

# EVENT PROGRAM

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



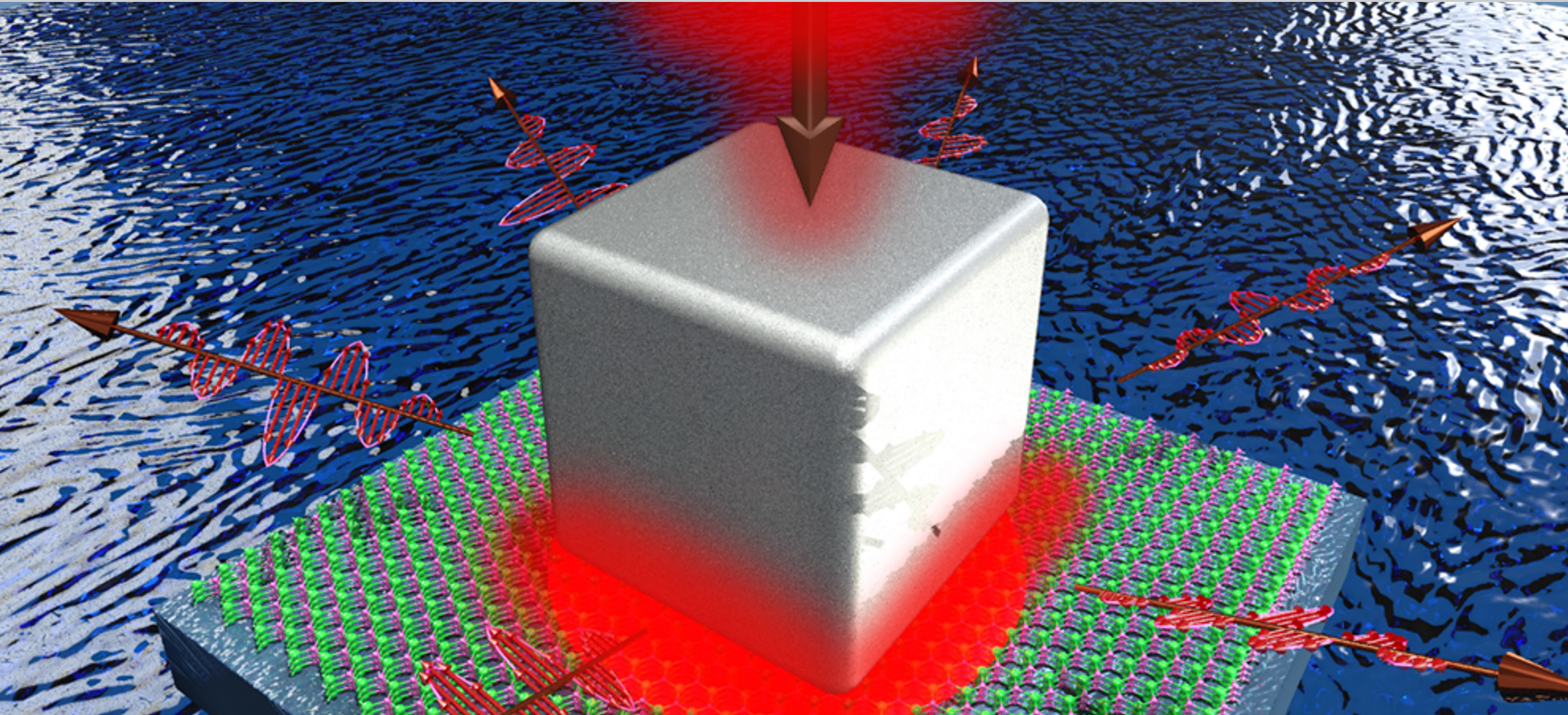
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2024 Nebraska Research & Innovation Conference

## DIAMOND QUANTUM SENSING: CHALLENGES & OPPORTUNITIES

MARCH 14 | LINCOLN, NEBRASKA





**SPECIAL THANKS  
to Nebraska EQUATE's  
External Review Panel  
for time and expertise  
in service to the National  
Science Foundation, ensuring  
the quality and fidelity of this  
project's progress with its  
approved goals.**

**Axel Hoffmann, Chair**

**Michael Flatté**

**Ilya Krivorotov**

**Allan Macdonald**

## Message from the Nebraska EPSCoR Director

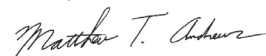
Welcome to the 2024 Nebraska Research & Innovation Conference (NRIC)! Thank you to our speakers for sharing their time and expertise with us, and thanks to EQUATE's partner organizations -- the University of Nebraska System, and the University of Nebraska-Lincoln Office of Research and Economic Development.

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 3, this symposium gathers a stellar slate of thought leaders, with topic coordination by FRG2 leader Abdelghani Laraoui.

Please enjoy NRIC's knowledge transfer and networking opportunities, including the morning and afternoon poster sessions, for further topics.

Best,



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

P.S. When posting to social media about this event, please use:  
#NebEQUATE and/or #NRIC24.

## Notes:

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### EQUATE Leaders

Scientific Director -- Christian Binek, Ph.D. (UNL)  
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](http://equate.unl.edu)

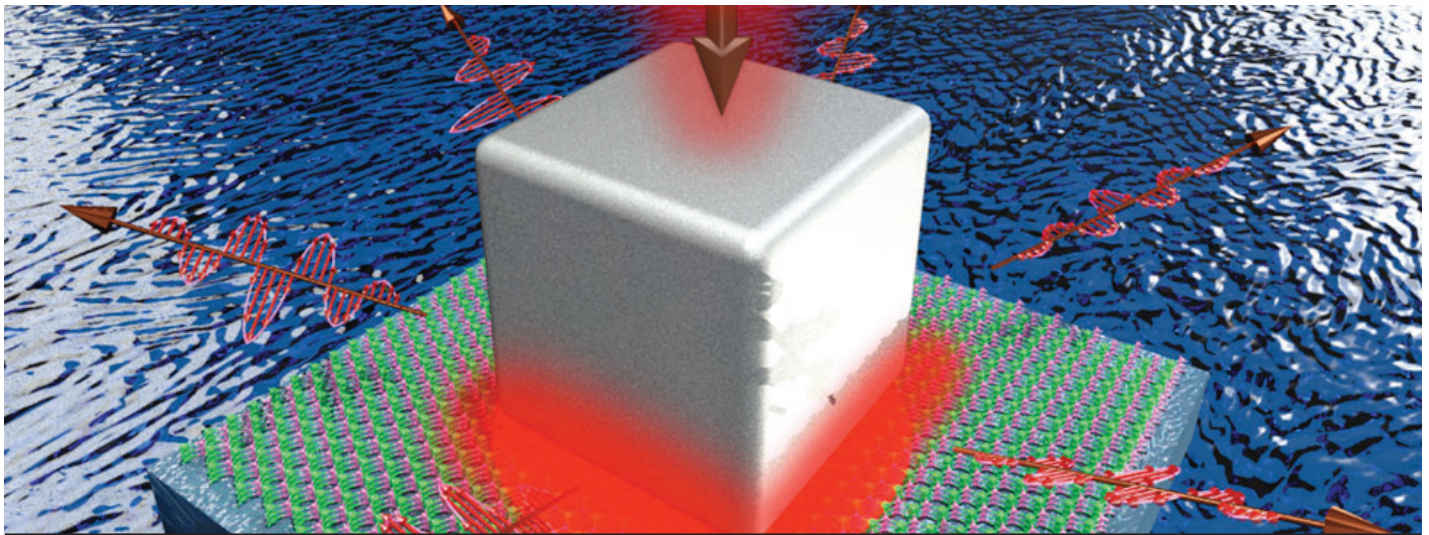
### Nebraska EPSCoR Staff

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

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### COVER ART: IMAGE ACKNOWLEDGEMENT

*Research from a collaboration by Nebraska engineers and scientists--Mohammadjavad Dowran, Andrew Butler, Suvechhya Lamichhane, Adam Erickson, Ufuk Kilic, Sy-Hwang Liou, Christos Argyropoulos, and Abdelghani Laraoui--depicts Plasmon Enhanced Quantum Properties of Single Photon Emitters with Hybrid Hexagonal Boron Nitride Silver Nanocube Systems and was produced with funding via Nebraska's NSF-funded EQUATE project, OIA-2044049. The image appeared on the back cover of Advanced Optical Materials, Volume11, Issue16, from August 21, 2023.*  
<https://doi.org/10.1002/adom.202370062>



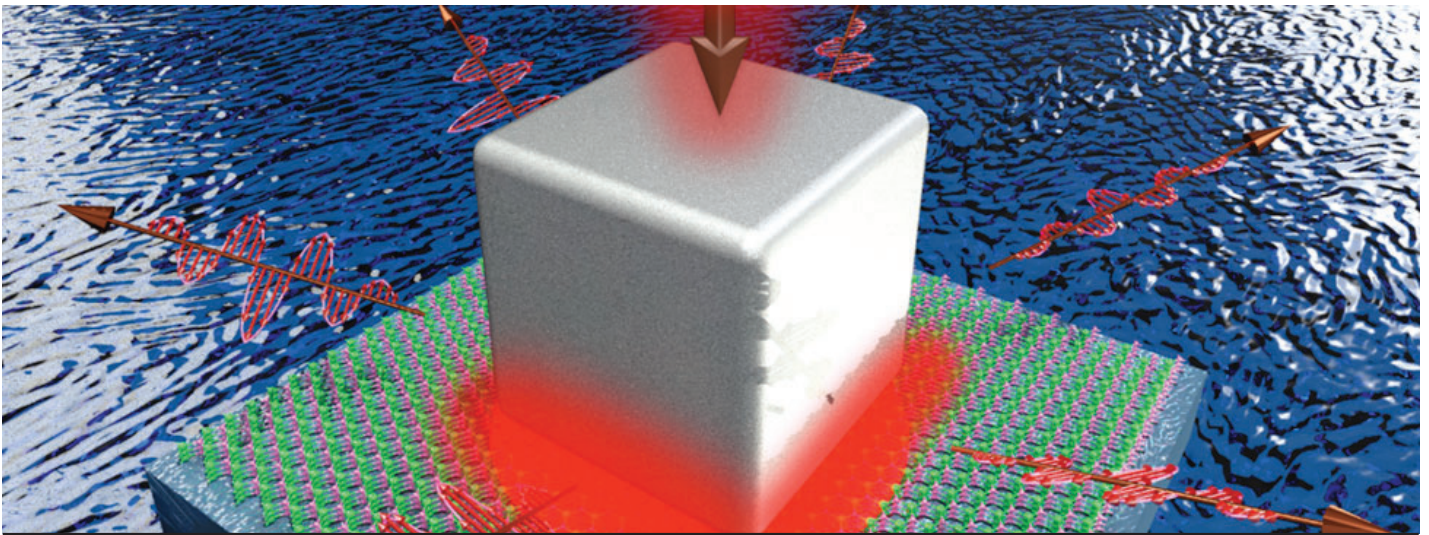
## **NRIC 2024 | DIAMOND QUANTUM SENSING: CHALLENGES & OPPORTUNITIES**

### **AGENDA — THURSDAY, MARCH 14** **WiFi Network: HiltonHonorsMeeting, Password: Embassy2**

- 7:30 - 8:00 AM Conference Check-In: Materials Pick-Up, Poster Setup & Continental Breakfast
- 8:00 - 8:15 Event Welcome and Introductions – Regents A ballroom  
Matthew T. Andrews, Ph.D. - Nebraska EPSCoR Director and Abdelghani Laraoui, Ph.D. - EQUATE FRG2 Leader
- 8:15 - 9:45 **SESSION I** -- Host: Abdelghani Laraoui, Ph.D.  
8:15 - 9:00 a.m. -- Nathalie de Leon, Princeton University  
Nanoscale covariance magnetometry with diamond quantum sensors  
9:00 - 9:45 a.m. -- Chunhui (Rita) Du, Georgia Institute of Technology  
Quantum Sensing of Two-Dimensional Magnetism
- 9:45 - 11:15 **MORNING POSTER SESSION & REFRESHMENTS**, Regents B ballroom – *ODD-numbered poster presentations*
- 11:15 - 12:00 **SESSION 2**---Host: Sy-Hwang Liou, Ph.D.  
11:15 a.m. - Noon -- Michael Flatté, University of Iowa  
Charge and spin noise for spin-1 qubits in diamond and silicon carbide
- 12:00 - 1:00 PM **LUNCH** – Hotel Atrium
- 1:00 - 1:45 **SESSION 3**---Host: Rebecca Lai, Ph.D.  
1:00 - 1:45 p.m. -- Peter Maurer, University of Chicago  
Interfacing Biomolecules with Coherent Quantum Sensors
- 1:45 - 3:15 **AFTERNOON POSTER SESSION & REFRESHMENTS**, Regents B ballroom – *EVEN-numbered poster presentations*
- 3:15 - 4:45 **SESSION 4**---Host: Abdelghani Laraoui, Ph.D.  
3:15 - 4:00 p.m. -- Carlos Meriles, City College of New York  
Characterization and control of sub-diffraction color centers clusters in diamond  
4:00 - 4:45 p.m. -- Shimon Kolkowitz, University of California Berkeley  
Studying and multiplexing nitrogen-vacancy centers in diamond
- 4:45 PM **CONFERENCE ENDS - THANK YOU FOR COMING!**

On X (formerly Twitter), follow @NebraskaEPSCoR and use #NRIC24 and #NebEQUATE in your tweets related to this event.





## NRIC 2024 | DIAMOND QUANTUM SENSING: CHALLENGES & OPPORTUNITIES

8:00 - 8:15 A.M.

### EVENT WELCOME & INTRODUCTIONS

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

### SESSION 1 -- Host: Abdelghani Laraoui, Ph.D.

8:15 - 9:00 A.M.

#### Nanoscale covariance magnetometry with diamond quantum sensors

NATHALIE DE LEON, PRINCETON UNIVERSITY

Correlated phenomena play a central role in condensed matter physics, but in many cases there are no tools available that allow for measurements of correlations at the relevant length scales (nanometers - microns). We have recently demonstrated that nitrogen vacancy (NV) centers in diamond can be used as point sensors for measuring two-point magnetic field correlators [1]. NV centers are atom-scale defects that can be used to sense magnetic fields with high sensitivity and spatial resolution. Typically, the magnetic field is measured by averaging sequential measurements of single NV centers, or by spatial averaging over ensembles of many NV centers, which provides mean values that contain no nonlocal information about the relationship between two points separated in space or time. We recently proposed and implemented a sensing modality whereby two or more NV centers are measured simultaneously, from which we extract temporal and spatial correlations in their signals that would otherwise be inaccessible. We demonstrate measurements of correlated applied noise using spin-to-charge readout of two NV centers and implement a spectral reconstruction protocol for disentangling local and nonlocal noise sources. This novel quantum sensing platform will allow us to measure new physical quantities that are otherwise inaccessible with current tools, particularly in condensed matter systems where two-point correlators can be used to characterize charge transport, magnetism, and non-equilibrium dynamics.

[1] "Nanoscale covariance magnetometry with diamond quantum sensors," J. Rovny, Z. Yuan, M. Fitzpatrick, A. I. Abdalla, L. Futamura, C. Fox, M. C. Cambria, S. Kolkowitz, N. P. de Leon, Science 378, 6626 1301-1305 (2022).

9:00 - 9:45 A.M.

#### Quantum Sensing of Two-Dimensional Magnetism

CHUNHUI (RITA) DU, GEORGIA INSTITUTE OF TECHNOLOGY

Two-dimensional (2D) van der Waals crystals with unconventional magnetic and electrical properties have been a rising topic of modern magnetism and spintronics research over the past years. Currently, there is ongoing intense activity to develop and understand this new family of magnetic materials, as well as to create new ones. The success of these efforts relies simultaneously on advances in theory, material synthesis, and development of new, sensitive metrology tools capable of evaluating the key material properties at the unprecedented length scale. Nitrogen-vacancy (NV) centers, optically active atomic spin defects in diamond, are naturally relevant in this context due to their excellent quantum coherence, highly competitive spatial and field sensitivity, and remarkable functionalities over a broad range of experimental conditions. In this talk, I will present our recent work on using NV centers to perform nanoscale quantum sensing and imaging of 2D magnetic quantum matter. Specifically, we have utilized NV centers to visualize the exotic spin properties of layered magnetic materials [1, 2] and moiré magnetism hosted by twisted van der Waals magnets [3], revealing the rich physics underlying exotic spin transport and dynamic behaviors in reduced dimensionality. Lastly, I will also briefly discuss our ongoing efforts on exploring next-generation van der Waals quantum sensing technologies using color centers beyond NVs [4].

References:

- [1] N. J. McLaughlin et al., Nano Lett. 22, 5810 (2022).
- [2] M. Huang et al., Nano Lett. 23, 8099 (2023).
- [3] M. Huang et al., Nat. Commun. 14, 5259 (2023).
- [4] M. Huang et al., Nat. Commun. 13, 5369 (2022), heterostructure which can be tuned by two orders of magnitude via the gate voltage.

9:45 - 11:15 A.M.

## MORNING POSTER SESSION & REFRESHMENTS

REGENTS BALLROOM B

### SESSION 2 -- Host: Sy-Hwang Liou, Ph.D.

11:15 A.M. - NOON

#### Charge and spin noise for spin-1 qubits in diamond and silicon carbide

MICHAEL FLATTÉ, UNIVERSITY OF IOWA

I will describe some general theoretical features of charge and spin noise on coherent spin-1 centers embedded in wide bandgap hosts (e.g. diamond and silicon carbide), including effects on optical linewidths[1] and spin coherence times[2,3]. We see that the spin coherence times of sensing qubits may be able to quantitatively identify the diffusive motion of nearby charge carriers through an analysis of the spatio-temporal correlations of the noise[2]. We find unusual effects of electric/charge noise, often producing effects that in simpler models are assigned to magnetic noise alone[3]. Similar simulations permit us to identify the effect of coating diamond nanoparticles, which lengthen the coherence times of NV- spin centers to near bulk values[4]. In media that provide highly coherent magnetic excitations (magnons) these magnons may be of use for qubit entangling gates[5]; recent measurements have identified the back-action of these excitations on the coherence times of a single qubit[6]. Work supported by DOE BES.

[1] PRXQ 2, 040310 (2021)

[2] arXiv:2112.15581

[3] arXiv:2303.13370

[4] arXiv:2305.03075

[5] PRXQ 2, 040314 (2021)

[6] PNAS 121, e2313754120 (2024).

12:00 - 1:00 P.M.

## LUNCH

EMBASSY SUITES HOTEL, ATRIUM

### SESSION 3 -- Host: Rebecca Lai, Ph.D.

1:00 - 1:45 P.M.

#### Interfacing Biomolecules with Coherent Quantum Sensors

PETER MAURER, UNIVERSITY OF CHICAGO

Quantum metrology enables some of the world's most sensitive measurements. When applied to biophysical systems, diamond-based quantum sensors have the potential to probe processes that cannot be accessed by conventional technologies. Examples of such processes range from cancer research to neuroscience to developmental biology. However, interfacing coherent qubit sensors with fragile biological target systems has remained an outstanding challenge that has severely limited applications. In this talk, I will discuss a novel approach that combines single-molecule biophysics technology with quantum engineering to interface intact biomolecules on a diamond quantum sensor without impacting qubit coherence and bio-functionality. In a second part, I will discuss our recent work on engineering highly coherent quantum sensors based on diamond nanocrystal. Such nanosensors can readily be taken up by cells and integrated into intact organisms. However, coherence in these nanocrystal sensors is limited by surface noise, which severely reduces the sensor's sensitivity. In our work we developed a new approach to engineer spin coherence in core-shell nanostructures which leads to a 50-fold improvement in qubit sensitivity. Finally, potential future applications of quantum sensing to biophysics and diagnostics will be discussed.

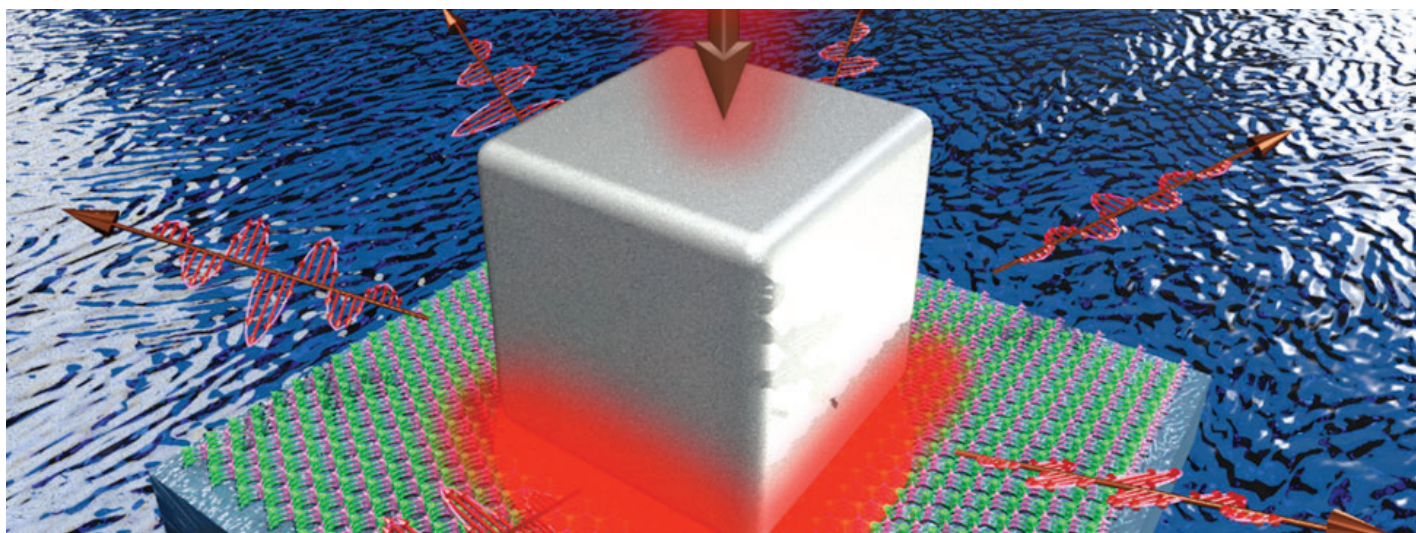
1:45 - 3:15 P.M.

## AFTERNOON POSTER SESSION & REFRESHMENTS

REGENTS BALLROOM B

CONTINUES, NEXT PAGE





## NRIC 2024 | DIAMOND QUANTUM SENSING: CHALLENGES & OPPORTUNITIES

**SESSION 4 -- Host: Abdelghani Laraoui, Ph.D.**

**3:15 - 4:00 P.M.**

### **Characterization and control of sub-diffraction color centers clusters in diamond**

**CARLOS MERILES  
CITY COLLEGE OF NEW YORK**

Under cryogenic conditions, color centers in wide-bandgap semiconductors feature a collection of “atomic-like” absorption resonances that can be exploited to examine and control their charge states in novel ways. In the first part of this talk, I will discuss how the local heterogeneity of these resonances can be leveraged to individually manipulate and readout the charge state of nitrogen-vacancy (NV) centers in diamond sharing the same diffraction-limited volume. I will also examine how to capitalize on the spectral diffusion of individual NVs in sub-diffraction clusters to establish statistical correlations between the temporal frequency shifts in each of the spectra, and ultimately map out proximal trapped charge in three dimensions. All in all, these results open intriguing opportunities for information processing in the form of devices with enhanced optical storage capacity and for the manipulation of nanoscale spin-qubit clusters connected via electric and/or magnetic couplings.

**4:00 - 4:45 P.M.**

### **Studying and multiplexing nitrogen-vacancy centers in diamond**

**SHIMON KOLKOWITZ  
UNIVERSITY OF CALIFORNIA BERKELEY**

The nitrogen-vacancy (NV) center in diamond has been widely adopted as a quantum sensor, and is now even used in undergraduate instructional labs as a model quantum system. However, despite its ubiquity and popularity, basic properties of the NV center remain poorly understood. In addition, most work has been restricted to measurements of one NV center at a time, or to globally averaged measurements of ensembles of many of NV centers. In this talk I will first present a recent experimental and theoretical study of temperature and spin-state-dependent spin-phonon relaxation rates in the electronic ground state spin-triplet of NV centers in diamond, and will discuss how these new insights could lead to magnetometers with enhanced sensitivity. I will also explain how these results led us to a simple, analytical, physically motivated expression for the temperature dependence of the zero-field splitting of the NV center electronic ground state, with applications to nanoscale thermometry. I will then briefly present our experimental demonstration of spatiotemporal magnetic field correlation measurements with pairs of NV centers, including the ability to distinguish between global and local noise sources, and the capability to measure signals of interest using free precession times beyond the apparent single NV coherence time in certain regimes. Finally, I will present on a new experimental platform we have developed for simultaneously manipulating and independently measuring many single NV centers in parallel.

# POSTERS

## ELECTRONIC AND MAGNETIC QUANTUM MATERIALS, POSTERS 1-20

Syed Qamar Abbas Shah, Ather Mahmood, Arun Parthasarathy, Christian Binek

### Search for magnetoelectric monopole response in Cr2O3 powder

POSTER #1

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 nonvanishing 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 field product. In accordance with our refined theory, a strong dependence of the functional form of  $\alpha$  vs T of Chromia powders on the ME field cooling protocol is observed. It shows that Chromia powder is not generically an isotropic ME effective medium but provides a pathway to realize the elusive isotropic ME response.

Syed Qamar Abbas Shah, Ather Mahmood, Jamie Weaver, Will Echtenkamp Jeffrey W. Lynn, Peter A. Dowben, Christian Binek

### Post annealing x-ray photoemission spectroscopy depth profiling investigating B-concentration in B:Cr2O3 thin films

POSTER #2

Chromium Oxide (Cr2O3) is a magnetoelectric antiferromagnetic material with a Néel temperature i.e.,  $T_N \sim 307$  K. Doping Cr2O3 with Boron (B) increases the antiferromagnetic transition temperature (TN). The enhancement of TN from B-doping facilitates the operation of B:Cr2O3 based devices in CMOS environments. In addition, B-doping turns Cr2O3 into a multifunctional single-phase material which enables the 90° Néel vector rotation in the absence of applied magnetic field. In context of antiferromagnetic spintronics, this peculiar nonvolatile voltage driven Néel vector rotation makes B:Cr2O3 an extremely good candidate for ultra-low power, ultra-fast, nonvolatile memory and logic device applications. In our work we prepare 200 nm thick B:Cr2O3 films grown epitaxially on Al2O3 (0001) substrates by using pulsed laser deposition. We utilize x-ray photoemission spectroscopy depth profiling to independently confirm data from cold neutron depth profiling which reveal thermally activated B-accumulation at the B:Cr2O3/ vacuum interface within a layer of about 50 nm thickness. We attributed the stable B-enrichment to surface segregation. Financial support by NSF/EPSCoR RII Track-1: Emergent Quantum Materials and Technologies, OIA-2044049 is acknowledged. The research was performed in part in the NNF: NNCI and the NCMN, supported by NSF under ECCS:2025208, and the NRI. Contributions of the National Institute of Standards and Technology are not subject to copyright.

Jaeil Bai, Renat Sabirianov, Wai-Ning Mei, Ahamad Alsaad

### Bound states in single and double Y-junction quantum dot

POSTER #3

We present the solution of quantum-mechanical problem of a particle in Y-junction quantum dot. The single bound state with Dirichlet Laplacian is described. The bound state presence is examined for the case of junction being asymmetric, i.e. going from C3V to C2v group when the width of one of the ligament is increased. We further investigated the solution of two connected Y-junction with two bound states. These finding could be useful for building 2D two-level systems for quantum qubits or quantum waveguide applications.

Hamed Vakili, Moaz Ali, Alexey A. Kovalev

### Field Free Anomalous Josephson effects in chiral superconductors

POSTER #4

We study the anomalous Josephson effects in superconductor/semiconductor heterostructure based on cuprate superconductors, which can operate at higher temperatures. The twisted cuprate superconductors are expected to have  $d+id'$  and  $d+is$  superconducting pairings depending on the chemical potential and temperature. By breaking appropriate symmetries, anomalous Josephson effects appear in the junction. We show that by rotating the planes and breaking the rotational symmetries, a large, field and SOC free Josephson diode effect can be realized. The  $d+id'$  superconductors host chiral edge states unlike  $d+is$ , which have unique properties. We show that by using a Josephson junction with modified geometry, and looking at the diode effect we can distinguish between these two superconducting pairings.

Bharat Giri, Xiaoshan Xu

### Observation of giant topological Hall effect in Pt/NiCo2O4 heterostructure over wide temperature range

POSTER #5

The spin configuration of materials significantly influences their transport characteristics. To investigate the potential emergence of novel spin structure in heterostructure of strongly spinorbit coupled metal Platinum (Pt) deposited on ferrimagnetic NiCo2O4 (NCO)/MgAl2O4 (001) films with perpendicular magnetic anisotropy (PMA)[1], we studied the spin transport properties at various temperature with different NCO thickness (8-30nm). In addition to the anomalous Hall effect expected from NCO, we observed topological Hall effects (THE) before the coercive field (HC). The magnitude of THE increases with increasing T and vanishes near transition temperature of NCO. These results indicate that interfacial Dzyaloshinskii Moriya interactions (iDMI) of NCO/Pt comes to play, and strong spin orbit coupling enhances the iDMI[2] and becomes influential to compete with exchange interaction to form skyrmions. Based on the measured THE, the maximum estimated skyrmion density is  $103 \mu\text{m}^{-2}$  at 270K for 16 nm thick NCO sample. Acknowledgment: This research was primarily supported by US DOE (DE-SC0019173). [1] C. Mellinger, J. Waybright, X. Zhang, C. Schmidt, and X. Xu, "Perpendicular magnetic anisotropy in conducting NiCo2O4 films from spin-lattice coupling," Phys. Rev. B, vol. 101 no. 2 [A. Fert, V. Cros, and J. Sampaio, "Skyrmions on the track," Nat. Nanotechnol., vol. 8, no. 3, pp. 152-156, 2013]

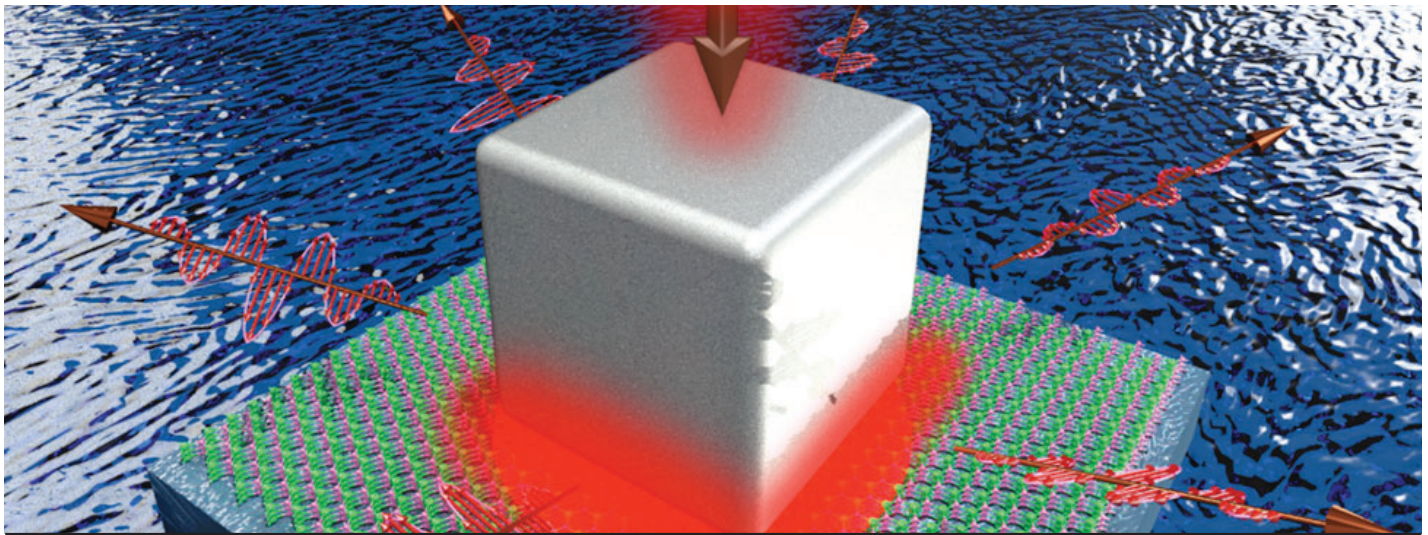
Arjun Subedi, Detian Yang, Xiaoshan Xu, Peter Dowben

### Reversible electronic phase transition and Debye temperature of NiFe2O4 thin film surface

POSTER #6

In X-ray photoelectron spectroscopy (XPS) of NiFe2O4 thin film, the Ni and Fe 2p3/2 core level binding energies show strong indications that reversible transition between a more dielectric and a more metallic phases of NiFe2O4 film is possible. The XPS of Ni and Fe 2p3/2 core levels for the NiFe2O4 thin film at room temperature showed large photovoltaic surface charging leading to core level binding energy shifts, characteristic of a highly dielectric (or insulating) surface of NiFe2O4 thin film at room temperature. This photovoltaic charging, seen in the XPS binding energies of the Ni and Fe 2p3/2 core levels, decreased with increasing temperature, indicating that the NiFe2O4 thin film became more metallic at elevated temperatures. The photovoltaic surface charging was absent at 520 K indicating metallic nature of the film. When the thin film was cooled down to room temperature, the core level binding energy shifts, due to photovoltaic surface charging, were observed again. This indicates that there exists reversible non-metal to metal phase transition of the NiFe2O4 thin film with temperature. This work illustrates a route to regulate the surface metal-to-insulator transition in NiFe2O4 thin film. Furthermore, effective surface Debye temperature has been estimated for the NiFe2O4 thin film.





**NRIC 2024 | DIAMOND QUANTUM SENSING: CHALLENGES & OPPORTUNITIES**

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 #7**

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  $\text{Sm}_{0.5}\text{Nd}_{0.5}\text{NiO}_3$  (SNNO),  $\text{NdNiO}_3$  (NNO), and  $\text{LaNiO}_3$  (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.

Yifei Hao, Xuegang Chen, Le Zhang, Myung-Geun Han, Wei Wang, Yue-Wen Fang, Hanghui Chen, Yimei Zhu, Xia Hong

**POSTER #8**

**Record high room temperature resistance switching in ferroelectric-gated Mott transistors unlocked by interfacial charge engineering**

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  $\text{Sm}_{0.5}\text{Nd}_{0.5}\text{NiO}_3$  (SNNO),  $\text{NdNiO}_3$  (NNO), and  $\text{LaNiO}_3$  (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.

Edward Schwartz, Alexey Kovalev

**Elliptical Skyrmion Dynamics**

**POSTER #9**

Magnetic skyrmions are chiral spin textures which are often stabilized by the inter-facial Dzyaloshinskii-Moriya interaction in heavy metal / ferromagnet multilayers. Such systems have approximate rotational symmetry, leading to rotationally invariant, circular skyrmions. Symmetry breaking due to applied fields, or due to the crystallographic structure of the material, may lead to skyrmions with a distorted shape. This distortion can modify the dynamics of skyrmions, in ways which may impact skyrmion based devices and measurements. Here we present an analytical approach to modelling the distortion of skyrmions and antiskyrmions into elliptical shapes. We then apply these results to investigate some of the consequences of distortion on skyrmion dynamics.

Gauthami Viswan, Alexey Lipatov, Alexander Sinitskii, Jose Avila, Takashi Komesu, Maria C. Asensio, Archit Dhingra, Peter A. Dowben

**The electronic band structure and conduction band formation of HfSe3**

**POSTER #10**

The anisotropic structure of Group 4 transition metal trichalcogenides (TMTCs) have gained significant interest due to various optoelectronic applications. In this work, the band structure of quasi one-dimensional  $\text{HfSe}_3$  is investigated with nano-spot angle resolved photoemission spectroscopy (nanoARPES). The effective hole mass extracted from the band structure was compared with that of  $\text{TiS}_3$  and  $\text{ZrS}_3$  from prior studies. X-ray absorption spectroscopy (XAS) has been used to characterize the unoccupied states of  $\text{HfSe}_3$  and will be compared to the XAS spectra of  $\text{HfS}_3$  and  $\text{TiS}_3$  and  $\text{ZrS}_3$ . The metal chalcogenide hybridization for Hf differs from the Ti and Zr trichalcogenides. This may be due to the increase in effective atomic number leading to strong spin-orbit interaction of Hf based TMTCs.

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

**POSTER #11**

**Néel temperature tuning in Magnetolectric B-doped Cr2O3 films**

Multi-functional thin films of boron (B) doped  $\text{Cr}_2\text{O}_3$  exhibit voltage-controlled and nonvolatile Néel vector  $\pi/2$  rotation in the absence of a magnetic field. Isothermal toggling of antiferromagnetic states is demonstrated in prototype device structures at CMOS compatible temperatures between 300 K and 400K. Néel vector rotation is detected with the help of heavy metal (Pt) Hall-bars in proximity of pulsed laser deposited B:Cr2O3 films. Cold neutron depth profiling (cNDP), performed at National Institute of Standards and Technology, reveals thermally activated B-accumulation at the B:Cr2O3/ vacuum interface in thin films deposited on  $\text{Al}_2\text{O}_3$



substrates. This work uses cNDP, X-ray Photoemission spectroscopy (XPS) and Spin Hall measurements [1] to demonstrate a shift in TN towards higher values of  $\approx 477$  K, associated with the increase in B-concentration within an interfacial layer of about 50 nm. The research was performed in part in the NNF: NNCI and the NCMN, supported by NSF under ECCS:2025208, and the NRI. Contributions of the National Institute of Standards and Technology are not subject to copyright. [1] A. Mahmood et al., Adv. Physics. Res., 2023, 2300061

Takashi Komesu, Amit Jadaun, Yudai Miyai, Shiv Kumar, Kenya Shimada, Christian Binek, Peter A. Dowben

### **The spin polarization of Palladium on Magneto-Electric Cr2O3**

**POSTER #12**

The spin polarized electronic band structure is essential to the implementation of spintronic materials; surface-interface is a key to the device. The tool of spin polarized inverse photoemission spectroscopy (SPIPES) combined with spin polarized photoemission is the most complete approach for developing a full understanding of magnetic materials in electronic structure point of view. Furthermore, SPIPES is hugely surface sensitive, which is an advantage of characterizing the boundary polarization. We have developed angle-resolved SPIPES [1,2], the time reversed process to SPES, specifically to characterize the unoccupied state band structure. Here, we present several results of SPIPES and the value of complementing PES, Angled Resolved PES, leading to the next step to Spin Polarized PES, including the latest on-going Pd covered Cr2O3 investigation. The Pd/ Cr2O3 results show evidence of magnetic behavior in Pd suggesting that Pd on Cr2O3 is more than just a paramagnetic with an induced polarization arising from the chromia boundary polarization. This be leading the voltage-controlled spintronic memory devices.

Yuanyuan Zhang, Kun Wang, Yifei Hao, Le Zhang and Xia Hong

**POSTER #13**

### **Large Tunneling Electroresistance in Epitaxial Ferroelectric Tunnel Junctions Enabled by a Narrow Gap Mott Insulator Electrode**

Ferroelectric tunnel junctions (FTJs) based on epitaxial complex oxide are promising building blocks for developing low power nanoelectronics. However, previous studies exploiting a singlelayer ferroelectric barrier only yield moderate tunneling electroresistance (TER) at room temperature. Here, we report large TER at 300 K by exploiting a narrow-gap spin-orbital Mott insulator as the bottom electrode. We work with epitaxial ferroelectric tunnel junctions composed of 2.8-4 nm PbZr<sub>0.2</sub>Ti<sub>0.8</sub>O<sub>3</sub> tunnel barriers, and correlated oxides LaNiO<sub>3</sub> and Mott insulator Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub> as electrodes. A large, nonvolatile TER of 6,600% has been observed at 300 K, and this value escalates to over 105 % at 100 K. The significant temperature dependence of TER indicates the presence of defect-mediated conduction in our junction. The on-state temperature dependence of conductance is within the interpretation of a direct tunneling model, while the offstate temperature dependence of conductance is fitted with the Glazman-Matveev inelastic tunneling model. Our study provides important material parameters for developing all-oxide FTJs with large TER.

Monirul Shaikh, Aleksander L. Wysocki

### **First principles studies of Fe adatoms on two-dimensional ferroelectric In2Se3 layer**

**POSTER #14**

Magnetic adatoms on surfaces may exhibit long-lived spin quantum states and function as single atom magnets with significant remanent magnetization and coercivity at low temperatures [1]. Such systems can have potential applications in high-density magnetic memory and quantum information science technologies if adatom magnetization can be reliably controlled and detected. Here, we use density functional theory, ab initio multireference quantum chemistry methods, and effective spin Hamiltonian technique to study magnetic properties of various adatom surface combinations including rare-earth ions on graphene and Fe adatom on two-dimensional ferroelectric  $\alpha$ -In<sub>2</sub>Se<sub>3</sub>. Preferred adsorption sites are identified and the adatom hopping energy barriers are computed. Electronic structure and magnetic anisotropy are calculated, and the stability of low-lying spin states is investigated. The effects of electric field and gate voltage are further studied and electrical control of the adatom spin states is demonstrated. [1] F. Donati, S. Rusponi, S. Stepanow, et al. Science 352, 318 (2016). This work is supported by the NSF EPSCoR Cooperative Agreement OIA-2044049, Nebraska's EQUATE collaboration.

Qiuchen Wu, Kun Wang, Xuegang Chen, Yifei Hao, Tianlin Li, Xia Hong

### **Topological Hall Effect in Free-standing NiCo2O4 Membranes**

**POSTER #15**

We report the observation of topological Hall effect (THE) in 30 nm suspended NiCo<sub>2</sub>O<sub>4</sub> (NCO) membranes. Free-standing NCO (001) membranes are achieved via epitaxial growth on Sr<sub>3</sub>Al<sub>2</sub>O<sub>6</sub> (SAO) buffered (001) LaAlO<sub>3</sub> (LAO) substrates via off-axis RF magnetron sputtering followed by water etching. X-ray diffraction measurements confirm the single crystalline phase of the membranes. The NCO membranes are then transferred on SiO<sub>2</sub>/Si substrate and patterned into Hall bar devices. We have studied the magnetoresistance (MR) and Hall effect in both NCO/SAO/LAO films and NCO membranes. The samples exhibit insulating temperature dependence, and the Curie temperature TC are above 300 K. Below TC, we observe anomalous Hall effect (AHE), which shows a nonmonotonic temperature dependence and reverses sign at about 240 K. For NCO membranes, topological Hall effect (THE) signal emerges below 10 K upon magnetic field cooling, a phenomenon that is absent in epitaxial NCO thin films. The THE signal changes sign when the magnetic field is reversed. The MR, AHE, and THE in suspended NCO membranes point to the intricate roles of strain and disorder in determining the magnetic properties of NCO. This work was supported by NSF (OIA-2044049) and Nebraska Center for Energy Sciences Research.

Mohamed Elekhtiar, Gautam Gurung, Ding-Fu Shao, Evgeny Y Tsymlal

**POSTER #16**

### **Emergence of 100% Spin Polarization in Non-Collinear Magnets**

Recently, large tunneling magnetoresistance (TMR) effects have been predicted and demonstrated in antiferromagnetic tunnel junctions (AFMTJs) with non-collinear antiferromagnetic (AFM) electrodes, that is promising for future information technology applications. These results indicated a very large transport spin polarization provided by AFM metals, which is unexpected due to the non-collinearity of their magnetic moments. In this work, we elucidate the origin of this giant spin polarization using simple tight-binding models and calculations based on density functional theory (DFT). Using tight-binding Hamiltonians to describe an infinite 1D chain of non-collinear magnetic moments and a 2D Kagomi lattice in a non-collinear AFM phase, we show that fully spin-polarized conduction channels appear in these systems and reveal their origin. Using DFT calculations, we further demonstrate the presence of 100% spin-polarized states in noncollinear AFM antiperovskites XNMn<sub>3</sub> (X = Ga, Sn, ...) leading to giant TMR values in AFMTJs based on XNMn<sub>3</sub> electrodes. Our results demonstrate great potential of non-collinear AFM metals for spintronics, boost accurate designs for next-generation sensors, and for other optoelectronic and photonic devices.

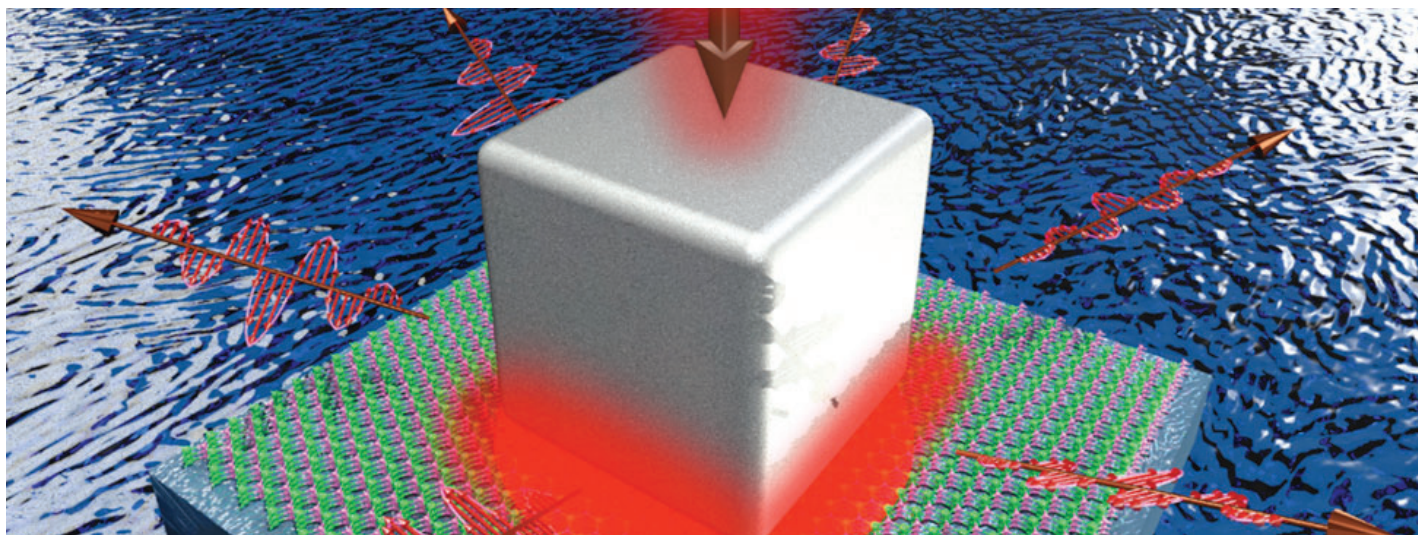
Tianlin Li, Hanying Chen, Kun Wang, Yifei Hao, Le Zhang, Kenji Watanabe, Takashi Taniguchi, and Xia Hong

**POSTER #17**

### **Transport Anisotropy in One-dimensional Graphene Superlattice in the High Kronig-Penney Potential Limit**

In this work, we investigate the transport signature of one-dimensional (1D) superlattice (SL) in monolayer graphene induced by prepatterned periodic domains in a ferroelectric bottom gate. We work with 50 nm single crystalline ferroelectric Pb(Zr,Ti)O<sub>3</sub> (PZT) films deposited on (La,Sr)MnO<sub>3</sub> buffered SrTiO<sub>3</sub> substrates, and create periodic polarization up (Pup) and down (Pdown) stripe-domains on PZT using conductive atomic force microscopy. The domain periodicity varies from 200 nm to 300 nm, and the number of periods changes from 30 to 50. We then transfer h-BN-graphene stacks onto the pre-patterned domains and fabricate them into top-gated field-effect devices. The difference in carrier density between the two polarization regions reaches around  $3 \times 10^{13}$  cm<sup>-2</sup> at 2 K due to the pyroelectric effect. Applying voltage to the h-BN top gate reveals extra Dirac points in R(Vg), which is attributed to the modified band structure via the SL. We discuss the effects of the SL period and the width ratio between the Pup and Pdown domains on the position of the extra Dirac points, and the magnetotransport properties of the 1D SLs.





## NRIC 2024 | DIAMOND QUANTUM SENSING: CHALLENGES & OPPORTUNITIES

Shuo Sun, Ather Mahmood, Bo Zhang, Syed Qamar Abbas Shah, Christian Binek, Yinsheng Guo

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

POSTER #18

We report the Raman signatures emerging from B doped Cr2O3 poled by an external electric field. Comparison between Raman scattering of pristine and B: Cr2O3 show phonon broadening and a broad two-magnon scattering peak, which is further verified via polarized Raman analysis, in the antiferromagnetic (AFM) phase at room temperature. Poled by an external E field, phonon mode of B:Cr2O3 qualitatively change, as well as the two-magnon mode line-shape changes with redistributed intensities. Inspired with pervious report, a non-interacting two-magnon density of states was first stimulated, and the experimental results were qualitative matched with a partial non-interacting DOS stimulation. These spectral signatures reveal information on magnon-magnon and magnon-phonon interactions in voltage-switchable antiferromagnets. Furthermore, the behavior of phonon mode is sensitive to the density of laser irradiation is found during Raman spectral acquisition, this found might be interested to laser fabrication industry

Naafis Ahnaf Shahed, Kartik Samanta, Chang-Beom Eom, Evgeny Tsybmal

### Prediction of ultra-flat bands in twisted moiré oxides

POSTER #19

The emergence of flat bands in moiré superlattices of twisted bilayer structures has recently gathered significant attention. Flat bands feature new phases and electronic behavior due to strong electronic correlations. In this work, driven by the recent experimental demonstrations of free-standing oxide membranes [1,2], we explore electronic properties of twisted oxide membranes. These membranes are expected to provide a much stronger coupling between the layers than typical two-dimensional van der Waals structures and thus may lead to a broader spectrum of exotic properties. We consider a prototypical oxide, SrTiO3, and design SrTiO3 bilayers with a relative twist between the layers. Using calculations based on density functional theory, we predict the emergence of ultra-flat bands in these bilayers at relatively high twist angles. These bands are formed due to the strong localization of electronic states exhibiting moiré periodicity. Using a tight-binding approach, we create simple toy models which qualitatively explain our results. With proper doping, the flat bands at the Fermi energy may give rise to superconductivity, Mott insulating phases, and other strongly correlated properties. 1. D. X. Ji et al., Nature 570, 87 (2019). 2. H. S. Kum et al., Nature 578, 75 (2020).

A. Lipatov, J. Dai, P. Wilson, M. Shekhirev, J. Teeter, X.C. Zeng, A. Sinitskii

### Quasi-1D TiS3 nanoribbons for electronic applications

POSTER #20

Two-dimensional layered materials have received much interest in recent years due to their ease of miniaturization by exfoliation techniques and very diverse physical properties. Quasi-one-dimensional (quasi-1D) materials, while seeing considerably less interest, can express many of the same desirable properties as conventional layered materials, with an added dimension of anisotropy. A representative example of quasi-1D materials is titanium trisulfide (TiS3), a layered n-type semiconductor composed of chains of trigonal sulfur prisms with Ti4+ centers. Because of its moderate bandgap of about 1 eV, which is comparable to that of silicon, and theoretically predicted electron mobilities of up to 10,000 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>, TiS3 is a promising material for electronic applications. In this study, we investigated the preparation of nanoscale TiS3 chains and their vibrational and electronic properties. We demonstrate that TiS3 has highly anisotropic properties and is a competitive electronic material in the family of transition metal chalcogenides.

## QUANTUM SENSING, QUANTUM COMPUTING -- POSTERS 21-28

Suvechhya Lamichhane, Kayleigh McElveen, Shuo Sun, Cody Schultz, Adam Erickson, Rupak Timalisina, Yinsheng Guo, Sy-Hwang Liou, Rebacca Lai, Abdelghani Laraoui

### Nitrogen Vacancy magnetometry of the weak paramagnetic molecules

POSTER #21

Many biomolecules and spin complexes exhibit paramagnetic behavior, generating weak magnetic stray fields. Nitrogen Vacancy (NV) center in diamond has emerged as a sensitive magnetometer with a very good magnetic sensitivity. Recently, we imaged spin crossover (SCO) nanorods and nanoparticles (size ~ 20 nm - 1 μm) using NV microscopy [1]. SCO materials are expected to be diamagnetic at room temperature (RT) and paramagnetic above 380 K. We observed weak paramagnetic behavior at RT, with a volume susceptibility of approximately  $1.58 \times 10^{-4}$  in the low spin state [1], possibly originating from the surface oxidation along the SCO nanorods. Additionally, we conducted NV relaxometry on Cytochrome C (Cyt-C), a protein involved in energy production in mitochondria. At RT, the heme group remains in the Fe+3 paramagnetic state. We performed NV-T1 relaxometry on a functionalized diamond chip and varied the concentration of Cyt-C from 2.6 μM to 54 μM, resulting in a decrease of T1 from 1.2 ms to 150 μs, respectively. This reduction is attributed to spin-noise originating from the intracellular Fe spins in the Cyt-C [2]. [1] Lamichhane, S., et al., (2023) ACS Nano, 17(9), 8694–8704. [2] Lamichhane, S., et al., (2024) Nano Letters, 24(3), 873–880.



**Development of Potassium Dipole Trap with Octupolar Trapping Symmetry**

Much novel work has been done towards generating a Bose-Einstein condensate of potassium, which has proven more difficult than other typical atoms used for BECs (e.g. 87Rb). Sub-Doppler cooling techniques have been developed for potassium but require a release of the atoms in order to exert sub-Doppler forces onto them. With these limitations in mind, our group has been pioneering an octupolar symmetry trap for the MOT; this field symmetry allows for both trapping (due to the magnetic field gradient at the edges of the trap) as well as sub-Doppler cooling of the trap center (where the magnetic field gradient approaches zero). We have previously demonstrated successful trapping and sub-Doppler behavior of such a MOT. Recent progress has been towards building the dipole trap for 41K, having recently installed and commissioned the 1550-nm laser used in the crossed dipole trap. We will describe the progress made towards the trapping and sympathetic cooling of atoms necessary to reach BEC.

Rupak Timalisina, Haohan Wang, Bharat Giri, Suchhit Saran, Suvechhya Lamichhane, Adam Erickson, Jeffrey E Shield, Sy-Hwang Liou, Xiaoshan Xu, and Abdelghani Laraoui

POSTER #23

**Study of spin wave transport in ferrimagnetic insulator TmIG thin films**

The propagation of spin waves in materials featuring perpendicular magnetic anisotropy (PMA) has attracted a significant interest for novel and energy-efficient spintronic devices [1]. Thulium iron garnet (TmIG:  $\text{Tm}_3\text{Fe}_5\text{O}_{12}$ ), ferrimagnetic insulator with PMA, is a promising candidate due to its unique magnetic properties and spin transport characteristics [2]. In this work we used broadband ferromagnetic resonance (FMR) spectroscopy, spin-wave (SW) electrical transmission spectroscopy (ETS), and nitrogen vacancy (NV) magnetometry to study SW transport properties in TmIG thin films (thickness of 7-35 nm) grown on gadolinium-gallium-garnet (GGG) and substituted-GGG (sGGG) substrates. We performed FMR and SW-ETS measurements on different TmIG thin films and studied the effect of thickness and substrate on the SW transport properties [2]. We also examined non-reciprocal propagation of surface and volume spin waves [2]. Furthermore, we used NV magnetometry to image the surface propagating spin waves at the sub-micrometer scale, observed by the amplification of the local microwave magnetic field due to the coupling of NV spins with the stray-field produced by the SWs [3]. [1] A. V. Chumak, et al., Nature Physics 11, 453–461 (2015), [2] R. Timalisina, et al., under preparation. [3] R. Timalisina, et al., Advanced Electronic Materials 2300648 (2023).

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

POSTER #24

**Study of the Interaction of a Static Impurity within a Dipolar Environment**

Information on the relaxation dynamics in quantum systems is essential to understand many-body systems. These dynamics are not only necessary for quantum mechanics but also important to understand several open questions in areas like high-energy physics, cosmology, and quantum data processing [1]. In the present work, we explore these dynamics using a static impurity in a quantum environment as our model. We delve into this by placing a static impurity into a three-dimensional Bose-Einstein Condensate made of dipolar gases. The Hamiltonian of the system was transformed in the frame of impurity, which led to a modified Gross-Pitaevskii equation (GPE). This modified GPE was then solved using both analytical methods and numerical solutions through the split-step Crank-Nicolson method [2]. We then calculated different properties of the static impurity, including its self-energy and density distribution. Additionally, we examined the effects of anisotropic impurities on density results by deforming the impurity. Further, by changing the orientation of the impurity at different deformations, we observed the density profile at several angles, revealing unique shifts due to the impurity's shape changes, emphasizing its complex interaction with the surrounding condensate.

Adam Erickson, Qihan Zhang, Hamed Vakili, Suvechhya Lamichhane, Lanxin Jia, Ilya Fescenko, Edward Schwartz, Sy-Hwang Liou, Alexey Kovalev, Jingsheng Chen, Abdelghani Laraoui

POSTER #25

**Direct Observations and Characterization of Topological Spin Textures in Gradient Engineered CoPt Thin Films at Room Temperature**

Magnetic skyrmions are nanoscale spin textures characterized by a topological charge and possess functionality for numerous contemporary applications [1]. Skyrmions can occur as two-dimensional ground states in magnetic systems where strong spin orbit coupling (SCO) and broken inversion symmetry lead to Dzyaloshinskii-Moriya interaction (DMI) [1]. Recently, sizable bulk DMI was measured in composition engineered ferromagnetic/heavy metal (HM/FM) single layer films. The resulting gradient DMI is believed to originate from bulk magnetic asymmetry and SCO and has a sign and proportionality dependence with the magnetization gradient [2]. In a novel demonstration, we employ nitrogen vacancy (NV) magnetometry and magnetic force microscopy and to directly image room temperature skyrmions in gradient engineered CoPt single layers. Skyrmions remain stable at a wide range of applied magnetic fields and are confirmed to be Bloch type from micromagnetic simulation and analytical magnetization reconstruction. Furthermore, we observe the stabilization of skyrmion pairs and discuss their possible origins. Our findings expand the family of materials hosting magnetic skyrmions at room temperature. [1] A. Fert et al., Nat. Nanot. 8, 152–156 (2013). [2] Qihan Zhang et al., Phys. Rev. Lett. 128, 167202 (2022) [3] A. Erickson et al., submitted to Nature Communications

Owen Root, Maria Becker

**Efficacy Testing IBM Quantum Computers via Statistical Randomness**

POSTER #26

The fundamental principles of quantum mechanics, such as its probabilistic nature, allow for the theoretical ability of quantum computers to generate statistically random numbers, as opposed to classical computers which are only able to generate pseudo-random numbers. This ability of quantum computers has a variety of applications, one of which provides the basis for a method of efficacy testing Quantum Computers themselves. We introduce this testing method and utilize it to investigate the efficacy of nine IBM Quantum Computer systems. The testing method utilized four different quantum random number generator algorithms and a battery of eighteen statistical tests. Only a single quantum computer-algorithm combination was found to be statistically random, demonstrating the power of the testing method as well as indicating that further work is needed for these computers to reach their theoretical potential

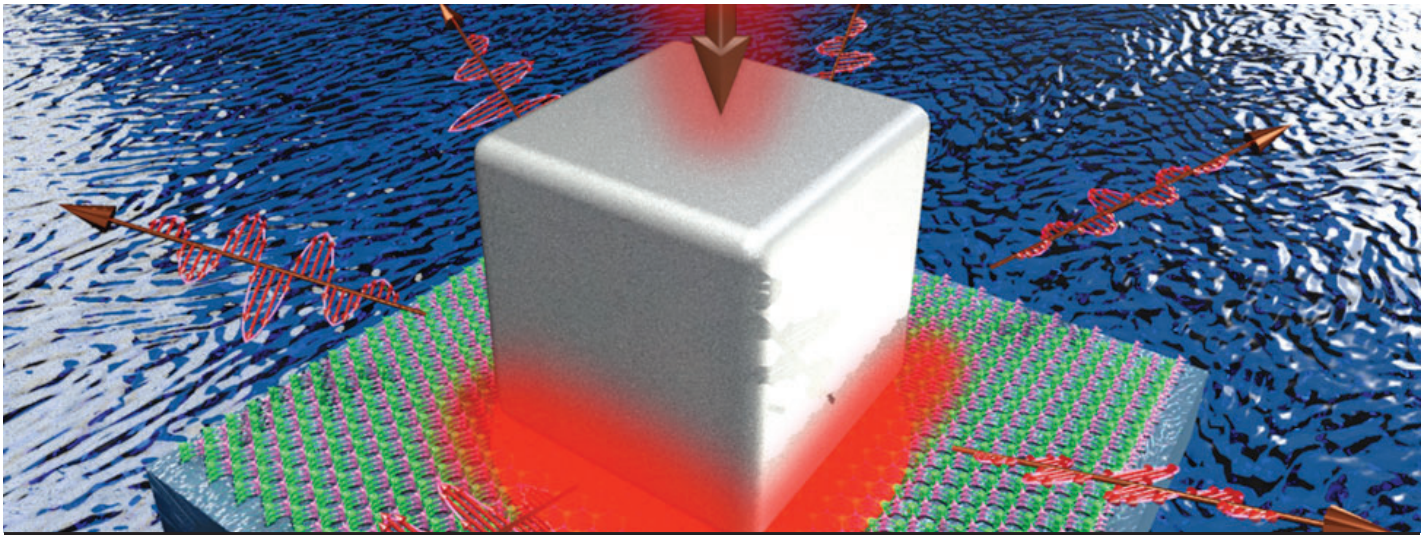
Abhilash Mishra, Ather Mahmood, Renat Sabirianov, Wai-Ning Mei, Christian Binek

**Crossroad quantum dots in Graphene**

POSTER #27

In this study, we present the fabrication and characterization of quantum dots (QDs) based on a cross-road structure where geometric confinement and the specific cross-road architecture are expected to lead to two discrete electronic states separated from a continuum. These QD devices are fabricated from few-layer graphene films with the help of e-beam lithography technique aiming at widths of the individual graphene ribbons of about 80 nm. The resulting structures exhibit novel properties that we investigate through electric transport measurements, allowing us to probe the energy levels within these devices. The combination of graphene's high carrier mobility with the geometrically tunable level spacing of the QDs offers a promising platform for diverse quantum device application. This research advances understanding of low-dimensional QD systems and paves the way for the development of next-generation quantum technologies. National Science Foundation funding via EPSCoR RII Track-1: Emergent Quantum Materials and Technologies (EQUATE), OIA-2044049 is acknowledged. The research was performed in part in the Nebraska Nanoscale Facility: National Nanotechnology Coordinated Infrastructure and the Nebraska Center for Materials and Nanoscience, which are supported by NSF under Award ECCS: 2025298, and the Nebraska Research Initiative.





## NRIC 2024 | DIAMOND QUANTUM SENSING: CHALLENGES & OPPORTUNITIES

Raman Kumar, Chandan Nagadi, Svetlana Kiriushechkina, Anton Vakulenko, Alexander B. Khanikaev, and Carlos A. Meriles

### Near-field sensing of a topological photonic waveguide via scanning color center probes

POSTER #28

As the ability to control electromagnetic (EM) fields through engineered photonic structures grows, so does our need for field mapping techniques with subwavelength resolution, an area thus far dominated by approaches relying on tips designed to collect or scatter light with nanoscale precision. Here, we use a ~100-nm-diameter diamond crystal at the apex of an atomic force microscopy probe to investigate the interplay between the emission of nanoparticle-hosted nitrogen-vacancy (NV) centers and a proximal topological waveguide. We show the NV photoluminescence serves as a local, spectrally broad light source to characterize the waveguide response, both in terms of its working wavelength bandwidth as well as the correspondence between locality of light injection and directionality of wave propagation. Further, we show that near-field coupling between the emitters and the chiral modes supported by the waveguide influences the ellipticity of the NV photoluminescence, hence allowing us to reveal nanostructured light fields with a spatial resolution defined by the nanoparticle size. Our results pave the route to exploiting color centers as photonic sensors able to probe nanostructured EM fields, an approach that also promises opportunities in the development of on-chip devices integrating single-photon emitters and quantum optics.

### OPTICAL QUANTUM MATERIALS AND PHENOMENA, POSTERS 29-37

Preston Sorensen, Ufuk Kilic, Yousra Taouli, Rafal Korlacki, Eva Schubert, Mathias Schubert

POSTER #29

### Elevated Temperature Model Dielectric Function of InAs Determined by Spectroscopic Ellipsometry

We report the elevated temperature (30-250°C) dielectric function of InAs across the spectral range of the near infrared to deep ultraviolet (0.73eV to 5.0eV) by way of spectroscopic ellipsometry. InAs is a III-V zincblende structure semiconductor used in long wavelength optoelectronic devices due to its direct bandgap of 0.355eV [1,3,4]. Determining the thermal evolution of its optical properties, like bandgap energy and band to band transitions, allows for predictable ellipsometry monitored growth of InAs device architectures at higher temperatures. Thermal perturbation of a crystal results in a small increase in the lattice constant of the material, altering the band structure, and therefore its dielectric function [4]. Spectroscopic ellipsometry allows us to directly measure the dielectric function of InAs. In-Situ measurements were taken from 30°C to 250°C at a single angle of incidence. We measured the sample again ex-situ at room temperature at multiple angles of incidence to identify any surface roughness or surface oxide layer present. We identified a general surface roughness layer and a secondary surface mode present at elevated temperatures. The resulting pseudodielectrics retrieved from the ellipsometric measurements were modeled using the critical point function method [2,3]. We augmented a complex phasor relationship for the critical point functions to mimic anharmonic broadening. The parameters of the functions in each model were then tabulated to find their evolution over the temperature spectrum. We find linear evolution of the features in the dielectric function versus temperature, thus making it easier to predict material behavior across elevated temperature use cases. References: [1] S. T. Schaefer, et al. "Absorption edge characteristics of GaAs, GaSb, InAs, and InSb" Journal of Applied Physics (2020). [2] E. Montgomery, et al. "Temperature dependent model dielectric function of highly disordered Ga<sub>0.52</sub>In<sub>0.48</sub>P" Thin Solid Films (2010). [3] S. Adachi. "Optical dispersion relationships for GaP, GaAs, GaSb, InP, InAs, InSb, Al<sub>x</sub>Ga<sub>1-x</sub>As and In<sub>1-x</sub>Ga<sub>x</sub>As<sub>y</sub>P<sub>1-y</sub>." Journal of Applied Physics (1989). [4] P. T. Webster, et al. "Measurement of InAsSb bandgap energy and InAs/InAsSb band edge positions using spectroscopic ellipsometry and photoluminescence spectroscopy" Journal of Applied Physics (2015).

Joshua Barker, Mohammadjavad Dowran, Suvechhya Lamichhane, Adam Erickson, Ufuk Kilic, Christos Argyropoulos, Sy-Hwang Liou, Abdelghani Laraoui

### Quantum properties of single photon emitters in thin hexagonal boron nitride flakes integrated with plasmonic nanocavities

POSTER #30

Two dimensional materials such as hexagonal boron nitride (hBN) emerge as promising hosts of single photon sources (SPEs) which exhibit favorable optical properties (high brightness, optically accessible spin states, high quantum efficiency), making them highly desirable elements for integrated quantum photonics [1]. In this work, we created SPEs in thin (thickness ≤ 20 nm) hBN flakes deposited on Si/SiO<sub>2</sub> substrates by using a high-temperature (1100 °C) annealing and plasma irradiation under O<sub>2</sub> flow. We characterized their quantum properties using a home-built confocal fluorescence microscope. We demonstrated a plasmonic enhancement of SPE properties from Au nanograins, manifested by an increase of the emitter fluorescence by ~ 392% [4]. To enhance further the quantum properties of SPEs on a selected thin hBN flake, we spin coated silver nanocubes (SNCs) with size of 100 nm on the Au/Si substrate [3]. We observed plasmon nanocavity enhancement of SPE properties manifested by a decrease of emitter lifetime by 100%, and a fluorescence enhancement of 200% [4]. [1] M. Atatüre et al., Nat Rev Mater 3, 38–51 (2018). [3] M. Dowran, et al., Advanced Optical Materials 11 (16), 2370062 (2023). [4] M. Dowran et al., Laser and Photonics Reviews, under review.

Ahmad Alsaad, Jaeil Bai, Wai-Ning Mei, Carolina C Ilie, Peter A Dowben, Renat Sabirianov

### Proximity effect of Optically Active h-BCN nanoflakes

POSTER #31

Hexagonal BCN (h-BCN), an isoelectronic counterpart to graphene, exhibits chirality and offers the distinct advantage of optical activity in the vacuum ultraviolet (VUV) region, characterized by significantly higher wavelengths compared to graphene nanoflakes. h-BCN possesses a wide band gap and demonstrates desirable

semiconducting properties. In this study, we employ Density Functional Theory (DFT) calculations to investigate the proximity effects of adsorbed hBCN flakes on two-dimensional (2D) substrates. The chosen substrates encompass monolayers of 3d-transition metals and WSe<sub>2</sub>, as well as a bilayer consisting of WSe<sub>2</sub>/Ni. Notably, the hydrogen-terminated h-BCN nanoflakes retain their planar configuration following adsorption. We observe a robust interaction between h-BCN and fcc-based monolayers such as Ni(111), resulting in the closure of the optical band gap, while the adsorption energy on WSe<sub>2</sub> is notably weaker. In the latter case, the system maintains an approximate gap of 1.4 eV. Furthermore, we investigate the magnetism induced by the proximity of adsorbed chiral h-BCN molecules, as well as the chiral-induced spin selectivity within the proposed systems.

*Yusra 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 ALD Recipe Optimization and Critical Point Model Dielectric Function Analysis of Atomic Layer Deposited ZnO ultrathin film**

**POSTER #32**

In this work, we employ in-situ Spectroscopic Ellipsometry (SE) to real-time monitor the growth of ZnO ultrathin films fabricated by Plasma-Enhanced Atomic Layer Deposition (PE-ALD). The process involves the utilization of a Zn(CH<sub>3</sub>)<sub>2</sub> organometallic precursor and oxygen plasma as the primary reactant and co-reactant, respectively. The investigation introduces a recently suggested dynamic dual-box model, offering a comprehensive understanding of cyclic surface modifications and continuous growth mechanisms of ZnO ultrathin films. Furthermore, we anticipate the applicability of this model approach for evaluating in-situ SE data obtained during the deposition of various oxide materials. Hence, we acquired in-situ SE data during the growth of ZnO ultrathin films across the spectral range of 1.7-4 eV, with a 67.9° angle of incidence.

Moreover, this model proves invaluable for the optimization of a robust ALD recipe in-situ by understanding the influence of the substrate temperature on the growth per cycle as one of the key ALD parameters. By applying the dynamic dual-box model approach, we also obtained the temperature dependent dielectric function spectra, in-situ. Furthermore, we then incorporate the critical point model dielectric function analysis. This allows us to identify band-to-band transitions for ZnO ultrathin films, offering crucial insights into the optical properties.

*Raymond Smith, Ufuk Kilic, Dmitry Kalanov, Erik Rohkamm, Carsten Bundesmann, Frank Frost, Mathias Schubert, Eva Schubert*

**POSTER #33**

**Ion Energy Distributions in Broad Beam Kaufman Ion Sources**

Broad beam Kaufman ion sources, devices that can produce positively charged particles at precise energies, are a valuable resource in many fields. There is an ever-growing list of applications for broad beam ion sources, including nanostructure manufacturing and ion thrusters. When used for nanostructure fabrication, knowledge of which conditions within the source produce the corresponding beam containing ions of a desired composition and energy is essential for accurate and efficient fabrication. While using Argon and Oxygen as source gases, we systematically varied parameters of the ion source and collected data on the energies of the produced ions with an energy selective mass spectrometer. We analyzed the ion energy distributions and found that the energy value of low energy ions is more stable across varying parameters when using a filament to produce negative charges that counteract the positive charge of the ion beam.

*Sema Guvenic Kilic, Ufuk Kilic, Mathias Schubert, Eva Schubert, Christos, Argyropoulos*

**POSTER #34**

**Chirality Enhancement of Helical Metamaterials Through Topologically Protected Resonance Revealed by 1D Photonic Crystal**

Our research aims to enhance the chirality response of a plasmonic nanohelical heterostructure metamaterial platform comprising gold (Au) and silicon (Si) helical sub-segments. Through series of systematic finite element modeling simulations, we demonstrate the control of chirality amplitude and spectral location by varying the turn rate of Au sub-segment in a one-turn nanohelical structure. To further enhance chirality, we propose incorporating a topological interface using a 1D photonic crystal composed of multiple TiO<sub>2</sub> and SiO<sub>2</sub> layers, serving as a bandpass filter. Introducing a 1D lattice mismatch at the interface results in an ultra-narrowband leak mode within the photonic band gap region, with spectral characteristics aligned with the edge mode in the energy dispersion band diagram. Finally, positioning a Si-Au plasmonic nanohelical structure at the interface center leads to a significant enhancement in chirality. We envision that the substantial enhancement in chirality achieved through our on-chip friendly topological insulator design can significantly advance applications in waveguide systems, quantum information technologies, and next-generation photonic integrated circuits [1-2]. References: 1- Lustig, Eran, et al. Nature 609.7929:931-935, (2022). 2- Alfieri, Adam, et al. Advanced Materials 35.27: 2109621(2023).

*Ian Green, Preston Sorensen, Alex Ruder, Rafal Korlacki, Mathias Schubert*

**Terahertz Electron Paramagnetic Resonance Ellipsometry with Field Flattened Split-Coil Magnet**

**POSTER #35**

Terahertz Electron Paramagnetic Resonance Ellipsometry, within a flattened magnetic field induced by a superconducting split-coil electromagnet, is explored. Idealistic and experimental motivations for the development of instrumentation is provided. A general theory of operation, applications of the system, and research opportunities are discussed.

*Shawn Wimer, Mathias Schubert*

**Sum rules for the dielectric function in monoclinic materials**

**POSTER #36**

The sum rules are reconsidered for complex valued response functions in materials with monoclinic and triclinic symmetry. An eigendielectric displacement vector summation approach [M. Schubert et al., Phys. Rev. B 93, 125209 (2016)] is used to represent physical excitation mechanisms such as phonon and exciton polaritons, and to render the dielectric permittivity tensor and their inverse for demonstration. The superconvergence theorem is used to derive additional sum rules and we show by comparison with recent results obtained by experiment their validity for lattice vibrations in monoclinic crystals.

*S M Nayeem Arefin, Sanchaya Pandit, Yanan (Laura) Wang*

**Integrated Photonics Empowered by Lead- Halide Perovskites: Opportunities and Challenges**

**POSTER #37**

Lead halide perovskite (LHP) is a family of emerging photonic materials that share similar crystalline structures (APbX<sub>3</sub> for three-dimensional phase, APb<sub>2</sub>Br<sub>5</sub> for two-dimensional phase, and A<sub>4</sub>PbX<sub>6</sub> for zero-dimensional phase). Due to the unique excitonic transitions, high tunability of photophysical properties, and the easiness of synthesis through hydrothermal reactions, LHP has been employed in photovoltaic and optoelectronic applications. On the other hand, the complex phase equilibrium and the chemical instability pose significant challenges in patterning LHP into sophisticated photonic structures by conventional lithography and etching techniques. In this work, we advocate for a novel synthesis method combining soft-lithography and self-assembly, in which a patterned template with asymmetric wettability is exploited to control nucleation and crystal growth. The demonstration of patterned LHP structures with high crystallographic order will pave the way to the realization of integrated photonic devices based on LHP through a feasible and scalable approach.

**CHEMICAL AND OTHER QUANTUM SYSTEMS, POSTERS 38-42**

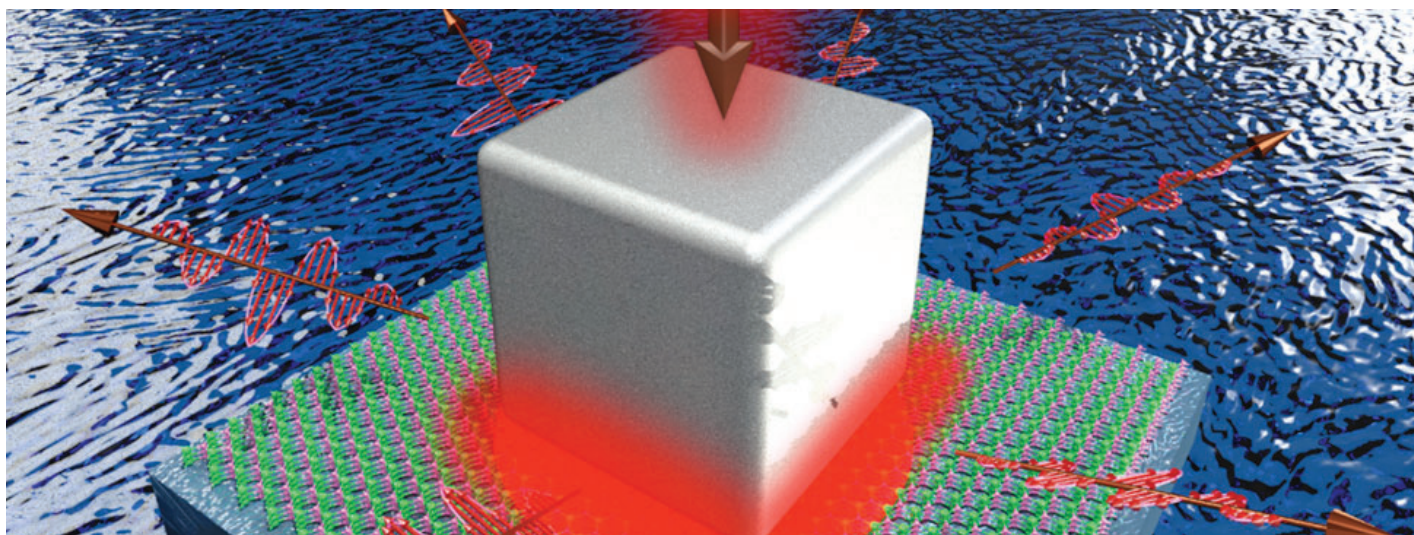
*Yuanyuan Ni, Yifan Yuan, Jing Li and Xiaoshan Xu*

**Effect of Capping Layer on Organic Thin Film**

**POSTER #38**

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 deposition of lithium fluoride (LiF) as capping layer. The





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effect of the capping layer on the evaporation of MBI films in different vacuum environments has been studied by measuring the change of remanent polarization of MBI at room temperature. The results show that the LiF layer effectively minimizes the loss of MBI films on the substrate in high vacuum of  $10e-7$  Torr for hours while in an environment with a pressure of  $10e-2$  Torr, the MBI thin film can remain highly stable for days.

Katherine Johnson, Shuo Sun, Kayleigh McElveen, Binny Tamang, Rebecca Lai, Yinsheng Guo

POSTER #39

### Optical studies of the spin crossover complex $[\text{Fe}(\text{Htrz})_2(\text{trz})](\text{BF}_4)$

Spin crossover (SCO) complexes possess the distinct capability to undergo spin transitions from the diamagnetic state to the paramagnetic state and vice versa when exposed to external stimuli such as heat, light, and pressure. This quality gives SCO materials an advantage in the fields of data storage, sensors, and actuators, as their optical, magnetic, and structural properties are also altered upon any electronic transition. One such SCO compound,  $[\text{Fe}(\text{Htrz})_2(\text{trz})](\text{BF}_4)$ , lends itself well to optical measurements, specifically via Raman spectroscopy. New sizes of  $[\text{Fe}(\text{Htrz})_2(\text{trz})](\text{BF}_4)$  were recently synthesized, including nanoparticles and nanorods. Here, the effects of size, environment, and damage on the spin crossover properties of these nanoscale samples are explored through optical techniques.

Greg Acosta, Malachi Hood, Mohammad Ghashami

POSTER #40

### Precision measurement of subcontinuum gas conduction within microconfinements

Subcontinuum gas conduction is an essentially important phenomenon in disparate fields of applications ranging from aerospace vehicles to biomedical sensors. It has been the focus of many computational studies over the past decades. These studies predicted that the energy exchange mechanisms are driven by gas-surface interactions, strongly dependent on the gas and surface characteristics. Despite its fundamental and practical importance, thermal transport via gas conduction at non continuum regimes mostly remains experimentally unverified. Here, we report precision measurements of subcontinuum gas conduction within parallel microcavities and elucidate its dependence on the gas and surface characteristics. More importantly, we demonstrate a systematic approach for extracting the energy accommodation coefficient (EAC), which is necessary to establish gas-surface scattering kernels or develop diffusive-specular solutions to the Boltzmann transport equation. EACs are also required for calculating the temperature jump coefficient in near-continuum conditions to solve classical hydrodynamical equations. We show a correction to the kinetic theory in the transition to near-continuum regimes (particularly for nonmonatomic gases) by extracting a physical parameter representing the intermolecular collisions within the Knudsen layer. Our results agree well with the kinetic theory predictions and are expected to inform the development of thermal switches, gas sensors, and light-driven actuators.

Clint Evrard Ph.D.

POSTER #41

### Programmable Electronic Structures of Transition-Metal Oxide Doped Photoactive Materials

Single-site photocatalysts constructed from transition-metal oxide clusters imbedded into the surface of bulk semiconductors have been found to be a class of materials that have demonstrated the ability to selectively oxidize methane to methanol with high photoactivity in ambient conditions. 1-6 The photocatalytic selective oxidation of methane is driven by long-lived electronic excited states. Long-lived excited states allow for the methane molecule to be able to effectively interact with the electronic structure of the photocatalytic material leading to the activation of the H-C bonds on the methane molecule. These long-lived excited states are achieved due to intersystem crossing events centered on the transition-metal oxide photoactive species which lead to the photocatalytic material crossing from a singlet to a triplet electronic spin state. These intersystem crossings will allow the electronic structure of the photocatalysts to avoid relaxation back to the initial  $S_0$  singlet ground state through the interaction of the excitation orbitals based on their spatial structure as stated by the El Sayed rules and through strong spin-orbit coupling events. 2,9-11 The interactions between shifts in the electronic structures and spin-orbit coupling in materials can lead to technologies that are highly programmable based on their inherent quantum mechanics. 1. [10.1021/bk-2019-1331.ch015](https://doi.org/10.1021/bk-2019-1331.ch015); 2. <https://doi.org/10.1021/acs.jpca.3c04289>; 3. <https://doi.org/10.1021/acs.jpcc.3c00663>; 4. <https://doi.org/10.1134/S0020168519110013>; 5. [10.1039/C8CS90119H](https://doi.org/10.1039/C8CS90119H); 6. <https://doi.org/10.1016/j.jcat.2021.07.014>; 7. <https://doi.org/10.1016/j.jphotochem.2013.05.005>; 8. <https://doi.org/10.1016/j.egypro.2012.09.035>; 9. <https://pubs.rsc.org/en/content/articlepdf/1950/df/df9500900014>; 10. <https://doi.org/10.1021/jp111892y>; 11. <https://doi.org/10.1002/wcms.83>

Binny Tamang, Kayleigh A. McElveen, Wai Kiat Chin, Peter A. Dowben, and Rebecca Y. Lai

### Synthesis of Spin Crossover Complex $\text{Fe}(\text{phen})_2(\text{NCS})_2$ and Fabrication of Composites with Polyaniline and Magnetite POSTER #42

$\text{Fe}(\text{phen})_2(\text{NCS})_2$  is an Fe(II) spin crossover (SCO) complex with a well-defined and reversible LS to HS transition with hysteresis between 180 and 190 K. In this study, we focused on the synthesis of  $\text{Fe}(\text{phen})_2(\text{NCS})_2$  and the fabrication of bi-composites with polyaniline (PANI) and tri-composites with PANI and  $\text{Fe}_3\text{O}_4$ . When analyzed using vibrating sample magnetometry, a slight increase in the thermal hysteresis loop was observed for the  $\text{Fe}(\text{phen})_2(\text{NCS})_2/\text{PANI}$  bi-composite when compared to the pure  $\text{Fe}(\text{phen})_2(\text{NCS})_2$  sample. The presence of PANI did not appear to have altered the SCO behavior of  $\text{Fe}(\text{phen})_2(\text{NCS})_2$ . Furthermore, tri-composites containing  $\text{Fe}(\text{phen})_2(\text{NCS})_2$ , PANI, and different amounts of  $\text{Fe}_3\text{O}_4$  were made and systematically characterized. Despite the superparamagnetic contribution from  $\text{Fe}_3\text{O}_4$ , the SCO signature of  $\text{Fe}(\text{phen})_2(\text{NCS})_2$  was still apparent in the magnetometry results. The addition of  $\text{Fe}_3\text{O}_4$ , even at a concentration up to 10% by weight, did not have a major negative impact on the system. These results are significantly different from those obtained from similar tri-composites fabricated with PANI,  $\text{Fe}_3\text{O}_4$ , and  $[\text{Fe}(\text{Htrz})_2(\text{trz})](\text{BF}_4)$ , an Fe(II) SCO polymer. It is possible that there is no major phase separation between the three components in the current tri-composites. It is worth noting that the tri-composite with 5%  $\text{Fe}_3\text{O}_4$  showed rather different responses both in magnetometry and I(V) analysis. The observed discontinuity in the current upon voltage sweep indicates that there is a voltage-controlled switching behavior, which is desirable for SCO systems and SCO-based devices.