry with bulk-sensitive vibrating sample magnetometry reveals the spatial, angular, and temperature dependence of the magnetization and magnetic anisotropy. Low-temperature films possess a uniaxial strain-induced anisotropy which vanishes in room-temperature specimens. These properties are tested for various thicknesses, compositions, cappings, and seed layers.

Bryce Herrington, Ruthi Zielinski, Nhat Nguyen, Szu-Fan Wang, Allen A. Sweet, and Robert Streubel

Ferromagnetic resonances in yttrium iron garnet films prepared by metal-organic decomposition epitaxy

POSTER #14

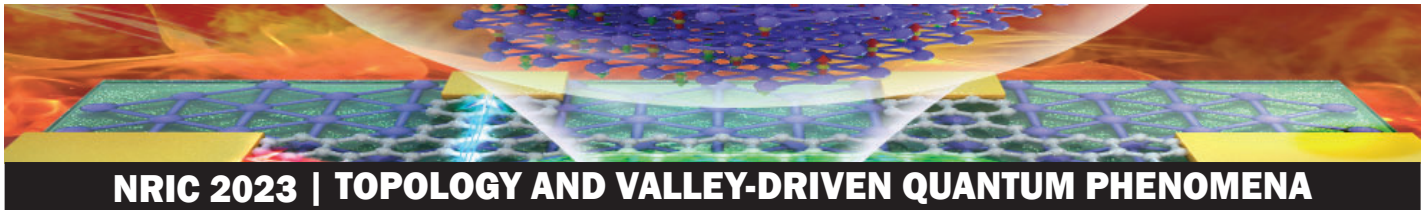
The magnetic and structural properties of yttrium iron garnet (YIG) films synthesized by a novel wet chemical deposition technique were investigated using magnetometry, ferromagnetic resonance spectroscopy, and electron backscatter diffraction. Films on gadolinium gallium garnet substrates are single-crystal on the millimeter scale with regions near the edge and corner exhibiting worse structural/chemical order, larger thickness, and larger coercive field and spin damping. The central regions possess quality factors similar to those obtained in films prepared with physical depositions.

Ather Mahmood, Jamie L. Weaver, Syed Qamar Abbas Shah, Will Echtenkamp, Jeffrey Lynn, Christian Binek

Effects of Boron surface accumulation on the Néel temperature revealed in B-doped Cr_2O_3 films

POSTER #15

Multi-functional thin films of boron (B) doped Cr_2O_3 grown by pulsed laser deposition exhibit voltage-controlled and nonvolatile Néel vector reorientation in the absence of a magnetic field. Isothermal toggling of antiferromagnetic states is demonstrated in prototype device structures at CMOS compatible temperatures up to 400 K. A strict determination of T_N remained elusive due to a thermally activated runaway effect of the Néel temperature. This behavior is understood by considering the B-enrichment due to the phenomenon of surface segregation. Cold Neutron Depth Profiling (cNDP), performed at National Institute of Standards and Technology, points at progressing depletion of B in the bulk and B-accumulation near the surface. By using Spin Hall measurements, we demonstrate a shift in T_N towards higher values of ≈ 477 K, associated with increase in B-concentration within an interfacial layer of 70 nm.



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Nhat Nguyen, Bryce Herrington, Anil Adhikari, Ruthi Zielinski, Shireen Adenwalla, and Robert Streubel

Angle-dependent magnetization relaxation in Co/Pt multilayers

POSTER #16

The temporal evolution of the magnetization in perpendicular magnetized Co/Pt multilayer stacks is investigated by means of magnetometry relaxation measurements at variable temperature and angles with respect to the surface normal. The analysis of hysteresis loops and relaxation data reveals insight into the switching mechanism mediated by, i.e., domain wall nucleation and propagation. The larger pinning site density and anisotropy of the thinner film cause domain wall nucleation to be dominant, while the opposite is true for the thicker film.

Arjun Subedi, Detian Yang, Xiaoshan Xu, Peter Dowben

A model for electronic phase transitions of CoFe₂O₄ and NiCo₂O₄ thin film surfaces: Temperature dependent X-ray photoemission studies of CoFe₂O₄ and NiCo₂O₄ thin films

POSTER #17

We observed large binding energy shifts of Co and Fe 2p_{3/2} core levels in X-ray photoemission spectroscopy (XPS) of CoFe₂O₄ thin films at room temperature due to large photovoltaic surface charging. This shows that the films can be dielectric. Temperature dependent XPS of the CoFe₂O₄ thin film showed that core level binding energies (BE) decreased with increasing temperature (T), but above 200 °C, during heating of the sample, shifts in the core level binding energies were not observed. This suggested that an evolution of the film to conducting after annealing to 200 °C. The dielectric nature of the film was restored only when the film was annealed in sufficient oxygen, indicating that the oxygen vacancies play a role in the transition of the film from dielectric (or insulating) to conducting. In contrast, similar studies on NiCo₂O₄ thin films showed that heating of NiCo₂O₄, which was observed to be a conductor, could make it insulator, and original more metallic character of the NiCo₂O₄ film could be restored only when the sample was annealed in sufficient oxygen. A model which could describe the phase transitions in both CoFe₂O₄ and NiCo₂O₄ is thus proposed:

$$|\Delta BE| = A \exp[-E_f / (R |\Delta T|)]$$

Van der Waals Materials, Posters 18 - 23

Yibo Wang, Sajib Kumar Saha, Tianlin Li, Yanwei Xiong, Kyle Wilkin, Anil Adhikari, Michael Loes, Jehad Abourahma, Bibek Tiwari, Xia Hong, Shireen Adenwalla, Xiaoshan Xu, Martin Centurion

Ultrafast electron diffraction instrument for gas and condensed matter samples

POSTER #18

We report a modified ultrafast electron diffraction (UED) instrument for both gas and condensed matter targets, where a time-resolved experiment with femtosecond resolution is demonstrated with solid state samples. The instrument relies on a hybrid DC-RF acceleration structure to deliver femtosecond electron pulses on the target, which are synchronized with femtosecond laser pulses. The laser pulses and electron pulses are used to excite the sample and to probe the structural dynamics, respectively. The new system is added with capabilities to perform transmission ultrafast electron diffraction on thin solid samples. It allows for cooling samples to cryogenic temperatures and to carry out time-resolved measurements. We tested the cooling capability by recording diffraction patterns of temperature dependent charge density waves in 1T-TaS₂. The time-resolved capability is experimentally verified by capturing the dynamics in photoexcited single-crystal gold. With this instrument, we plan to investigate the structural dynamics of organic ferroelectric materials after an ultrafast interaction with femtosecond laser pulses.

Jia Wang, Yifei Hao, Qiuchen Wu, Kun Wang, Takashi Taniguchi, Kenji Watanabe, and Xia Hong

Ferroelectric field effect in few-layer CrCl₃ tunnel junctions top-gated by PbZr_{0.2}Ti_{0.8}O₃ membranes

POSTER #19

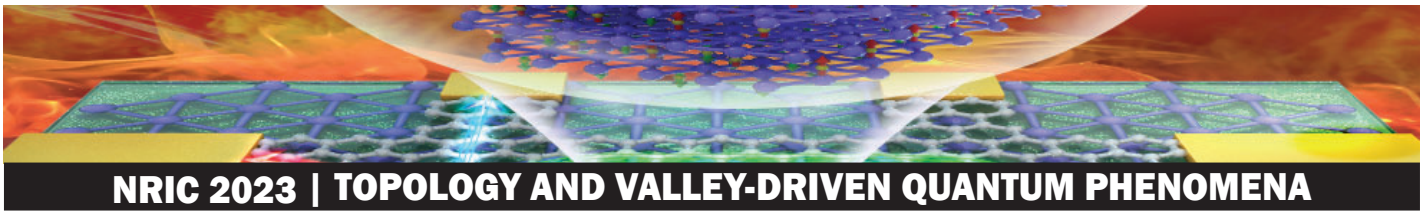
We report the ferroelectric gating control of few-layer antiferromagnetic CrCl₃ tunnel junctions. High-quality CrCl₃ flakes are synthesized on mica by the physical vapor transport technique. Epitaxial ferroelectric PbZr_{0.2}Ti_{0.8}O₃ (PZT) films (50 nm) are deposited on Sr₃Al₂O₆ (SAO) buffered (001) SrTiO₃ substrates and suspended via dissolving the SAO layer in water. Selected few-layer CrCl₃ flakes are fabricated into graphite/CrCl₃/graphite tunnel junctions by the all-dry stamping transfer method, which are encapsulated by either PZT membranes or h-BN flakes. Using conductive atomic force microscopy, we pole the PZT top-layer to uniformly polarized up and down states. Polarization reversal leads to nonvolatile modulation of the tunneling current, with an on/off ratio of 106 obtained at room temperature. Compared with h-BN encapsulated devices, the PZT-gated CrCl₃ tunnel junctions exhibit distinct magnetotransport properties. The tunneling magnetoresistance changes sign at low temperature, suggesting a change of magnetic state. Our study provides an effectively strategy to design CrCl₃-based nonvolatile memory and spintronic applications.

Kun Wang, Du Li, Jia Wang, Yifei Hao, Hailey Anderson, Li Yang, and Xia Hong

Engineering ferroelectricity and quadruple-well state in CuInP₂S₆ via interfacial PbZr_{0.2}Ti_{0.8}O₃

POSTER #20

Layered van der Waals CuInP₂S₆ exhibits room-temperature ferroelectricity with unconventional quadruple-well states. Its high mobility of Cu ions makes it challenging to achieve nanoscale polar control. Here we report the enhanced domain formation and piezoelectric response of CuInP₂S₆ via interfacial epitaxial ferroelectric oxide PbZr_{0.2}Ti_{0.8}O₃ films. Piezoresponse force microscopy (PFM) studies revealed spontaneous domains formed in CuInP₂S₆ flakes on Si and Au substrates, while thin flakes on PZT exhibit uniform polarization. This polar alignment effect vanishes with increasing CuInP₂S₆ thickness (t_{CIPS}). We further extracted the piezoelectric coefficient d₃₃ of CuInP₂S₆ flakes (d₃₃ CIPS) on the three types of substrates. The change of d₃₃ CIPS on PbZr_{0.2}Ti_{0.8}O₃ can be divided into three distinct regions. Compared with the results on Si and Au, the magnitude of d₃₃ for thin CuInP₂S₆ on PbZr_{0.2}Ti_{0.8}O₃ is significantly enhanced, and the sign of d₃₃ changes to positive. *In situ* PFM studies also revealed a Curie temperature of ~200 °C for CuInP₂S₆ on PbZr_{0.2}Ti_{0.8}O₃, which is much higher than the bulk value (42°C). The unconventional evolution of d₃₃ CIPS can be attributed to the interface-mediated structure distortion in CuInP₂S₆. Our study points to a new strategy to engineer the nano-domain structure and piezoelectric response of the two-dimensional ferroelectric CuInP₂S₆.



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Sanchaya Pandit, Yanan Wang

Design of Robust h-BN Microdisk Cavities Toward Integrated Quantum Photonics

POSTER #21

Quantum emitters based on defect centers in hexagonal boron nitride (hBN) have emerged as prominent light sources for integrated quantum photonic applications. Especially, the defect centers with single-photon emission around 635 nm have been demonstrated to exhibit lifetime-limited linewidth even at room temperature. This work explores the monolithic integration of this type of h-BN emitters with the whispering gallery mode (WGM) in the microdisk cavity. By optimizing the cavity design, strong coupling between the emitter and cavity has been predicated analytically. Furthermore, coherent energy transduction has been visualized as Rabi splitting and vacuum Rabi oscillation through the Quantum toolbox in python (Qutip) simulation. The robust cavity design and methodology developed will provide valuable guidelines for the realization of scalable and integrated quantum photonic circuits based on h-BN defect centers.

Hamed Vakili, Alexey Kovalev

Conductance Fluctuations in graphene with correlated disorder

POSTER #22

We investigate the conductance fluctuation of a graphene strip in presence of disorder. We use the correlated Gaussian function to represent a smooth disorder on the scale of the atomic scale to account for electron-hole puddles. We introduce spin-orbit coupling and magnetic field terms to see how they contribute to the conductance fluctuations. We further compare our results with the Altshuler-Lee-Stone theory of universal conductance fluctuations (UCF), which agrees well with the Anderson disorder model. The UCF in graphene (or any metallic system in general), depend on the number of symmetries protected degeneracies of the system. The introduction of the first and second-neighbor spin-orbit interactions modifies the amplitude of the UCF as it lifts the spin degeneracy. In the case of graphene, due to the presence of valleys, another degree of degeneracy exists. Finally, we compare the conductance fluctuations in zigzag and armchair graphene strips, which show different behavior near the Dirac point in the presence of magnetic disorder.

Renat Sabirianov, Jaeil Bai, Mengying Bian, Chang Huai, and Hao Zeng

The anomalous Hall conductivity of bulk and 2D Cr₂Te₃

POSTER #23

Chromium telluride (Cr₂Te₃) is an inorganic chemical compound that exhibits ferromagnetic properties ($T_c=195$ K) and a large perpendicular anisotropy of 7×10^5 J m⁻³. Recently, ferromagnetic Cr₂Te₃ nanorods were synthesized that exhibit hard and soft phase coexistence (Nanoscale, 2018, 10, 11028). We present the density functional study of the anomalous Hall effect of bulk and 2D Cr₂Te₃. The effect of magnetic texture is investigated as these layered materials show possibility of canting of the Cr moments in the ordered vacancy layers. We discuss these results in view of recent anomalous Hall effect measurement.

Optical Quantum Materials and Phenomena, Posters 24 - 29

Ufuk Kilic, Yousra Traouli, Matthew Hilfiker, Khalil Bryant, Stefan Schoeche, Rene Feder, Christos Argyropoulos, Eva Schubert, and Mathias Schubert

Unraveling the aspect-ratio driven evolution of anisotropic homogenization parameters of slanted columnar nanostructures from a wide variety of materials

POSTER #24

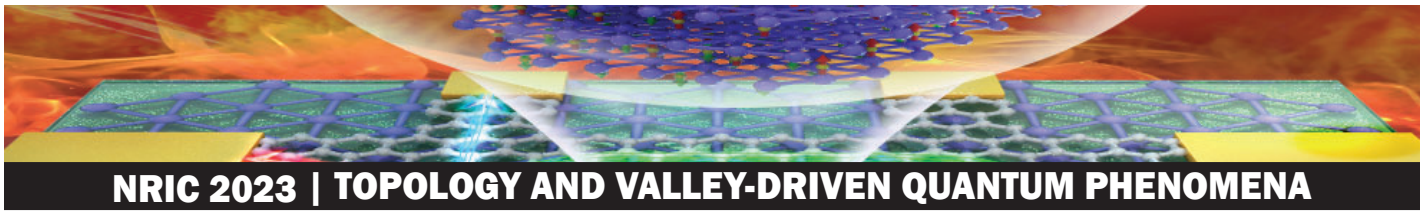
As a universally applicable homogenization method, the anisotropic Bruggeman effective medium approach (AB-EMA) can provide access to render anisotropic optical and structural properties of columnar nanostructures. In this study, by using a custom-built ultra-high vacuum electron beam evaporation glancing angle deposition, we fabricated sets of slanted columnar thin films (SCTF) from a wide variety of materials such as ultra-wide-bandgap (zirconia), low bandgap (silicon), zero-bandgap (titanium), and magnetic metal alloy (permalloy) materials. For each fabricated thin film, we acquired Mueller matrix generalized spectroscopic ellipsometry data from near-infrared (0.72 eV) to deep ultraviolet (6.5 eV) for multiple angles of incidence and one complete in-plane sample azimuthal rotation. As a result of the systematic AB-EMA based spectroscopic ellipsometry data analysis, we determine the anisotropic dielectric function and depolarization factors for each STCF. The depolarization factors provide information about the shape of the columnar inclusions and are extremely sensitive to changes in critical dimensions along major polarizability axes. Hence, we found that depolarization factors asymptotically evolve with the column lengths which are obtained from ellipsometry data analysis, and which are in an excellent agreement with results from high-resolution scanning electron microscopy image analysis. We propose an empirical relationship for structural dependent depolarization factors to predict the evolution of anisotropic optical properties for different thin film scenarios. Furthermore, we show and discuss the effective birefringence and dichroism as a function of thin film thickness for each material combination. We believe that our findings can boost accurate designs for next-generation sensors, and for other optoelectronic and photonic devices.

Ufuk Kilic, Matthew Hilfiker, Shawn Wimer, Alex Ruder, Christos Argyropoulos, Eva Schubert, and Mathias Schubert

Engineering the broadband enhanced chiral response of L-shaped metamaterials

POSTER #25

As a symmetry breaking phenomenon, chirality or handedness, has recently gained remarkable attention owing to its diverse applications in polarization optics, sensing, catalysis, stereochemistry, quantum information systems, and spintronics. Optical activity and circular dichroism form the optical manifestations of chirality and enable us to understand handedness in molecules and the control of the spin angular momentum in photons. While the chirality found in nature is very weak and emerges in deep ultraviolet part of the spectrum, it is difficult to be made tunable. Recent studies showed that one can obtain strong and tunable chiral response using subwavelength scale structures so-called metamaterials. As an emerging large-scale area, bottomup 3D nanomorphology fabrication method, glancing angle deposition (GLAD) is envisioned to be a promising route to the experimental realization of strong and tunable chiroptical responses.



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In this study, we propose a new class of metamaterials so called all-dielectric silicon-based L-shaped metamaterials. Using combined reflection and transmission mode Mueller matrix spectroscopic ellipsometry, we performed the chiroptical characterization of this new metamaterial platform. Hence, we experimentally demonstrate and theoretically verified that the proposed metamaterial can achieve tunable and strong broadband chirality with simplistic variations in its geometry parameters. Our investigation lays out a comprehensive road map for design, optimization, and fabrication of new chiral metamaterials with unprecedentedly high and broadband chiroptical properties that can be used in a plethora of diverse emerging classical and quantum optical applications.

Preston Sorensen, Ufuk Kilic, Sean Murray, Mohammed Ghashami, and Mathias Schubert

Tunable localized surface phonons SiC nanopillar metamaterial platform

POSTER #26

Artificially engineered structures with subwavelength scale dimensions, so-called metamaterials, are thought to be an area of great promise due to their ability to modulate, control, and confine incoming light. Of particular interest, these platforms can provide an enhanced thermal radiation in the near-field regime which leads to a myriad of applications, for example: thermophotovoltaic devices, optical elements, radiative cooling systems, thermo-electronic devices, thermal imaging. A strong candidate for such platforms is 6-H SiC, as it possesses negative permittivity in the infrared region and TO/LO phonon modes in the spectral neighborhood of typical thermal emissions.

In this study, by using the inductively coupled plasma reactive ion etching method, an array of conical frustum-shaped nanopillars is carved from a single slab of 6H-Silicon Carbide. The resulting metamaterial can operate as a nano diffraction grating, which scatters the components of a polychromatic beam of light away from the angle of incidence as a function of their respective wavelengths. We perform scanning electron microscopy image analysis in order to extract the dimensions of the nanopillars which feed our finite element modeling (FEM) based theoretical calculations. In order to perform optical characterization of SiC substrate and the nanopillar metamaterial platform, we acquire Mueller matrix spectroscopic ellipsometry (MM-SE) data from near-infra-red to deep-ultra-violet for multiple angles of incidence and full azimuthal sample rotation. As a result, we determine the uniaxial dielectric functions of both substrate and the nanopillars. We also perform a systematic FEM based theoretical characterization of thermal emissivity performance of the nanopillar metamaterial design as a function of geometrical parameters including radius, height, and spacing between neighboring pillars. As a next step, we will perform MM-SE based optical analysis of our metamaterial design by expanding our spectrum to the far infrared and implement the anisotropic Bruggeman effective medium approach-based model to unravel the anisotropic dielectric function and homogenization factors.

Megan Stokey, Rafał Korlacki, Matthew Hilfiker, Teresa Gramer, Jenna Knudtson, Steffen Richter, Sean Knight, Alexis Papamichail, Alyssa Mock, A. Mauze, Y. Zhang, J. Speck, R. Jinno, Y. Cho, H. G. Xing, D. Jena, Y. Oshima, K. Khan, E. Ahmadi, K. Irmscher, Z. Galazka, Vanya Darakchieva, and Mathias Schubert

Evolution of anisotropy and order of band-to-band transitions, excitons, phonons, static and high frequency dielectric constants including strain dependencies in alpha and beta phase $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$

POSTER #27

The rhombohedral alpha and monoclinic beta phases of gallium oxide both make promising candidates for ultra-wide bandgap semiconductor technology. Of particular interest are alloyed films and the evolution of anisotropic optical properties with respect to both alloy composition and strain induced effects. Here, we study alpha and beta phase $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ via a combined density functional theory and generalized spectroscopic ellipsometry approach across a range of alloying. Infrared-active phonon properties, static dielectric constants and midband gap indices of refraction are quantified. Strain and alloying effects are shown and compared to previous theoretical works. Bandgaps, excitons, and high-frequency dielectric constants are also investigated in the visible to vacuum-ultra-violet (VUV) spectral range. We identify a switch in band order where the lowest band-to-band transition occurs with polarization along the ordinary plane in $\alpha\text{-Ga}_2\text{O}_3$ whereas for $\alpha\text{-Al}_2\text{O}_3$ the lowest transition occurs with polarization in the extraordinary direction. With this, we present the most comprehensive picture of optical properties' evolution along composition and strain currently available.

Shawn Wimer, Ufuk Kilic, Mathias Schubert, Eva Schubert

Incorporating species-specific interactions in Monte Carlo ballistic simulations

POSTER #28

Simulation methods that incorporate the differences in interactions between particles of specific species in heterostructure and compound material GLAD deposition in discrete space, discrete areas, and continuous space are presented. The effects of the modifications on structure shape, film density, growth front evolution, and structure inclination angles are presented. Space partitioning methods used in the continuous space simulations allow for efficient physical deposition and reasonable times taken in the diffusion process, permitting realistic and accurate simulations.

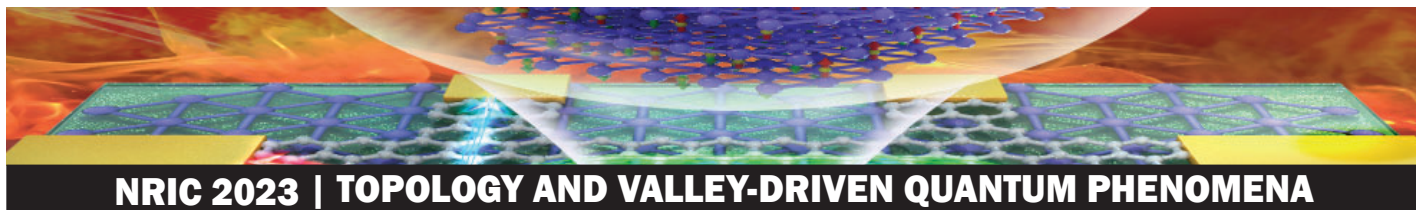
Yousra Traouli, Ufuk Kilic, Sema G. Kilic, Matthew Hilfiker, Alyssa Mock, Derek Sekora, Giselle Melendez, Daniel Schmidt, Mathias Schubert, and Eva Schubert

In-situ spectroscopic ellipsometry-based real-time growth monitoring of oxygen plasma enhanced ZnO atomic layer deposition process

POSTER #29

Thin film deposition techniques are continuously evolving given the growing amount of research being done on the advancement of nanotechnology. Atomic Layer Deposition (ALD) has been one of the most promising methods for growing metal-oxide ultra-thin films with pronounced conformality and uniformity. Zinc oxide (ZnO) is one of the propitious semiconductors with a wide range of useful applications in energy harvesting, electronic devices, and pharmacology. The need for an accurate and precise growth monitoring technique is necessary to obtain the critical dimensions of such material fabricated by ALD. One of the prominent in-situ thin film growth monitoring methods is spectroscopic ellipsometry (SE), an optical, non-invasive approach that can be integrated into ALD processes.

In this study, we successfully performed a systematic optimization of the oxygen plasma-enhanced ALD recipe for ZnO material. We utilized $\text{Zn}(\text{CH}_3)_2$ organometallic precursor as the main reactant, Oxygen plasma as the co-reactant, and Argon as the purging gas. Thanks to the integration of the SE instrument to our deposition chamber, we acquired *in-situ* SE data during the growth of ZnO ultra-thin films within the spectral range from 0.7-3.4 eV at 67.9° angle of incidence. We also



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proposed a simplistic model so-called dynamic dual box model which consists of five phases (substrate, mixed native oxide interface layer, metal oxide thin film layer, surface ligand layer, ambient) including two of them that function as dynamic parameters (metal oxide thin film layer thickness and surface ligand layer void fraction). Hence, the cyclic surface modifications and continuous ZnO ultra-thin film growth mechanisms are unraveled. Our proposed dynamic dual box model leads us to gain an in-depth understanding of the complex ALD growth process and enables the creation of robust ALD recipes *in-situ*. Moreover, we predict that the model can also be potentially applicable to analyze the *in-situ* SE data, acquired during the deposition of other oxide materials. Complementary crystallographic, chemical, and morphological investigations were performed by using x-ray diffraction, x-ray photoelectron spectroscopy, and atomic force microscopy, respectively.

Atomic and Molecular Quantum Systems, Posters 30 - 37

Md Rashedul Hasan

POSTER #30

Android Malware Classification Addressing Repackaged Entities By The Evaluation Of Static Features And Multiple Machine Learning Algorithms

Expanded usage and prevalence of Android apps allows developers of malware to create new ways in various applications to unleash malware in various packaged types. This malware causes various leakage of information and a loss of revenue. In addition, the discovered software is repeatedly launched by unethical developers after classifying the program as malware. Unluckily, the program still remains undetected even after being repackaged. In this research the topic of repackaging was discussed, emphasizing the implementation based on source code using the Bag-of-Words algorithm and testing the findings through machine learning. The findings of the assessment demonstrate comparatively improved result in this aspect than the existing implantation based on source code by adapting the Bag-of-words strategy and implementing some supplementary dataset pre-processing. A vocabulary for identifying the malicious code has been developed in this study. Bag-of-words was used to classify malware trends using custom implementation. The findings were instantiated using various algorithms of machine learning. The concept was eventually implemented in a practical application, too. The suggested method sets out a new methodology for examining source code for Android malware to tackle repackaging of malware.

Corbyn D. Mellinger, David Loos, Benjamin DalFavero, Chance Persons, Joe Klomp, and Jonathan Wrubel

POSTER #31

Design and Commissioning of an Octupole Magnetic Trap for Sub-Doppler Cooling of ^{39}K

Potassium is a difficult atom to Bose-condense, with initial condensates coming about due to sympathetic cooling from other species, e.g. ^{87}Rb . The difficulty with achieving a high phase-space trap is largely due to the hyperfine atomic structure of potassium, with splitting between the $^2P_{3/2}$, $F=3$ and $F=2$ levels only 20 MHz (3.3 Γ) in ^{39}K and about 17 MHz (2.8 Γ) in ^{41}K , preventing the use of dark-spot magneto-optical traps (MOTs). Low density and high photon rescattering make loading a potassium optical dipole trap challenging. Sub-Doppler cooling techniques have been developed for potassium, but dipole trap loading remains inefficient.

To this end, we have developed and built a trapping field using an octupole magnetic field, which combines elements of both near-zero fields at the trap center for sub-Doppler cooling and restoring forces at the boundary to generate cold atoms for long enough times to load an optical dipole trap at high density. In this talk, we discuss the design and construction of our octupole symmetry trap from two sets of quadrupole symmetry anti-Helmholtz coils. This work allows for more consistent and rapid loading of an optical dipole trap for atoms with poorly resolved hyperfine structure such as potassium.

Neelam Shukla, Artem G. Volosniev, and Jeremy R. Armstrong

POSTER #32

Properties of an Asymmetric Impurity Implanted into Dipolar Media

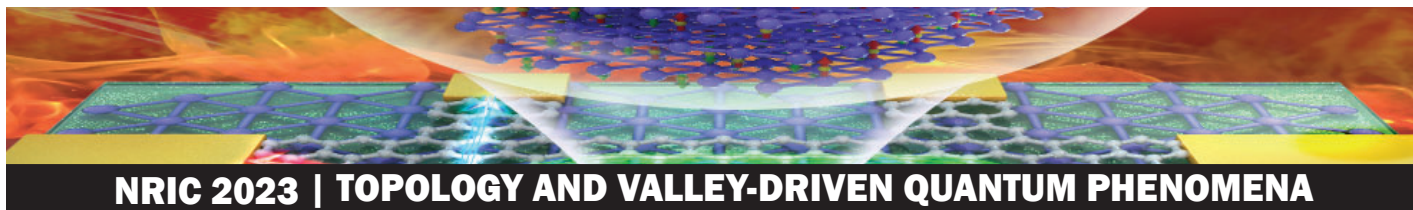
Relaxation dynamics in closed quantum systems are responsible for some of the most difficult issues in many-body physics. Understanding these dynamics is crucial for quantum statistical physics, but it is also an open question in many other disciplines, such as cosmology, quantum information, and high-energy physics. An ideal model to answer those problems is an impurity interacting with a quantum environment. The impurity has at least one different property from the medium, such as a distinct hyperfine state, mass, or dipole moment. The medium, in this case is a three dimensional (3D) dipolar Bose gas. The constituents of the dipolar medium have their dipole moments aligned along the z-axis by an external field. The dipole-impurity system could exhibit attractive and repulsive interactions depending on the direction, as the dipole-dipole interaction is anisotropic and long-range. For this purpose, we used the split-step Crank-Nicolson method to solve the modified Gross-Pitaevskii (GP) equation. The impurity is a repulsive Gaussian particle with different widths along the z-axis and the in xy-plane. We probe the effects on the system density in response to the implantation of the impurity. Without an impurity, the system is elongated along the z-axis with the maximum density predictably in the centre. The impurity causes the central density to fragment in different ways, depending on the symmetry of the impurity. The effect of the relative strength of the dipole-dipole interaction and the Gaussian repulsion is also examined. The GP equation incorporating temporal dynamics was then solved in three dimensions in order to examine the development and temporal response of the gas to the presence of the impurity.

Aleksander L. Wysocki, Karolina Janicka, and Kyungwha Park

POSTER #33

Optical control of nuclear spin states in a nonmagnetic Eu-based molecular qubit

Realization of a coherent spin-photon interface in spin-qubit materials is an exciting prospect with many potential applications in nanophotonics and quantum information science technologies. Molecular systems are promising spin-qubit materials thanks to their scalability and easily tunable properties. Achieving coherent spin-light interface in magnetic molecules is, however, challenging due to strong coupling of molecular electronic spins to the environment. Recently, super-narrow homogeneous optical linewidths have been experimentally obtained by considering nuclear spin states in a nonmagnetic Eu-based molecular crystal [Serrano et al., Nature 603, 241 (2022)] with evidence of their coherent optical control. Here, we investigate electronic ground-state and excited-state multiplets, nuclear spin spectra, and optical properties for the Eu-based magnetic molecule by employing first principles multireference quantum chemistry



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methods including spin-orbit coupling. The nuclear quadrupole coupling parameters are computed and an ab-initio effective nuclear spin Hamiltonian is constructed for ground and excited electronic states. Electric dipole transition probabilities between nuclear states that belong to different nondegenerate electronic multiplets are calculated and various mechanisms for optical control of nuclear spin states are discussed.

Yuanyuan Ni, Yifan Yuan, Jing Li, and Xiaoshan Xu

Effect of Capping Layer on Molecular Ferroelectric Thin Film

POSTER #34

Molecular crystal of 2-methylbenzimidazole (MBI) belongs to the family of organic ferroelectrics, which become increasingly important for capacitors, piezoelectrics, and memory devices because they are lightweight, flexible, and environment friendly. However, device fabrication using MBI films is challenging due to its high volatility in vacuum. We have grown MBI films using physical vapor deposition at low temperature followed by the single-layer and multi-layer capping using lithium fluoride (LiF). The effect of the capping layer on the evaporation of MBI films in high vacuum has been studied by measuring the change of remanent polarization of MBI in $1e-7$ Torr pressure at room temperature. The results show that one-micrometer-thick LiF layer effectively minimizes the loss of MBI films on the substrate for hours. The effect of multi-layer LiF is being investigated.

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Fabrication of Conducting Polymer Composites of Polyaniline with Spin Crossover Coordination Polymer [Fe(Htrz)₂(trz)](BF₄) with the Addition of Magnetite

POSTER #35

Composites of conducting polymer polyaniline (PANI) A and B were generated with spin crossover (SCO) polymer [Fe(Htrz)₂(trz)](BF₄) using a direct approach. PANI A was synthesized in the presence of hydrochloric acid and no attempt to dedope and redope the polymer were attempted, while PANI B was purchased and converted to the conducting emeraldine salt form using p-toluene sulfonic acid. Superconducting quantum interference device (SQUID) measurements confirmed that the thermal hysteresis narrowed in the presence of PANI, a result of reduced Fe-Fe interactions. Transport measurements demonstrated that the conductivity for composites in the low spin (LS) state were higher than in the high spin (HS) state. PANI A composites had a much higher conductivity likely due to the extent of doping being better controlled during the synthetic protocol than as a post-synthetic transformation. To improve the magnetometry results, magnetite (Fe₃O₄) was added to the [Fe(Htrz)₂(trz)](BF₄)/PANI A composite in 1% w/v, and the thermal hysteresis opened up to 53 K, likely due to Fe-Fe coupling. Also, despite the superparamagnetic behavior of Fe₃O₄, the SCO for [Fe(Htrz)₂(trz)](BF₄) was still apparent in the moment/g versus field measurements. The addition of Fe₃O₄ did not have an impact on the transport measurements.

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Synthesis and Characterization of Polypyrrole and Polypyrrole/[Fe(Htrz)₂(trz)](BF₄) Composites

POSTER #36

Polypyrrole (PPy) is an organic conducting polymer that has been used in the fabrication of various electronic devices, including memory devices, switches, and actuators. It possesses properties similar to polyaniline (PANI) and is thus a suitable substitute for certain device applications. In this project, we focused on the synthesis of PPy and its characterization using several analytical techniques. In brief, PPy was synthesized via oxidative polymerization with ammonium persulfate as the oxidizing agent and polyvinyl alcohol (PVA) as the surfactant. The effects of PVA on the size of the resultant PPy were apparent; the addition of a higher amount of PVA resulted in smaller PPy nanoparticles. Furthermore, PPy/[Fe(Htrz)₂(trz)](BF₄) composites were made by combining the two reagents in a 1:1 (w/w) ratio and subsequently analyzed with a vibrating-sample magnetometer. All PPy/[Fe(Htrz)₂(trz)](BF₄) composites showed a thermal hysteresis loop and with transition temperatures similar to standard [Fe(Htrz)₂(trz)](BF₄). SEM images of PPy and the corresponding composites were collected to determine their sizes and sample homogeneity. Transport measurements were also performed on both PPy and PPy/[Fe(Htrz)₂(trz)](BF₄) thin films to verify their suitability for electronic device applications. With further optimization, the current system could produce thin films with properties comparable to the well-characterized PANI/[Fe(Htrz)₂(trz)](BF₄) system.

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Raman Observations of Voltage-controlled Antiferromagnetic Switching in Boron-doped Cr₂O₃

POSTER #37

We report Raman signatures of voltage-controlled antiferromagnetic (AFM) switching in B doped chromia (B:Cr₂O₃). Comparison of Raman scattering between pristine and B:Cr₂O₃ showed that B doping led to phonon broadening and the emergence of a broad two-magnon excitation peak, further verified via polarized Raman spectroscopy. Non-volatile spectral changes were observed in B:Cr₂O₃ poled by an external E field. Upon voltage poling, B:Cr₂O₃ phonons sharpened, the two-magnon lineshape changed and redistributed toward low energies. A non-interacting magnon dispersion model produced a two-magnon density of state that qualitatively matches spectral observations. These spectral signatures reveal information on magnon-magnon and magnon-phonon interactions in voltage-switchable antiferromagnets. In addition, high density laser irradiation was found to locally anneal B:Cr₂O₃. This laser annealing produced phonon softening and broadening while the two-magnon excitations largely remained intact, providing a laser writing method for micro/nano device patterning applications.