Emergent QUAntum materials and TEchnologies (EQUATE)
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Year 4 Narrative Report – February 2025
(Y4: 6/1/2024 – 5/31/2025)

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Participating Institutions: University of Nebraska-Lincoln, Creighton University, University of Nebraska at Omaha, University of Nebraska at Kearney, Little Priest Tribal College, Nebraska Indian Community College

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Overview

Much of modern scientific and technological advancement occurs where multiple disciplines intersect. Emergent Quantum Materials and Technologies (EQUATE) spans multiple campuses, with 20 investigators from the University of Nebraska's Lincoln (UNL), Omaha (UNO), and Kearney (UNK) campuses, as well as Creighton University (CU). The project also promotes STEM education (science, technology, engineering, and mathematics) by supporting undergraduate learning at two participating community colleges.

Materials science reaches a new phase with the second quantum revolution. A key discovery from the first quantum revolution is wave-particle duality, the concept that electrons can exhibit both particle-like and wave-like properties. The second quantum revolution focuses instead on macroscopic quantum phenomena that arise from strong electron-electron correlation, entanglement, non-trivial topological orders, and quantum effects including magnetism and non-trivial magnetic textures, ferroelectricity, and quantum confinement and proximity effects in low-dimensional materials.

The EQUATE research initiative adopts an interdisciplinary approach, structuring its work into three interconnected Focused Research Groups (FRGs). Each group is dedicated to specific thrust areas, combining theoretical, experimental, and engineering expertise to drive collaborative advancements.

FRG1 (Quantum Materials) establishes the project's foundation in fundamental materials science. Guided by theoretical insights, new quantum materials are designed, synthesized, and integrated into hybrid structures and prototype devices through nanofabrication. These materials are then characterized and modeled, with a continuous feedback loop between theory and experiment driving progress. Some of the quantum material platforms developed in FRG1 (Quantum Materials) have potential applications in FRG2 (Quantum Technologies) and FRG3 (Quantum Information Processing).

FRG1 explores materials where emergent quantum phenomena arise from non-trivial topologies, spin ordering, and strong electron correlations (Thrust 1). It leverages magnetoelectric coupling and the valley degree of freedom in low-dimensional systems and interfaces (Thrust 2). Additionally, it investigates novel molecular platforms for spin quantum bit (qubit) systems (Thrust 3).

FRG2 (Quantum Technologies) focuses on sensing and metrology, utilizing the extreme sensitivity of quantum systems (Thrust 1), as well as quantum communication, emphasizing the role of photons as quantum information carriers (Thrust 2).

FRG3 sits atop this hierarchy, focusing on quantum information processing through the development of quantum emulation (Thrust 1) and the long-term vision of general quantum computing (Thrust 2), with critical components currently under development.

Across all FRGs, senior investigators (SIs) from UNL, UNO, UNK, and CU contribute expertise spanning physics, chemistry, materials science, mechanical engineering, electrical engineering, and computer science. A key strength of the initiative is the well-established collaboration and continuous feedback loop between theory and experiment, fostering multi-campus exchanges and accelerating discoveries.

Development and application of quantum materials for quantum technologies in Nebraska is supported by the Nebraska Center for Materials and Nanoscience (NCMN). With faculty expertise, Nebraska competes in the competitive and economically significant race for leadership in quantum technologies.

Four years of EQUATE research have shown that the translation of fundamental research into commercial quantum technologies that represent the next major advancement, crucial in securing Nebraska's future economic prosperity. EQUATE helps create a highly skilled workforce for the American Midwest. The region will not attract a quantum-based industry without providing quantum engineers. EQUATE plays the leading role for Nebraska to develop this quantum workforce.

Executive Summary

EQUATE remains a key driver in the second quantum revolution, fostering discoveries, innovation, and workforce development. Its Year 4 results are a testament to the success of the center's interdisciplinary, multi-campus collaborative approach. Much of EQUATE's Year 4 advanced in accordance with the objectives set forth in the project's strategic plan.

Dr. Aleksander **Wysocki** at the University of Nebraska at Kearney (UNK) is now deeply integrated into EQUATE collaborations, including work with FRG1 PIs **Binek**, **Guo**, and **Dowben**, as well as FRG2 PI **Laraoui**. Wysocki' s contributions include theoretical explanations for the voltage dependence of the two-magnon Raman signal in boron doped chromia thin films. Additionally, he has built a robust research portfolio focused on ad-atoms on surfaces, exploring their potential applications as qubits. In Year 4, Dr. Zuocheng **Zhang** joined the Department of Physics and Astronomy at the University of Nebraska-Lincoln (UNL) as a faculty member and EQUATE PI, bringing expertise in two-dimensional materials and topological insulators. He has already collaborated with multiple senior FRG1 PIs on experimental efforts and has become an active contributor to several proposals (see Sustainability, page 41) that support the long-term sustainability of EQUATE research including the recent DoE EPSCoR proposal titled "Emergent Interface Phenomena Enabled by Ferroelectric Oxide Thin Films and Membranes" by lead PI and FRG1 leader **Hong** together with co-PIs **Dowben, Tsymbal, Zhang, and Xu**.

The departure of Dr. Wei **Bao** from the Department of Electrical and Computer Engineering at UNL to the Department of Materials Science and Engineering at the Rensselaer Polytechnic Institute in Troy, NY is now more than compensated for through integration of Dr. Laura **Wang** as the center's most recent Seed Awardee. In collaboration with former Seed Awardee Alexander **Sinitskii**, now FRG3 SI, she will advance research on non-equilibrium Bose-Einstein condensates in condensed matter to new heights. Her work will expand the concept of solid-state exciton-polariton BECs in distributed feedback resonators, by realizing an exciton-polariton photonic platform. Through leveraging Sinitskii's expertise in wide-bandgap materials and semiconducting exciton emitters, she aims to develop a fully integrated solution which circumvents many of the complexities in fabricating Bao's resonator cavities. The BECs investigated in FRG3, including those realized through the ultra-cold atom approach led by FRG3 leader Dr. Jonathan **Wrubel**, enable further advancements in quantum emulation methods. These developments build upon the emulation of model systems, such as the XY-Hamiltonian emulated by Bao.

Bolstered by the strategic innovations outlined above, EQUATE continues to establish itself as a leading center in quantum materials science and technology. This is exemplified by the participation of EQUATE Scientific Director Dr. Christian **Binek** as a panel member at the 28th NSF EPSCoR National Conference in 2024 in Omaha, NE. The panel, titled Quantum Research in EPSCoR Jurisdictions, also included Matt Doty, Director of the Quantum Science and Engineering Program at the University of Delaware; Liz Godwin, Assistant Professor of Electrical and Computer Engineering at the University of New Mexico; Chitro Chakraborty, Assistant Professor of Materials Science and Engineering at the University of Delaware; Marek Osinski, Professor of Electrical and Computer Engineering at the University of New Mexico; and Jake Douglas, Quantum Business Development Lead at Sandia National Laboratories.

EQUATE continues to be frequently consulted through in-person visits of high-ranking leadership representatives of the U.S. Strategic Command (STRATCOM) associated with the National Strategic Research Institute (NSRI). In addition to meetings coordinated by Allen Geist, the director of the Electromagnetic Spectrum Operations (EMSO) Programs at the NSRI which is the DOD-designated University Affiliated Research Center sponsored by STRATCOM, the scientific director of EQUATE is now frequently consulted by Marty Sikes, Associate Executive Director of the Chemical and Biological Defense Program at the National Strategic Research Institute.

In Year 4, FRG1's focus on quantum materials continues to achieve significant milestones, driving breakthroughs in fundamental quantum materials science for applications in quantum and spintronic devices. EQUATE's hallmark remains its highly collaborative approach, fostering strong partnerships within and across FRGs, as well as between experimentalists and theorists. One key example is the field of magnetoelectric antiferromagnetic oxides, where senior investigators from physics, engineering, chemistry, and national labs collaborate to pioneer Néel vector rotation through purely electric means. Another thriving area of FRG1 research is the study of topological spin textures for device applications, where theoretical and experimental efforts advance synergistically through the topological Hall effect.

As EQUATE matures, the boundaries between different FRGs are becoming increasingly fluid. We consider this a highly positive development that highlights the growing synergy between research groups and disciplines. A prime example is SI **Binek's** work in FRG1 on the lithographic fabrication of crosswire quantum dots based on graphene, which is directly inspired by theoretical predictions from FRG3 PIs **Sabirianov** and **Mei**. The objective is to demonstrate that these quantum dots possess precisely two discrete electronic energy levels, with tunable spacing controlled by the geometry (width) of the graphene nanoribbons. Complementing this effort, FRG3 PI **Sinitskii** explores alternative approaches by leveraging different 2D materials, including MXene, and investigating chemical synthesis as an alternative to lithographic top-down fabrication.

FRG2 continues to gain remarkable progress as well -- exemplified by the successful real-space mapping of periodic magnetization modulation induced by a specific spin wave excitation (Damon-Eshbach mode). This achievement was made possible through a quantum metrology approach that leverages FRG1's expertise in materials growth and FRG2's proficiency in NV-center microscopy. The work underscores the strong collaboration between senior investigators across FRGs and the integration of expertise from both physics and engineering. Further FRG2 highlights in Year 4 include the ongoing development of THz-electron paramagnetic resonance ellipsometry by SI **M. Schubert**, with applications in ultra-wide bandgap semiconductors for qubits, specifically through defects similar to nitrogen vacancies in diamond. There is also progress in the use of NV centers as quantum sensors for low-field magnetic resonance spectroscopy, with applications in detecting MetHemoglobin via spin noise detection. Further advancements have been made in nanophotonics, including second harmonic chiroptical scattering in Si nanohelices and the use of plasmonic nanocavities to enhance single photon emission.

FRG3 values the return of Dr. Tom **Wong** (Creighton University) as an active researcher, after three years at the National Quantum Coordination Office in Washington, D.C. His selection for this prestigious role highlights the strong reputation of EQUATE senior investigators and their contributions to the work done within EQUATE and FRG3. SI Wong's return has strengthened FRG3's efforts in quantum computing algorithms, in collaboration with FRG3 leader Dr. **Wrubel**. Their collaboration has already resulted in a publication. FRG3's work on BECs from ultra-cold atoms is progressing as planned, with successful laser cooling achieved in an octupole trap down to 40 μK. Simultaneously, complementary work on condensed matter BECs expands into a new nanophotonic direction with the assistance of Dr. **Sinitskii** and EQUATE's most recent seed awardee, Dr. Laura **Wang**. In 2024, the **Binek** group successfully fabricated the first graphene-based crosswire quantum qubits and partially characterized them through current-voltage measurements at low temperatures. The I-V data reveal the phenomenon of Coulomb blockade, with plateaus in I-V curves potentially indicating the presence of discrete energy levels. The theoretical analysis of this data is ongoing through a cross-FRG collaboration with Drs. **Sabirianov** (UNO) and **Mei** (UNO).

EQUATE's Education and Outreach activities remain outstanding in both scale and scope, with our partnership with two of Nebraska's community colleges serving as one notable example of this impressive initiative. Further details can be found in the Solicitation-Specific Project Elements section of this document, which builds upon the project's strong Education and Workforce Development efforts.

RESEARCH AND CAPACITY BUILDING

FRG1 – Quantum Materials (EQUATE Year 4: 2024-2025)

In its Thrust 1, an FRG1 team addresses Topology, SOC, and Correlation-Driven Phenomena in Emergent Ferroic Materials. With a goal to realize a range of emergent topology, spin, and correlation phenomena in novel ferroic materials, including topological antiferromagnets, 2D vdW magnets, and correlated oxides. In FRG1's Thrust 2: Magnetoelectric and Valley Control of Layered Two-Dimensional Materials, the team's goal is to achieve magneto-electric and valley control of layered 2D vdW materials.

Year 4 Accomplishments and Impacts

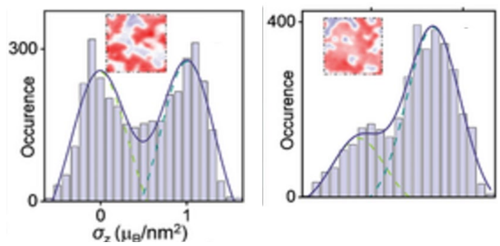

Figure 1: Change of the distribution of surface magnetization without (left) and after application of an electric field confirming the previously hypothesized 90 degree reorientation of boundary magnetization.

Thrust 1, Objective 1a aims to explore quantum materials for antiferromagnetic (AFM) spintronics. In Year 4, SI **Binek**'s group collaborated with FRG2 leader **Laraoui**, FRG1 SI **Guo**, and FRG3 SI **Wysocki** to achieve electrical rotation of Néel vector and have demonstrated via nitrogen vacancy (NV) center microscopy and Raman spectroscopy measurements (meets metric). This study builds upon prior work by the Binek group, which demonstrated that B-doped Cr_2O_3 not only exhibits an increased Néel temperature but also enables pure voltage-controlled rotation of the Néel vector without the need for an applied magnetic field. While earlier investigations hypothesized the mechanism behind this non-volatile rotation based on magnetotransport and magnetic force microscopy data, a recent breakthrough came with the application of NV microscopy by the Laraoui group, which provided microscopic evidence showing that voltage application alters the surface magnetization distribution, transitioning it between out-of-plane and in-plane orientations (meets metric). **Fig. 1** illustrates the probability of finding a surface region with a specific normal component of magnetization. The left panel displays a bimodal distribution, indicating an comparable presence of domains with in-plane magnetization (σ_z = 0) and out-of-plane magnetization (σ_z = 1). In contrast, the right panel, taken after voltage application, reveals a significant reduction in the number of in-plane magnetized domains and an increase in out-of-plane magnetized domains. This work has been published in *Advanced Functional Materials* (2024).

SI **Guo** conducted Raman investigations on the films from the Binek group, observing pronounced electric field effects, most notably a strong electric field dependence of a two-magnon mode. FRG3's **Wysocki** is currently simulating the two-magnon spectra and its modifications under an electric field. The investigation of domain switching dynamics in these systems is in progress.

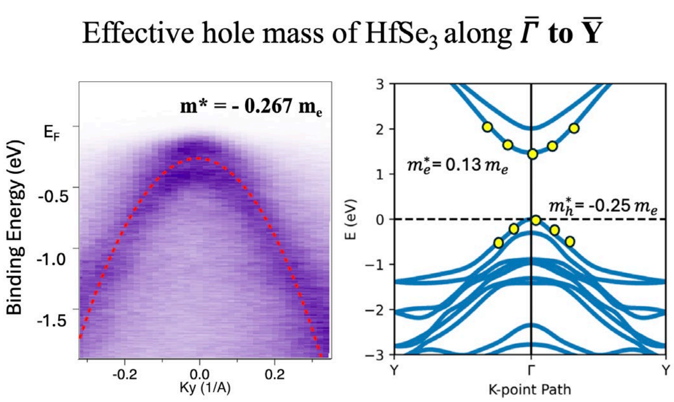

Figure 2. Experimental band mapping of $HfSe_3$(001), along the chain direction, from angle-resolved photoemission. The hole effective mass extracted from the experimental data is -0.27m_e and this is in good agreement with the calculated band strtucture (shown on the right), with an effective hole mass of -0.25m_e.

SI **Dowben** group fabricated 2D transition metal trichalcogenides, including TiS_3 and HfS_3, on chromia (meets metric). The band structure of the transition metal trichalcogenides $HfSe_3$(001) was investigated through high resolution angle resolved photoemission (ARPES) (**Fig. 2**). The effective hole mass is consistent with theoretical prediction, and we find from fitting theory to experiment, that $HfSe_3$ has more than 200 meV of spin-orbit coupling. The very light hole mass along the quasi-one-dimensional chains in turn suggest that the hole carrier mobility is very high (> 10,000 cm^2/Vs).

In collaboration with experimentalists at Stanford, SI **Tsymbal** showed using density functional theory calculations that the unconventional spin–orbit torques (SOTs) generated by AFM $MnPd_3$ thin films interfaced with a CoFeB ferromagnet are due to the AFM structure and low symmetry of the (114)-oriented $MnPd_3$ films. The theoretical search of other AFM candidates is in progress.

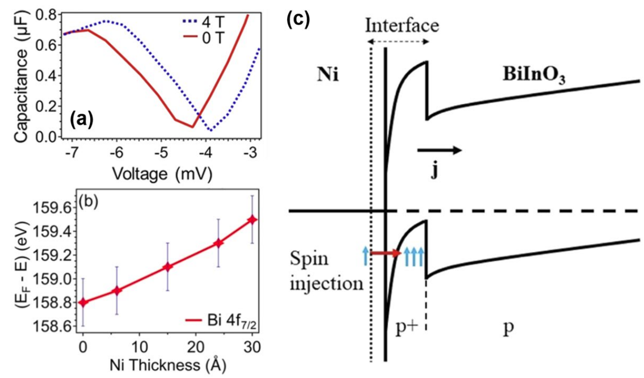

Fig. 3. (a) Room-temperature capacitance vs voltage with and without a perpendicular magnetic field applied. (b) Binding energy of Bi^{3+} $4f_{7/2}$ photoemission core levels as a function of Ni overlayer thickness on $BiInO_3$. (c) Schematic energy level diagram at the Ni to $BiInO_3$ interface.

<u>Thrust 1, Objective 1b</u> aims to probe and control topological spin textures in ferroic oxides. SI Peter **Dowben** collaborated with SIs Xia **Hong** and Robert **Streubel** and researchers at University of New South Wales to understand the polar properties of epitaxial $BiInO_3$ films on (Ba,Sr)RuO_3 buffered $NdScO_3$(110) substrates, and have quantified the magnetocapacitance effect (**Fig. 3a**). Structural characterizations show that strained $BiInO_3$ films are in the non-ferroelectric Pnma phase, which is consistent with the piezoresponse force microscopy (PFM) imaging results (meets metric).The team has showed that the formation of a p-type Schottky barrier (**Fig. 3b**) plays a critical role in the room temperature magneto-capacitance effect films, which can be explained by the tunneling induced interfacial spin accumulation at the interface between Ni and epitaxial non-polar $BiInO_3$ thin (**Fig. 3c**) (meets metric). The result demonstrates a significant magneto-capacitance effect at room temperature without involving multiferroic materials, paving the path for their applications in spintronics. This work is published in *ACS Appl. Mater. & Interfaces* (2024).

SI **Hong** group fabricated ferroelectric tunnel junctions (FTJs) with 2.8 nm and 4 nm ferroelectric Pb(Zr,Ti)O_3 (PZT) tunnel barriers sandwiched betwen a correlated metal $LaNiO_3$ (LNO) with a small bandgap Mott insulator $Sr_3Ir_2O_7$ (SIO) as electrodes (**Fig. 4a-b**) and showed that a giant a nonvolatile electroresistance (ER) of 6,500% can be achieved at room temperature by switching PZT polarization (**Fig. 4c**). Compared with previously reported all-oxide FTJs with single-layer tunnel barrier and correlated oxide electrodes, these values are one to three orders of magnitude higher than those of similar tunnel barrier thickness (**Fig. 4d**). The giant enhancement has been attributed to the polarization induced metal-insulator transition in the interfacial $Sr_3Ir_2O_7$, which leads to highly asymmetric tunnel barrier energy profile for the P_{up} and P_{down} states. The giant ER, nonvolatile, reversible switching, and superb retention make these all-oxide FTJs with narrow bandgap Mott electrodes highly competitive for nonvolatile memory and neuromorphic computing

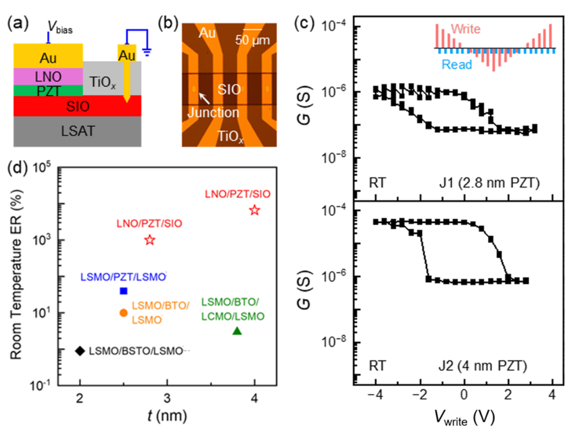

Figure 4. (a) Device schematic of LNO/PZT/SIO FTJs. (a). (b) Optical image of a sample patterned with four tunnel junctions. (c) Tunneling conductance G vs writing voltage V_{write} at room temperature for FTJs with 2.8 nm and 4 nm PZT barriers. (d) Room temperature ER vs tunnel barrier thickness t for various all-oxide FTJs.

applications. This work has been published in *Applied Physics Letters* (2024). The imaging of local tunneling current is in progress.

SI **Tsymbal** group performed theoretical modeling of the layer Hall effect and showed that it can be used to efficiently detect the Néel vector in centrosymmetric magnetoelectric antiferromagnets. This work has been published in *Physical Review Letters* (2024). SI **Zhang** has been constructing magneto-optical Kerr effect (MOKE) setup for measuring the valley polarization in tunneling devices, which is in progress.

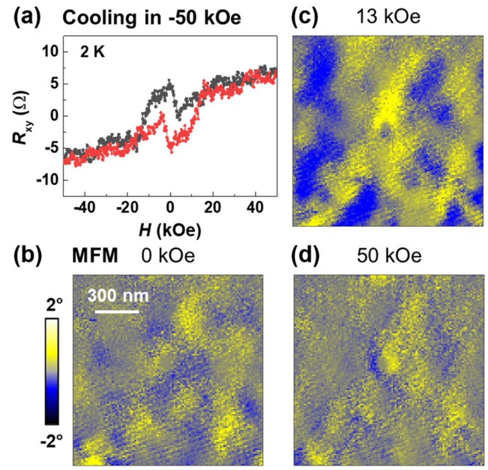

Figure 5. (a) THE in NCO membrane upon field cooling. (b-d) MFM phase imaging of NCO membrane in different magnetic fields.

SI Hong fabricated strain-free $NiCo_2O_4$ (NCO) membranes by depositing epitaxial NCO thin films on water soluble $Sr_3Al_2O_6$ buffered $LaAlO_3$ substrates followed by water etching. Magnetotransport studies showed that T_C of the sample is above 300 K. Topological Hall effect (THE) emerges in the membranes upon field cooling (**Fig. 5a**). Magnetic force microscopy (MFM) images reveal magnetic bubble domains, which only occur in the magnetic field range of the THE (**Fig. 5c-d**), providing clear evidence of their correlation (meets metric). These results show that strain can be utilized to engineer the THE response, providing critical material information for developing $NiCo_2O_4$-based topological devices.

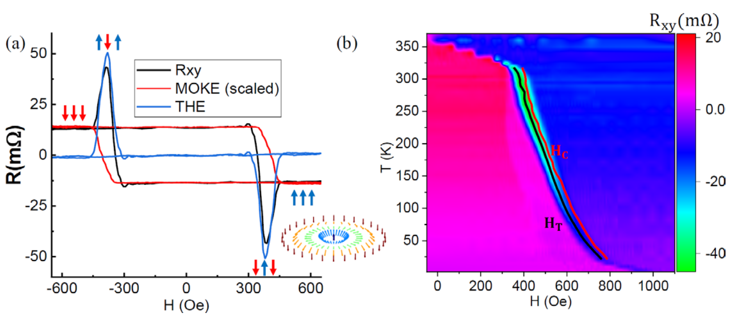

Fig. 6. (a) THE resistance extracted from the MOKE and Hall signal R_{xy} hysteresis loops. (b) Contour map of R_{xy} hysteresis loops *vs.* magnetic field and temperature.

SI **Xu** studied the giant THE as evidence of small skyrmions above room temperature in Pt/NCO Heterostructures. The bilayer system exhibits large perpendicular magnetic anisotropy, moderate exchange interaction, and modest magnetization. A giant THE has been observed across a wide temperature range 2–350 K in a Pt (3 nm) /NCO (15 nm) system (**Fig. 6**). The absence of THE in single layer Pt and NCO, and in Pt/Cu/NCO, as well as the reduction of THE in Pt/NCO of thicker NCO, suggests it originates from interfacial Dzyaloshinskii-Moriya interactions. The occurrence of THE maximum before coercivity suggests the skyrmions correspond to magnetic nucleation centers as their topological equivalence. According to the emergent-field model, the large THE in the Pt (3 nm) /NCO (15 nm) system indicates a high population density of small skyrmions, which is consistent with the apparently missing nucleation process measured by the scanning probe microscopies with a 30–50 nm spatial resolution. These results highlight heavy metal/conducting ferrimagnetic oxide thin films as a promising platform for exploring topological spin structures for spintronics applications. Theoretical modeling and electric field effect control of the THE effect are in progress.

SI **Kovalev** collaborated with FRG2 SIs **Laraoui** and **Liou** to achieve direct NV imaging of room temperature magnetic skyrmions in CoPt single layers with gradient engineered Dzyaloshinskii–Moriya interaction (DMI) (meets metric). In composition gradient-engineered CoPt single-layer films, skyrmions remain stable over a wide range of applied magnetic fields and are confirmed to be nearly Bloch-type from micromagnetic simulation and analytical magnetization reconstruction. Furthermore, we observe skyrmion pairs, which may be explained by skyrmion–antiskyrmion interactions. Our findings expand the family of magnetic materials hosting RT magnetic skyrmions by tuning g-DMI via gradient polarity and a choice of magnetic elements. This work is published in *ACS Nano* (2024).

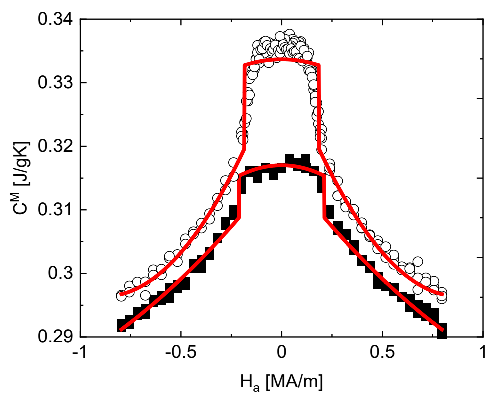

Figure 7. Magnetic field dependence of the heat capacity measured via relaxation calorimetry at T = 280K (squares) and T = 285 K (circles). Lines display single parameter best fits.

Thrust 1, Objective 1c aims to probe entanglement and correlation effect. SI **Binek** first focused on enhancing the fundamental understanding of magnetism and statistical physics, examining the high-oment (7 μ_B/atom), archetypical magnetocaloric material, gadolinium (Gd). While Gd is not considered a quantum material in the same sense as other materials studied in FRG1 such as those with topological order or strong electron-electron correlations, its properties and applications are deeply rooted in quantum mechanical principles, justifying its place in broader discussions of quantum materials. The key findings of this study are:

a) The softness of Gd gives rise to magnetic isothermal magnetic field loops which are virtually hysteresis free. This in turn enables the application of Maxwell relations from equilibrium thermodynamics in the regime of coexisting up and down domains.

b) The validity of the equilibrium thermodynamics approach is confirmed through independent measurement of the magnetic field dependence of the heat capacity.

c) Modeling of the magnetization data allows to calculate a functional description of the measured heat capacity data.

d) The study reveals that there is isothermal entropy change in the coexistence regime accompanying the demagnetization broadened first order isothermal phase transition.

e) The isothermal entropy change is associated with a non-zero adiabatic temperature change.

f) The observed effects originate from dipolar interaction and demagnetization effects in real samples with open boundaries. The entropy analysis of the fully demagnetized state suggests the presence of hitherto experimentally undetected magnetic fine structures on a scale of a few nanometers.

g) The general analytic approach which predicts the nanometric magnetic fine structure is tested with the help of a Monte Carlo simulation.

Fig. 7 shows the relaxation calorimetrically measured heat capacity, C_{H_a} vs H_a, data (symbols) for T=280 K (squares) and T=285 K (circles) together with single parameter best fits (lines) of functional forms obtained from modeling magnetization data. The result confirms that equilibrium thermodynamics can be used to determine from magnetization data the isothermal entropy change and from it the field dependent heat capacity. The entropy difference between the fully demagnetized state and the magnetic saturation can be utilized in an analytic approach to estimate correlation length scale of magnetic domains. The entropy approach is based on the assumptions that there is a vast configuration space of nearly degenerate domain structures and that the contribution of the domain wall energy to the total energy of the domain state in the presence of an applied field is small. A Monte Carlo study of a 3D Ising system with dipolar interaction and open boundary conditions allows to explore the cluster size distribution in the demagnetized state of this model system. The cluster size distribution of up magnetized clusters is utilized to calculate a typical/average cluster size and compare it with the cluster size obtained

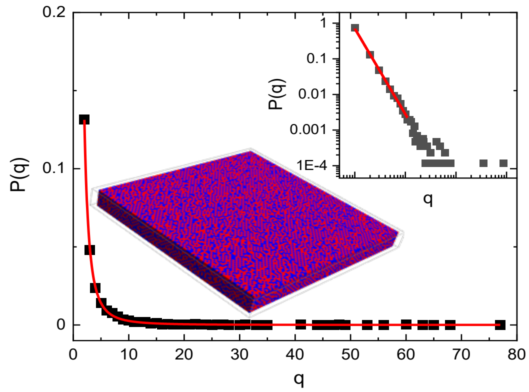

Figure 8. Cluster size distribution (squares) P versus q with P being the relative frequency of finding clusters of up spins forming connected groups of size q. Line is a best fit of a power law $P \propto q^{-s}$ with s=2.44. Inset show the same distribution in a log-log plot together with a linear best fit (line) of slope s.

from the entropy analysis validating the approach used to predict the presence of nanometer-sized magnetic structures in Gd.

Fig. 8 shows the magnetic cluster size distribution of a simulated hysteresis-free isotherm at $H_a = 0$ (squares). The distribution follows the power law behavior $P(q) \propto q^{-s}$ with q being the number of spins within a cluster and s being a temperature dependent exponent. The line shows a best fit of this power law behavior which yields $s = 2.44 \pm 0.01$. The depicted domain image shows the fully demagnetized state at T = 4K. The inset of Fig. 8 shows the corresponding log-log plot of the cluster size distribution with a linear region of slope s. This work is published in *J. Phys.: Condens. Matter* (2025).

SI **Binek** collaborated with FRG2 SI **Laraoui** to probe the domain distribution in the B:Cr_2O_3 using NV-microscopy. The NV images reveal a stronger magnetic exchange in B:Cr_2O_3 compared with the undoped chromia (meets metric). The NV imaging of voltage-enabled entanglement between chromia magnetization and NV spin is in progress.

To develop new quantum information protection platforms, SI **Kovalev** studied the superconductor/normal region/superconductor (S|N|S) Josephson junction formed using superconductors with d, $d+id'$, and $d+is$ superconducting pairings. We showed that the quality factor of the Josephson diode effect and its sign can be substantially tuned by the external magnetic field, the gate voltage, and the length of the junction for all three types of pairings (meets metric). We also identified the conditions under which the anomalous Josephson and Josephson diode effects can appear in the junction by analyzing appropriate symmetries. In particular, by breaking a π-rotation symmetry, we showed how a large field-free Josephson diode effect can be realized even in the absence of spin-orbit coupling. We also studied the role of edge states appearing in the case of chiral superconductor with $d+id'$ pairing. These results demonstrate that the Josephson diode effect in a planar geometry can be used as a signature of unconventional superconducting pairings. This work is published in *Physical Review B* (2024) and is selected as an Editors' Suggestion.

Thrust 2, Objective 2a aims to achieve magnetoelectric control of topological states in graphene. SIs **Binek** and **Dowben** obtained evidence of edge-state transport in graphene-on-chromia heterostructures in the absence of any external magnetic field, which result from the presence of substrate-induced spin-orbit coupling (SOC) in graphene. Low-temperature measurements in the non-local spin-Hall geometry reveal large ($\gg h/e^2$) resistance fluctuations as the Fermi level is swept through the graphene bands. The non-local features persist to much higher temperatures (> 60 K) than is typical for mesoscopic effects in normal metals and semiconductors (**Fig. 9**). They are moreover invariant to the application of magnetic fields as high as 7 T, pointing to the presence of edge-like modes. *T*. Spectroscopy studies of the Néel vector orientation and general spin structures and spin switching in chromia is in progress.

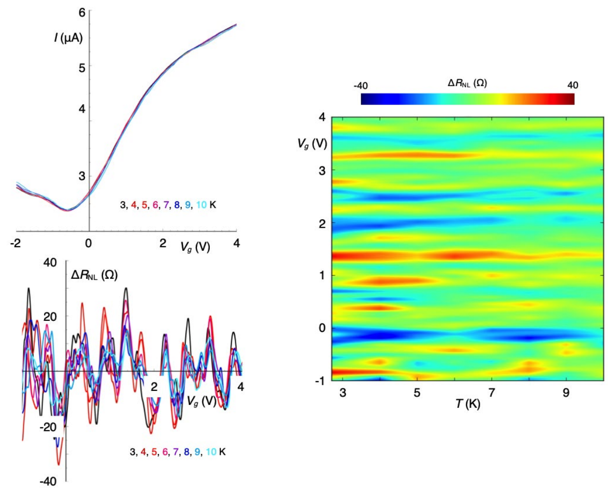

Figure 9. The variation of the non-local resistance, measured as a function of back-gate voltage at the left and temperature at the right. The quantum fluctuations in the non-local signal die out beyond 60 K, but are remarkably persistent up to 10 K.

SIs **Kovalev** and **Tsymbal** have predicted elliptical skyrmions and antiskyrmions and magnetoelectric control in 2D stacked CrI_3. Unlike the widely investigated skyrmions, antiskyrmions are rarely observed due to the required anisotropic DMI. We proposed that van der Waals (vdW) assembly of two-dimensional (2D) materials can break inversion symmetry and create conditions for anisotropic DMI. Based on density-functional theory (DFT) calculations, we predicted that polar layer stacking of two centrosymmetric magnetic monolayers of CrI_3 efficiently lowers 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 control of antiskyrmions by an electric field (meets metric). Furthermore, we showed that the magnetocrystalline anisotropy and DMI of CrI_3 can be efficiently modulated by Mn doping, creating a possibility to control the size of antiskyrmions. Using atomistic spin dynamics simulations with the parameters obtained from our DFT calculations, we predicted the formation of antiskyrmions in a $Cr_{0.88}Mn_{0.12}I_3$ bilayer and switching their spin texture with polarization reversal. Our results open a direction to generate and control magnetic antiskyrmions in 2D vdW magnetic systems. This work is published in *Physical Review B* (2024) and selected as an Editors' Suggestion.

SI **Dowben** studied the band structure of the transition metal dichalcogenides 2H-MoS_2(0001) through high resolution angle resolved photoemission (ARPES) (**Fig. 10**). ARPES of palladium adsorbed on 2H-MoS_2(0001), at a Pd film thickness of 5 monolayers, shows good agreement with the expectations of theory. The study of Au on MoS_2(0001) is in progress.

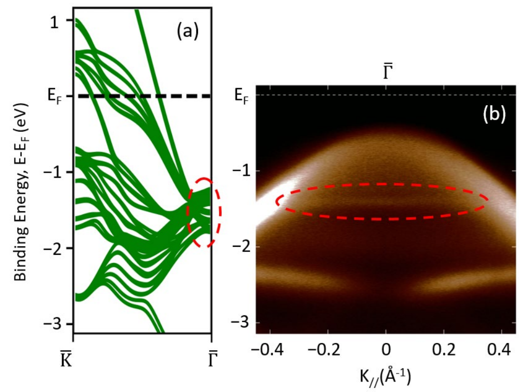

Figure 10. The electronic band structure of 5 monolayers of palladium on 2H-MoS_2(0001) crystal along $\overline{\Gamma}-\overline{K}$ direction. (a) DFT calculation. (b) Experimental band structure of 10 Å palladium on 2H-MoS_2(0001) crystal.

__Thrust 2, Objective 2b__ aims to explore emergent 2D materials for designing valley spin valves. SI **Tsymbal** has predicted the material choice of 2D non-volatile valley spin-valve (VSV). VSV utilizes a valley degree of freedom to modulate the spin configuration at the Fermi surface and create a spin valve. Valleys are separated energy extrema in the electronic band structure in the momentum space. A non-volatile VSV (n-VSV) based on 2D ferroic materials exhibiting valley spin polarization can potentially serve as the key element of low-power non-volatile memories and logic. The 2D ferroelectric 1H or 2H MoS_2 was identified as a promising candidate for realizing the n-VSV. The FRG3 SI **Sinitskii** collaborated with SI Tsymbal to demonstrate experimentally that a ferroelectric 1T'' phase of MoS_2. **Tsymbal** performed DFT and quantum transport calculations to show that the conductance ON/OFF ratio, $\eta = (G_{\mathrm{UP}} - G_{\mathrm{DW}})/G_{\mathrm{DW}}$, where G_{UP} and G_{DW} are conductance for the UP (ON) and DW (OFF) states, respectively, can reach as high as ~10^7 above the bandgap and ~10^6 below the bandgap in the presence of a domain wall due to locking between the spin and electric polarization and represents the key property of an n-VSV (**Fig. 11**). This advancement paves a new route for more energy-efficient and high-performance valleytronic devices, highlighting the importance of 2D ferroelectrics in future electronic applications. The fabrication of the VSV device by the Hong group is in progress.

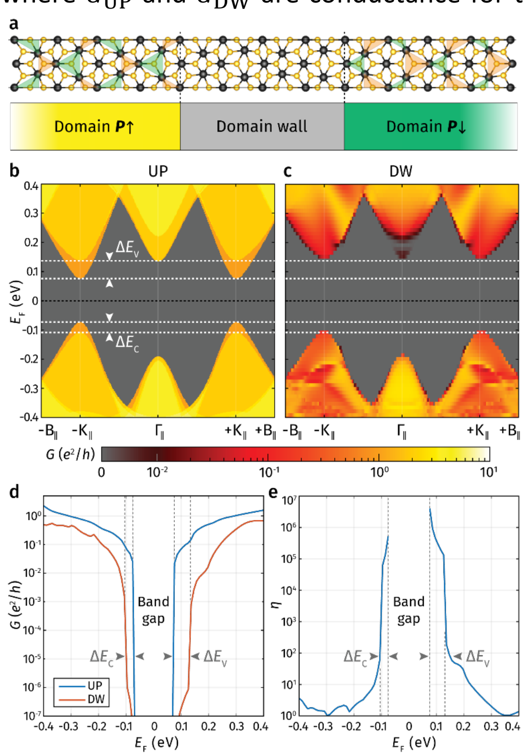

Figure 11. (a) Schematic n-VSV structure. (b,c) Conductance of the n-VSV in UP state (b) and DW state (c) *vs.* Fermi energy E_{F} and electron momentum perpendicular to the transmission direction ($k_{\parallel}$). (d) Total conductance as a function of E_{F} for the UP and DW states. (e) ON/OFF ratio as a function of E_{F}.

SI **Guo** spatially resolved ferroelastic domain structures in halide perovskites. As ferroelastic twin domain walls can guide internal reflections optically, domain wall imaging was achieved using unpolarized light (meets metric). This finding can lead to potential application in nonvolatile, switchable, position tunable guide for energy transport in perovskite optoelectronics. The study of substrate screening of carrier dynamics is in progress.

__Thrust 3, Objective 3__ aims to develop molecular system-based materials platforms for spin-qubit systems. The response SI **Streubel** collaborated with SIs **Lai** and **Dowben** shows that optical excitations of the ligand to metal charge transfer state can lead to conductance changes in tautomeric molecular Co spin crossover molecule (SCO) complexes (meets metric). The excitation is absence in red light while enabled by incandescent light, as the latter includes shorter wavelength light. The results was assessed by the conductance change at higher T . SIs **Guo** and **Lai** further explored optical driven spin crossover behavior in [Fe(Htrz)2(trz)](BF_4). The team also examined the impact of adding magnetic nanoparticles to spin-crossover polymer films to control the electronic transport properties. The team discovered that the magnetic nanoparticles couple either ferromagnetically or antiferromagnetically to the spin-crossover molecules, depending on the used molecular structure (meets metric). Initial magneto-transport measurements reveal a signature that may originate from this exchange coupling stimulating further detailed analysis of both longitudinal and transverse resistivity. The quantification of the exchange coupling is in progress.

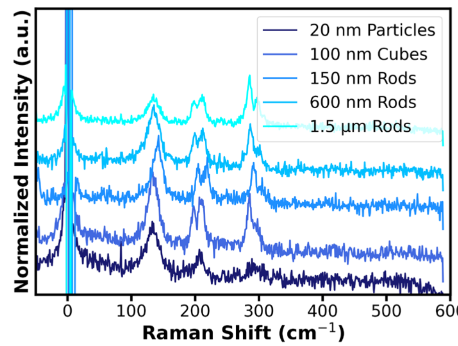

Figure 12. Size dependent collective structural dynamics, with intermolecular relaxational continuum below 100cm^{-1} and intramolecular metal-ligand vibrations from 100-300cm^{-1}.

SI **Guo**, in collaboration with SI **Lai**, identified vibrational signatures of spin states in spin-crossover (SCO) complexes using Raman spectroscopy, using Raman spectra of SCO complexes as optical readout of its spin state (meets metric). Their collaboration tuned the grain size of the SCO complexes via control of the crystallization process. Our low-frequency Raman spectroscopy provided access to collective lattice motion. We observed size-dependent collective structural dynamics (**Fig. 12**). The relaxational spectral continuum was pronounced in 20nm nanoparticles and absent in 1.5mm rods of the SCO complex crystal. At the same time, we observed the metal-ligand bond vibrational mode show broadened single mode in 20nm nanoparticles and clear split modes in 1.5mm rods. The correlated spectral signatures of intermolecular and intramolecular structural dynamics provided a detailed picture of how synthesis modifications affect cooperativity.

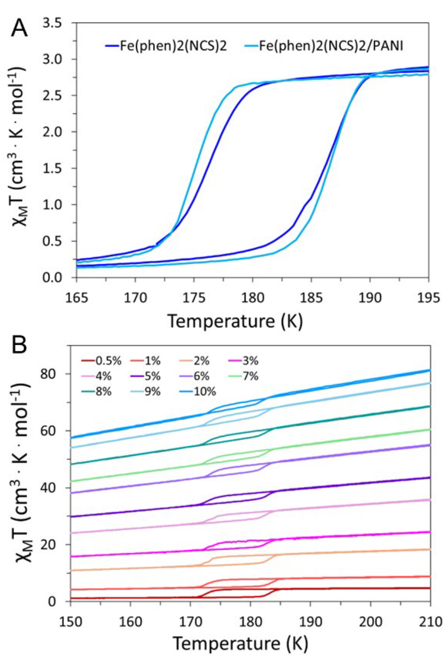

Figure 13. Temperature-dependent magnetic susceptibility of (a) $Fe(phen)_2(NCS)_2$ and $Fe(phen)_2(NCS)_2$/PANI bi-composite, and (b) $Fe(phen)_2(NCS)_2$/PANI/Fe_3O_4 tri-composites. The concentration range of Fe_3O_4 was from 0.5 to 10%.

SI **Lai** engineered SCO for devices with improved device characteristics using the strategies of combining appropriate SCO complex with a conducting polymer such as polyaniline (PANI) to create thin films that are less dielectric and thus better suited for device applications. We are interested in employing $Fe(phen)_2(NCS)_2$, an Fe(II) SCO complex with a well-defined and reversible low spin (LS) to high spin (HS) transition at ~187 K with hysteresis (**Fig. 13a**) for fabricating nonvolatile voltage controlled memory devices. However, the relatively high resistance of this SCO thin film has been a key impediment to creating a competitive memory device. To circumvent this, we incorporated PANI and Fe_3O_4 nanocomposites to engineer the conductivity and transition temperature of the SCO (**Fig. 13a-b**). Next, we will compare the behavior of the $Fe(phen)_2(NCS)_2$ tri-composites with the [Fe(Htrz)$_2$(trz)](BF_4) tri-composites we previously developed. The fabrication of SCO devices with improved characteristics is in progress.

SI **Guo** observed an optical hysteresis in spin crossover behavior that does not conform with standard mechanisms of photo-induced SCO phenomena: the SCO power threshold remained similar regardless of base temperature, which pointed to a non-thermal spin transition. Yet the width of the hysteresis loop reduced as base temperature decreases, which behaves opposite to the widely discussed light-induced excited state spin trapping (LIESST) mechanism. This unique observation may suggest an interplay between collective lattice motion and spin state transitions. We also observed a spin-state dependent reactivity of the [Fe(Htrz)2(trz)](BF4) complex with molecular oxygen. The reactivity of the SCO complex is changed by orders of magnitude by only the low spin to high spin transition. This observation may point to new strategies of spin control of interfacial electron transfer rate. The tuning of the structure and structural dynamics of SCO complexes using high pressure conditions generated inside a diamond anvil cell (DAC) is in progress.

The UNL Physics Department has successfully recruited a new faculty as part of EQUATE FRG1. Dr. Zuocheng **Zhang** is collaborating with SIs **Tsymbal** and **Hong** for optical spectroscopy studies of the tunneling anomalous Hall effect and valley spin valves in van der Waals heterostructures (meets metric).

In pursuing FRG1 research, team members also noted the following **Changes/Problems:**

- The project on oxides with persistent spin texture is concluded. The polar structure is not thermodynamically stable. In Year 5, the SIs will expand the efforts on realizing topological spin textures in complex oxides.
- The project on theoretical modeling of quantum spin fluctuation and field-gradient manipulation and quenching of quantum states in graphene on chromia is concluded. The graphene mobility on chromia is not sufficiently high for quantum transport studies. In Year 5, the SIs will expand efforts on theoretical modeling of chiral spin textures.
- Molecular magnets' film quality was insufficient to perform reliable electronic transport and ferromagnetic resonance spectroscopy measurements. In Year 5, SIs will expand efforts on SCO molecules.

Beyond the research above, FRG1 team members achieved the following **Other Accomplishments:**

- Over the past project year, EQUATE FRG1 research has been disseminated via more than 30 peer-reviewed papers, 1 patent, and over 30 conference presentations (meets metric).
- Approximately 12 graduate students, 6 undergraduate students, and 5 postdocs have been trained on modern computational techniques based on density functional theory and atomistic magnetic simulations and advanced experimental techniques, including materials synthesis, electron/x-ray diffraction/spectroscopy, PFM, MFM, FMR, Raman, MOKE, and magnetotransport, as well as data analysis, conference presentation, and paper writing.
- FRG1 graduate students Yifei Hao, Tianlin Li, Bo Zhang, and Kai Huang graduated with Ph.D. degrees.
  - In April 2024, Yinsheng Guo received NSF's CAREER Award. His award (#2339721), for $648,335, is titled, CAREER: Structural dynamics and optoelectronics of anharmonic soft semiconductors and will continue through 2029.
- Two undergraduate students co-authored a paper for EQUATE research: Ruthi Zielinski, Nhat Nguyen, **Robert Streubel**, *et al.*, *J. Phys.: Condens. Matter* 37, 045802 (2025).
- A team with **Guo** lab participants Andrea Phan and Bo Zhang was selected as an Explore Phase competitor in EnergyTech University Prize 2024 (EnergyTech UP 2024), organized by U.S. Department of Energy's Office of Technology Transitions (DOE OTT). They represented University of Nebraska-Lincoln among 117 competing schools and 225 teams.
- Two EQUATE-hosted REU undergraduate students participated in FRG1 research and presented posters at the Nebraska Summer Research Symposium in August 2024.

FRG2 – Quantum Technologies (EQUATE Year 4: June 2024 – May 2025)

The goals of FRG2 explore different quantum technologies based on solid-state spin qubits for quantum sensing and metrology, and photons for ultrafast, compact, and low-power quantum communication nanophotonic devices. The FRG is divided into two research thrusts. Thrust 1 (**Laraoui**, **Liou**, **M. Schubert**) focuses on studying spin-magnon interactions in magnonic waveguides, exploring hyperpolarization using hybrid diamond quantum sensors with ferromagnetic nanoparticles (FMN) for low-field (LF) magnetic resonance spectroscopy, and investigating new quantum defects in ultra-wide bandgap (UWBG) semiconductors. Thrust 2 (**Kilic**, **E. Schubert**, **Laraoui**) explores hybrid nanoscale optical nanostructures for generating single photon sources and entangled photon pairs. During Year 4, FRG2 investigators collaborated extensively with investigators from other thrusts in FRG2 and FRG1 (**Binek**, **Xu**, **Lai**, **Hong**, **Kovalev**). The scientific and educational achievements are detailed below.

In the area of **Thrust 1, Objective 1.a: Quantum Sensing and Metrology, Probing Spin-Magnon Interactions in Ferromagnetic (FM) Waveguides** is on track to meet its Year 4 commitment and made the following progress:

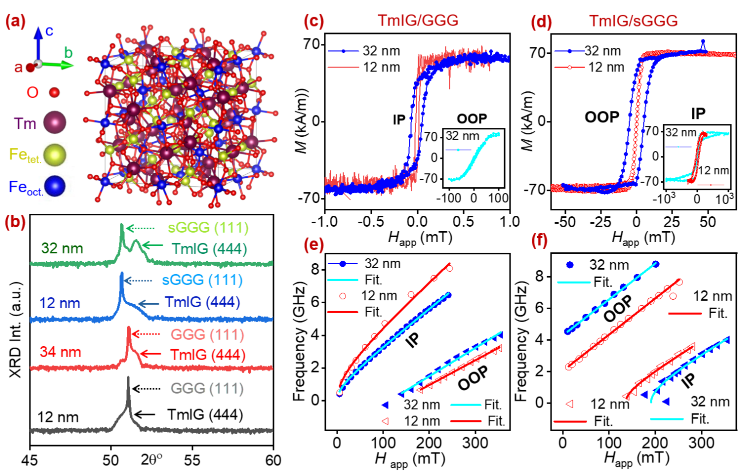

Figure 14. (a) schematic of the complex unit cell of TmIG showing tetrahedral Fe (light green) and octahedral Fe (blue) lattice along Tm (purple) and O (red) atoms. **(b)** Measured XRD spectrum of TmIG films (thickness of 12 – 32 nm) grown on 0.5 mm thick GGG and sGGG substrates. (c) IP *M-H* loops of TmIG (32 nm)/GGG (blue filled circles) and TmIG (12 nm) /GGG (red solid line). Inset of (c) OOP loop of TmIG (32 nm)/GGG (sky blue filled circles). (d) OOP *M-H* loops of TmIG (32 nm)/sGGG (blue filled circles) and TmIG (12 nm) /sGGG (red open circles). Inset of (d) IP loop of TmIG (32 nm)/sGGG (sky blue filled circles) and TmIG (12 nm)/sGGG (red open circles). (e) FMR IP curves of TmIG (32 nm)/GGG (blue filled circles) and TmIG (12 nm) /GGG (red open circles), and FMR OOP curves of TmIG (32 nm)/GGG (blue filled triangles) and TmIG (12 nm)/GGG (red open triangles), respectively. (f) FMR OOP curves of TmIG (32 nm)/sGGG (blue filled circles) and TmIG (12 nm) /sGGG (red open circles), and FMR IP curves of TmIG (32 nm)/sGGG (blue filled triangles) and TmIG (12 nm)/sGGG (red open triangles), respectively. All IP and OOP FMR measured curves are fitted with solid lines.

In Year 4, **Laraoui** collaborated with **Xu** (FRG1) to study the effect thickness and substrate on spin-wave (SW) propagation properties in Thulium Iron Garnet ($Tm_3Fe_5O_{12}$:TmIG) thin films. TmIG has attracted an increasing interest recently in spintronics and magnonics applications. TmIG has a ferrimagnetic behavior, originating from the super-exchange interactions between Tm^{+3} (Dodecahedral, Dod), Fe^{+3} (Tetrahedral, Tet), and Fe^{+3} (Octahedral, Oct) sublattices (see **Fig. 14a**). A series of TmIG thin films, with a thickness of 7 – 34 nm (deduced from x-ray reflectometry) were grown on (111) $Gd_3Ga_5O_{12}$ (GGG) and substituted GGG (sGGG) substrates, using pulsed laser deposition. **Fig. 14b** shows X-Ray diffraction (XRD) spectra for TmIG films of thicknesses 32 nm and 12 nm grown on GGG and sGGG substrates. For all TmIG films grown on GGG, the TmIG (444) peak is submerged within the GGG (444) peak due to the small lattice mismatch and/or the weak XRD signal obtained on thin (< 15 nm) films. The lattice mismatch between TmIG and sGGG is higher, resulting in distinct XRD peaks of TmIG and sGGG. The magnetic anisotropy for all TmIG films grown on GGG and sGGG substrates was investigated by vibrating-sample magnetometer (VSM) and Ferromagnetic resonance (FMR) spectroscopy. **Fig. 14c** shows in-plane (IP) *M-H* hysteresis loops of TmIG (32 nm)/GGG and TmIG (12 nm)/GGG films with a low saturation magnetic field ~1 mT. Out-of-plane (OOP)

M-H hysteresis loop is plotted in the inset of **Fig. 14c** for TmIG (32 nm)/GGG film with a saturation field ~100 mT and saturation magnetization M_S of 66 kA/m. No OOP VSM signal was detected from the TmIG (12 nm)/GGG film due to insufficient sensitivity. The VSM measurements confirm an in-plane easy axis for the TmIG films grown on GGG substrates, consistent with MOKE measurements (not discussed here). **Fig. 14d** displays OOP *M-H* hysteresis loops of TmIG (32 nm)/sGGG and TmIG (12 nm)/sGGG films with a saturation magnetic field ~30 mT and 10 mT, respectively, and M_S of 70 kA/m. Inset of **Fig. 14d** depicts IP *M-H* loops for TmIG (32 nm)/sGGG and TmIG (12 nm)/sGGG with a saturation magnetic field of 1 T and 0.3 T, respectively. The VSM measurements on TmIG/sGGG films confirm out-of-plane easy axis and perpendicular magnetic anisotropy (PMA). **Fig. 14e** shows IP and OOP FMR resonance vs H_{app} for TmIG (32 nm)/GGG and TmIG (12 nm)/GGG films. The resonance magnetic field is higher for OOP than IP measurements on TmIG/GGG films for the same FMR frequency, suggesting in-plane magnetic anisotropy. However, TmIG/sGGG films have the opposite behavior, *i.e.*, the resonance magnetic field is higher for IP than OOP measurements, suggesting PMA. The IP and OOP measurements in **Fig. 14e** and **Fig. 14f** were fitted with solid lines leading to gyromagnetic ratio γ of 22.4 GHz/T and M_S of 66 kA/m for TmIG (32 nm)/GGG film and γ of 22.87 GHz/T and M_S of 66 kA/m for TmIG (12 nm)/GGG film. For the TmIG/sGGG films, the linear fit of the OOP measurements in **Fig. 14f** gives M_s = 70 kA/m^{-1} (for both 12 nm and 32 nm films), a negative H_{app}-intercept of -198 mT and -99 mT for 32 nm and 12 nm films, respectively. The out-of-plane magnetic anisotropy values are 286 mT and 187 mT for 32 nm and 12 nm thick TmIG/sGGG films.

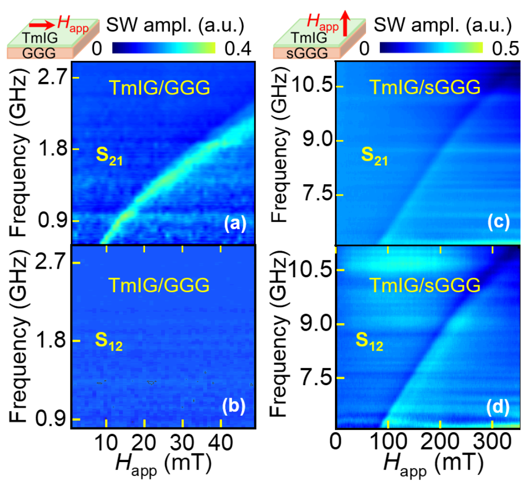

Figure 15. S_{21} **(a)** and S_{12} **(b)** intensity maps (MW frequency *vs* H_{app}) on TmIG (12 nm)/GGG films. S_{21} **(c)** and S_{12} **(d)** intensity maps (MW frequency *vs* H_{app}) for FVSWs propagation on TmIG (32 nm)/ sGGG at a separation distance S of 32 µm.

To measure the spin-wave transport properties of the TmIG films, SW electrical transmission spectroscopy was performed in the magnetostatic surface spin waves (MSSW) geometry, *i.e.*, H_{app} is applied in-plane and perpendicular to the SW propagation wavevector. The spin waves are excited by the microwave (MW) field, injected through the picoprobe to the CPW antennas to measure S_{21} and S_{12} parameters. **Fig. 15a** shows the S_{21} intensity map (MW frequency *vs* H_{app}) of MSSWs measured at a propagation distance S of 32 µm and at a MW power of 1 mW. One dominating SW mode is clearly seen with a wavevector k of 0.2 rad.µm^{-1}, given by the GSG geometry of the stripline. **Fig. 15b** depicts the S_{12} intensity map (MW frequency *vs* H_{app}) of MSSWs measured at a propagation distance S of 32 µm and at a MW power of 1 mW. No signal was observed due to the nonreciprocity behavior, explained by the difference in amplitude and of the CPW antenna produced stray magnetic fields along y (H_y) and z (H_z) directions. TmIG films grown on sGGG substrates have PMA (discussed above), and no SW transmission is observed in plane (*i.e.*, MSSW geometry). **Figs. 15c** and **15d** show the SW S_{21} and S_{12} intensity maps (MW frequency *vs* H_{app}) of TmIG (32 nm)/sGGG, respectively, measured in forward volume spin waves (FVSW) geometry (*i.e.*, magnetic field is applied perpendicular to the sample plane) at a propagation distance of 32 µm and MW power of 1 mW. The amplitude of the measured FVSW is weak in comparison to the MSSW measured on TmIG (12 – 34 nm)/GGG films. This can be explained by the large separation distance (3.5 µm) between the CPW antenna, compared to the short wavelength (< 500 nm) of the FVSWs, resulting in inefficient MW excitation. Indeed, the S_{21} parameter shows similar resonance and amplitude to S_{12} at 142 mT suggesting a bidirectional propagation of FVSWs. Similar strength and amplitude of S_{11} and S_{22} reflection spectra.

In addition to TmIG, we explored new magnetic materials/waveguides based on two dimensional magnets (2D) $CrTe_2$. Initial FMR measurements reveal low FMR frequencies (down to ~ 1 GHz) and Gilbert damping constant *α* of 0.08 in comparison to the undoped $CrTe_2$ with FMR frequency above 4 GHz and a damping constant *α* of 0.05. In collaboration with **Hong** (FRG1), we are studying the magnon properties of CrC_3 flakes using NV qubits in diamond at variable temperatures (3-300 K) with the goal to control its properties using multiferroic lead zirconate titanate (PZT) materials (meets metric).

Laraoui in collaboration with **Xu** (FRG1) studied the effect of thickness and substrate on the spin-wave properties of magnetic insulator TmIG thin films. **Laraoui** collaborated with **Hong** (FRG1) and studied the local magnetic properties of CrC_3 flakes using NV centers in diamond at variable temperatures (3 – 300 K).

With EQUATE FRG2 research, **Laraoui** trained a postdoc and a UNL freshman undergraduate student on cryogenic NV experiments on CrC_3 flakes. **Laraou**i and his students (PhD and undergraduate) gave multiple contributed talks and posters at local workshops, plus national meetings like the 2025 Joint MMM-Intermag and the joint March Meeting and April Meeting: Global Physics Summit 2025 (specifics provided in EQUATE Year 4 EDOCS reporting); this includes **Laraoui**'s two invited talks on studying Nanoscale Magnetic Phenomena in Magnetic Materials Using Diamond Quantum Sensing Microscopy at Single Photon Emitters and Spin-Based Quantum Sensors workshop at Oak Ridge National Laboratory and at the joint March Meeting and April Meeting: Global Physics Summit 2025. In addition, an EQUATE FRG2 team published a paper in *Advanced Electronic Materials* (IF = 7.65), titled "Effect of substrate on spin-wave propagation properties in ferrimagnetic thulium iron garnet thin films."

EQUATE FRG2's **Objective 1.b - Quantum Sensors for Low Field Magnetic Resonance Spectroscopy**, is on schedule to meet its commitments. During year 4 **Laraoui** and **Liou** used NV-low field magnetic resonance (LFMR) spectroscopy to study methemoglobin (MetHb, **Fig. 16a**) proteins synthesized by **Lai** (FRG1). Hemoglobin (Hb) is a multifaceted protein, classified as a metalloprotein, chromoprotein, and globulin. It incorporates iron, which plays a crucial role in transporting oxygen within red blood cells. Hb functions by carrying oxygen from the respiratory organs to diverse tissues in the body, where it releases oxygen to fuel aerobic respiration, thus supporting the organism's metabolic processes. Hb can exist in several forms, primarily distinguished by the oxidation state of the iron in the heme group, including MetHb. Measuring the concentration of MetHb is crucial because it cannot transport oxygen, hence higher concentration of MetHb in the blood causes methemoglobinemia. The Fe^{+3} spins in MetHb nanoclusters generate a fluctuating magnetic field that interacts with NV spins via dipolar magnetic interactions and increases its relaxation rate G_1, which depends on the dipolar interaction strength between Fe^{+3} and NV spins and the fluctuation rate of the Fe^{+3} spins as follows:

$$\Gamma_1 = \frac{2\langle B^2\rangle f_t}{f_t^2 + D^2}$$

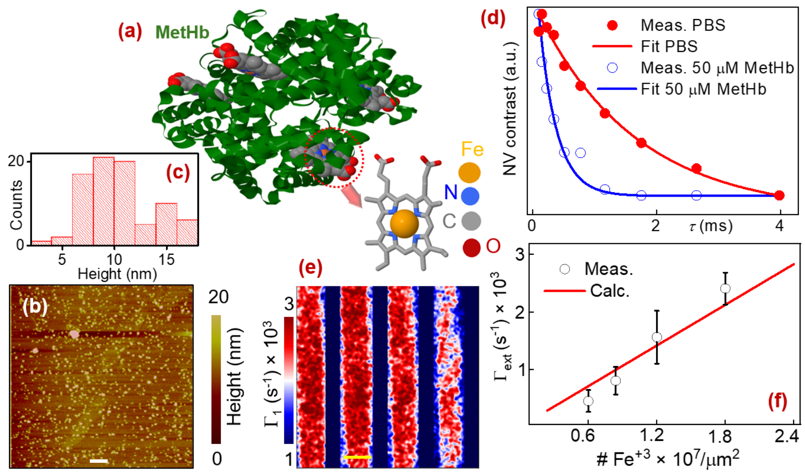

Figure 16: (a) Ribbon structure of Hb complex with the zoomed molecular structure showing the heme center. **(b)** AFM image of the MetHb nanoclusters. The scale bar in (b) is 1 mm. **(c)** AFM height distribution of the MetHb nanoclusters (concentration of 2 mM) drop-cased on top of the diamond substrate. **(d)** Measured NV contrast as function of t for a diamond with PBS (filled circles) and MetHb solution with a density of 50 μM (open circles). The measurements were fitted with exponential decay function (solid lines). **(e)** Γ_1 image of MetHb nanoclusters drop-casted on diamond with Fe^{+3} spins concentration of 1.8 × $10^7/\mu m^2$. The scale bar in (e) is 5 μm. **(f)** Measured (open circles) and calculated (solid line) Γ_{ext} as function of the density of Fe^{+3} spins in Hb adsorbed on diamond.

The concentration of MetHb was varied from 30 μM to 100 μM in a phosphate-buffered saline (PBS) buffer on a diamond chip. MetHb proteins were diluted in DI water (concentration of 2 mM with a pH of 7.60), drop-casted on the diamond surface. Atomic force microscopy (AFM) was used to measure the size and height of MetHb nanoclusters as shown in **Fig. 16b)**. The MetHb size analysis shows a variation of the nanocluster's diameter from 50 to 200 nm, whereas the height distribution shows an average height of ~ 10 ± 6 nm (see **Fig. 16c**). The diameter of MetHb in its physiological state is reported to be 5 nm that varies depending on the pH values. Prior to measuring MetHb diluted in a PBS buffer solution, NV relaxation spectroscopy on diamond was performed with (G_{bar} =1.1 × 10^3 s^{-1}) and without PBS (G_{buf} = 0.8 × 10^3 s^{-1}) at different locations using APD connected to the oscilloscope for T_1 spectroscopy readout. The variation of G_1, which is found to be ~ 20%, comes primarily from the inhomogeneous distribution of NVs within the diamond substrate, which can modulate the charge state of the NV centers and the phonon bath surrounding them, respectively. Next, NV T_1 relaxometry measurements on MetHb in a PBS solution were performed. G_1 is increased to 3.5 × 10^3 s^{-1} after adding 50 μM MetHb, **Fig. 16d**, explained by the increased spin noise due to Fe^{+3} spins. The equation in **Fig. 17** is used to fit the relaxation rate G_1 for the MetHb/PBS solution of various concentrations. For estimating the external relaxation rate, the relaxation rate of the PBS buffer G_{buf} was subtracted. In our calculation, the variance $\langle B^2 \rangle$ was derived from only the dipolar coupling between NV spins and Fe^{+3} spins present in MetHb as a variable parameter. This dipolar coupling field strength amounts to 0.27 mT for a concentration of 100 mM which gives a relaxation rate of 6.7 × 10^3 s^{-1}.

In the second set of the experiments, the relaxation rate induced by dried MetHb nanoclusters was imaged by using NV relaxometry. MetHb diluted in DI water was drop-casted on the diamond substrate similar to **Fig. 16b**. **Figure 16e** shows Γ_1 images of diamond with SiN grating with MetHb proteins adsorbed onto the diamond surface with a Fe^{+3} spin density of 1.8 ×$10^7/mm^2$. The region with SiN grating gives the intrinsic relaxation rate of G_{int} of the bare diamond, *i.e.*, surface effects reduced. **Fig. 16f** shows the G_{ext} plotted against the spin density demonstrated by open circles. The theoretical dependence (solid line in **Fig. 16f**) of G_{ext} *vs* the density of Fe^{+3} adsorbed centers per 1 mm^2 was calculated by using the equation in **Fig. 16**. For theoretical estimation, the variance $\langle B^2 \rangle$ obtained from the dipolar coupling of NV spins and external spins was kept as a free parameter. The dipolar coupling field strength is 0.107 mT and the fluctuation rate of MetHb is 0.5 GHz for the spin density of 1.7 × 10^7 Fe^{+3} adsorbed/ mm^2.

Also with this work, **Laraoui** developed additional NV-low field magnetic resonance (NV-LFMR) including NV-NMR with the goal to perform NV-NMR on single cells. Further, **Laraoui** trained a UNL PhD student in

LFMR and quantum biosensing. Within EQUATE FRG2, **Laraoui and Liou** groups hd weekly group meetings where students (5 graduates and 3 undergraduates) and a postdoc learn new aspects of quantum sensing technologies. This collaboration, in addition with FRG1's **Lai** (FRG1), submitted an abstract on NV sensing of MetHb nanoclusters for oral presentation (accepted) to be presented by an EQUATE graduate student at the joint March Meeting and April Meeting: Global Physics Summit 2025. This work has met its Year 4 metrics and improved the sensitivity and spectral resolution of LF-NV MR imaging setup by using FMN.

Additionally in this area, FRG2 is proud to note that a paper titled "Magnetic Relaxometry of Hemoglobin by Widefield Nitrogen-Vacancy Microscopy of MetHb" was published in the high impact factor (4) journal at *Applied Physics Letters*. And FRG2 PhD student, Suvechhya Lamichhane, presented a poster at the 28th NSF EPSCoR National Conference.

With **Objective 1.c Characterizing new solid-state Qubits in Ultrawide Band Gap semiconductors**, FRG2 successfully analyzed frequency-field scanning THz-EPR ellipsometry on EPR transitions in UWBG semiconductors and began developing dual-frequency THz modulation instrumentation for new THz

(a)

$$\boldsymbol{\mu} = \boldsymbol{I} + \sum_{j=1}^{2S} \begin{pmatrix} \frac{\chi_{0,j}\omega_{0,j}^2}{\omega_{0,j}^2-\omega^2} & i\frac{\chi_{0,j}\omega\omega_{0,j}}{\omega_{0,j}^2-\omega^2} & 0 \\ -i\frac{\omega\omega_{0,j}}{\omega_{0,j}^2-\omega^2} & \frac{\chi_{0,j}\omega_{0,j}^2}{\omega_{0,j}^2-\omega^2} & 0 \\ 0 & 0 & \chi_{0,j} \end{pmatrix}$$

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(b)

$$\mu_{\mathrm{dc}} = \prod_{j=1}^{2S} \frac{\omega_{\mathrm{LO}}}{\omega_{\mathrm{TO}}}$$

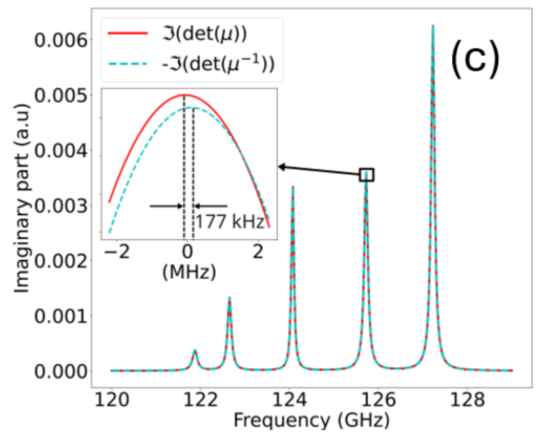

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Fig. 17. (a) Bloch equations for the magnetic susceptibility of for an ensemble of spins S as a function of frequency, derived by the Schubert team. (b) The analogue of the Lyddane-Sachs-Teller relationship originally derived fro dielectric resonances, here derived by the Schubert team for magnetic resonance. Notably, this relationship predicts the existence of longitudinal optical (anti-resonance) magnetic frequencies, which were also discovered by the Schubert team in Fe-doped GaN (c). The difference between resonance ("TO") and anti-resonance ("LO") frequency leads to splitting observable in the magnetic permeability and inverse permeability functions, which the team were able to measure for the first time. The results are accepted in Physical Review Letters and will be highlighted as Editor's Suggestion.

electron double magnetic resonance methods. The **Schubert** group published their paper reporting on the Fe-doped monoclinic gallium oxide results obtained using the newly developed frequency-scanning THz EPR ellipsometry setup [Phys. Rev. B 109, 214106 (2024)]. The paper was highlighted as an Editor's Suggestion. The group also published a seminal work on derivation of the Bloch equations for THz magnetic resonance ellipsometry [Phys. Rev. B 110, 054413 (2024)]. This paper derives and describes correct use for the first time of the frequency dependence of the magnetic resonance and its fundamental polarization properties which were unknown prior to this work. In another seminal paper likely to become history in the foundation of physics, the Schubert team published a paper discovering the magnetic Lyddane-Sachs-Teller relationship and demonstrating the existence of magnetic resonance loss modes. The paper is published in Phys. Rev. Lett. in January 2025 and highlighted as Editor's Suggestion. The **Schubert** group also investigated potential quantum emitters in UWBG metal oxides. **Fig. 17**. depicts a summary of the results published in the two important works by this team. Measurements are ongoing on Cr, Cu, Co, Cs, SI, and Al doped and co-doped Gallium Oxide and Sn and Ge doped AlGaO alloys in epitaxial layers. This research has met metrics and is on schedule for further work.

Also in this area, FRG2 advances in prototype frequency-scanning THz-EPR ellipsometer setup can be explored for further use in dual-frequency modulated THz EPR modes. The **Schubert** team is prototyping circuit boards and instrumentation to perform electron double nuclear resonance at THz frequencies (THz ENDOR-Ellipsometry). New potential quantum qubits are continued to be investigated including doped AlN, AlGaN, and Ga_2O_3 secured from collaborators at Lund University, Sweden, Leibniz IKZ Berlin, and UCSB. **M. Schubert** continued to work as organizing member of the AVS technical group Spectroscopic Ellipsometry at AVS 70 in Tampa, FL. **M. Schubert** was reappointed Commissioning Editor for Applied Physics Letters. **M. Schubert** is the recipient of a prestigious guest professorship in the Swedish Wallenberg Initiative for Sustainable Energy (WISE Professor, wise-materials.org) and will be appointed guest professor for four years at the Physics Department in Lund University, Sweden starting January 2025.

Regarding team development, FRG2 graduate student Ian Green continued development of THz EPR ellipsometry instrumentation at UNL in **M. Schubert**'s group. **M. Schubert** visited Lund and Linkoping Universities in Sweden, the Leibniz Institute for Chrystal Growth in Berlin, Germany, the physics department at the University of Stuttgart, Germany, the physics department at the Otto-von-Guericke University in Magdeburg, Germany, the Technical University in Ilmenau, the Felix Bloch Institute at University of Leipzig and presented seminars on THz EPR methods for quantum defect characterization. **M. Schubert** group trained new graduate students Preston Sorenson (ECE, UNL) and Sina Khayam (MME, UNL) in ellipsometry basics, basic instrumentation design, and fundamentals of quantum material engineering. Khayam is exploring the concepts of Planck's black body radiation of individual quantum emitters in the THz spectral range based on the Bloch equations and results from THz EPR Ellipsometry investigations of quantum defects in ultrawideband gap semiconductors.

In terms of disseminating project work, the **Schubert** group published a total of 20 peer-reviewed papers and 7 papers were also published on ArXiv. As one highlight, the **Schubert** group published three papers in the journals Nature Communications (IF 14.7), ACS Nano (IF 15.8), and Advanced Optical Materials (IF 10), on Controlling the broadband enhanced light chirality with L-shaped dielectric metamaterials (http://dx.doi.org/10.1038/s41467-024-48051-4), Chiroptical Second-Harmonic Light Scattering from Silicon Nanohelices (http://dx.doi.org/10.1021/acsnano.4c02006), and Nanocolumnar Metamaterial Platforms: Scaling rules for structural parameters revealed from optical anisotropy (http://dx.doi.org/10.1002/adom.202302767).

The **Schubert** team continued to investigate fundamental properties of ultrawideband gap semiconductor gallium oxide which is a host candidate for emerging quantum emitters, and published two papers in Phys. Rev.: Applied explaining the anisotropic Beer-Lambert law, and effects of domain texture onto the lattice mode properties. **M. Schubert** published an editorial in Applied Physics Letters leading the Special Collection on Wide- and Ultrawide-Bandgap Electronic Semiconductor Devices. The **Schubert** team published a new chapter on Characterization of semiconductors by spectroscopic ellipsometry as part of the Elsevier Comprehensive Semiconductor Science and Technology 2nd ed. The **Schubert** group presented over 65 EQUATE-relevant scientific talks at various in-person and online events at national and international conferences--including invited and plenary talks, for example, at the Compound Semiconductor Week in Lund, Sweden. As another highlight, graduate student Preston Sorensen presented his FRG2 research poster at the 28th NSF EPSCoR National Conference in Omaha. Also, 4 graduate students of the Schubert group participated at the Spectroscopic Ellipsometry Group Meeting during the AVS 70 International Symposium and Exhibition (AVS-70) in Tampa, FL, during November 2024.

At the 2025 American Physical Society March Meeting (Minneapolis, MN), two EQUATE FRG2 graduate students presented. The **Schubert** team also presented on EQUATE-relevant work at the following venues:

- 7th U.S. Workshop on Gallium Oxide (GOX 2024), Columbus, OH;
- AVS 70 International Symposium and Exhibition, Tampa, FL;
- CMD-General Conference of the Condensed Matter Division 31, Braga, Portugal,
- 63rd Rocky Mountain Conference on Magnetic Resonance, Copper Mountain, Co.;
- Materials Research Society (MRS) Spring Meeting, San Francisco, CA;
- CLEO 2024, Charlotte, NC;
- International Workshop on Gallium Oxide IWGO, Berlin, Germany;
- 66th Electronic Materials Conference (EMC 2024), College Park, MD; and
- 2024 Materials with Extreme Properties and Condensed Matter Physics Joint Review, Washington D.C.

With regard to FRG2's **Thrust 2, Objective 2.a, Quantum Communication: Transmitting Data with Single or Entangled Photons, Enhanced Non/linear Optical Effects at the Nanoscale** and **2.1.1 Scaling Rules for Optical Anisotropy of Columnar Metamaterials**: In EQUATE Year 4, FRG2's **E. Schubert, M. Schubert, and U. Kilic** made significant contributions to advancing the design of optically active nanostructures. Their collaborative efforts centered on the theoretical and experimental optimization, design, and fabrication of spatially coherent columnar nanostructures using the innovative glancing angle deposition technique. Utilizing the generalized spectroscopic ellipsometry technique, they extracted optical (e.g., dichroism, birefringence, complex dielectric function) and structural parameters (e.g., column fraction rate, slanting angle, column length) of columnar metamaterials from various materials, including zirconia (ZrO_2, ultra-wideband gap semiconductor), titanium (Ti, metallic), silicon (Si, semiconductor), and permalloy (NiFe, magnetic) (see **Fig. 18** for SEM images of columnar structures). The anisotropic Bruggeman effective medium approach (AB-EMA) was applied to analyze these parameters, providing insights into a rarely discussed set of optical properties known as anisotropic depolarization factors (qi, where i = a, b, and c, corresponding to the major polarizability axes of the columnar structures). Systematic analysis revealed that for columnar thin films of varying lengths, within the near-IR to ultraviolet spectral range, these parameters are highly sensitive and directly correlated to changes in critical dimensions (e.g., radius, column length) of the nanocolumns. These findings underscore the extreme sensitivity of optical anisotropy to dimensional variations in nanocolumns, paving the way for a novel class of nano-metrology tools.

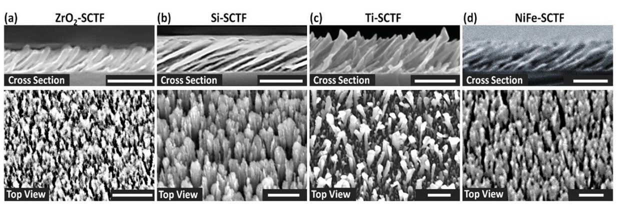

Figure 18: High-resolution cross section and top view scanning electron microscopy (SEM) images of slanted columnar metamaterial platforms from various material types: (a)ZrO_2 (b)Si, (c)Ti, and (d) NiFe. All scale bars are 200 nm.

As a forward-looking perspective, the research emphasizes the immense potential of these metamaterial platforms in advancing nanoparticle sensing and infiltration mechanisms. The manuscript was selected for the front cover image of the prestigious Advanced Optical Materials (see **Fig. 19**). The integrated spectral color variation patterns, displayed with a quarter-sized field of view in either reflection (left two quarters) or transmission (right two quarters) configurations, are critical for developing an anisotropic contrast optical microscope. The optical contrast was evaluated by comparing the responses of slanted nanocolumnar thin film samples before and after exposure to metal oxide (TiO_2) nanoparticles. Contrast variation was studied as a function of nanoparticle concentration (increasing from left to right) and column length (top to bottom). This study clearly demonstrates how the spectral controllability of the optical response depending on both fraction rate of infiltrated TiO_2 nanoparticles and column length of extremely birefringent underlying metamaterial platform.

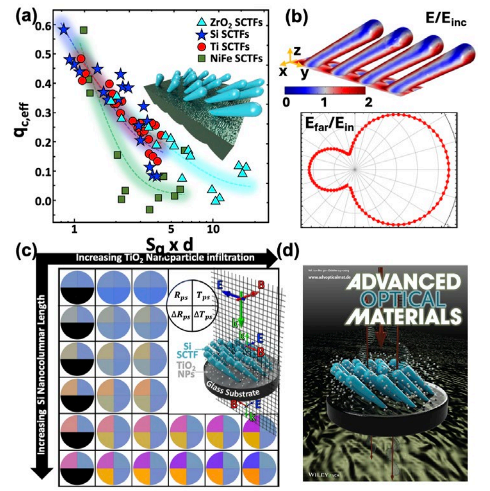

Figure 19: (a) Unveiling the generalized scaling rule for AB-EMA-based MM-GSE data analysis of optically anisotropic depolarization factors (qC, where "C" represents the major polarizability axis along the long axis of the columnar structure) as a function of the columnar structure length (L), with $d = L \cdot \cos(\theta_s)$ where θ_s is the slanting angle of the columnar structure. The analysis is performed for four material types: zirconia (ZrO_2, cyan triangles), silicon (Si, blue stars), titanium (Ti, red circles), and permalloy (NiFe, green squares). (b) Near- and far-field electric field characteristics of Ti columnar structures, derived from FEM simulations.(c) Integrated spectral color variation patterns generated with a quarter-sized field of view in either reflection (left two quarters) or transmission (right two quarters). These patterns are reported by comparing the optical responses of nanocolumnar thin film samples before and after exposure to metal oxide (TiO_2) nanoparticles.
(d) This work has been selected as the front cover image of Advanced Optical Materials (IF ~9).

With FRG2's <u>**Objective 2.1.2**</u> ***Unveiling the chiroptical second-harmonic Tyndall scattering from Si nanohelices***, the collaboration between E. Schubert, M. Schubert, and U. Kilic during years 2 and 3 focused on exploring nonlinear chiroptical responses in various nanostructure designs. By employing all-dielectric silicon (Si) helical structures fabricated via the glancing angle deposition technique, the team achieved an optimized chirality response with superior spectral control of chiral resonance modes (meets metric). This work emphasized the study of second-harmonic Tyndall scattering, a phenomenon that occurs in these high-refractive-index dielectric nanomaterials.

In collaboration with the team from the University of Bath, **Kilic**, **E. Schubert**, and **M. Schubert** demonstrated the chiroptical second-harmonic Tyndall scattering effect in Si nanohelices. For three different wavelengths of laser illumination, a clear dependence of second-harmonic scattered light on the chirality of the nanohelices and the handedness of circularly polarized light was observed. Specifically, the multiphoton emission intensity was measured at five distinct wavelengths when the Si(−) nanohelices were illuminated with 710, 730, and 750 nm light, using a fundamental laser power of 7 mW and left circularly polarized (LCP) light. In all cases, the second-harmonic emission was clearly resolved above the background multiphoton emission.

This research highlights the significance of second-harmonic Tyndall scattering in advancing nonlinear optical processes (**Fig. 20**). The findings have potential applications in energy harvesting, quantum communication, and photonic integrated circuit devices. By elucidating the mechanisms of optical harmonic generation in these nanostructures, the team contributed valuable insights to the development of chiroptical phenomena.

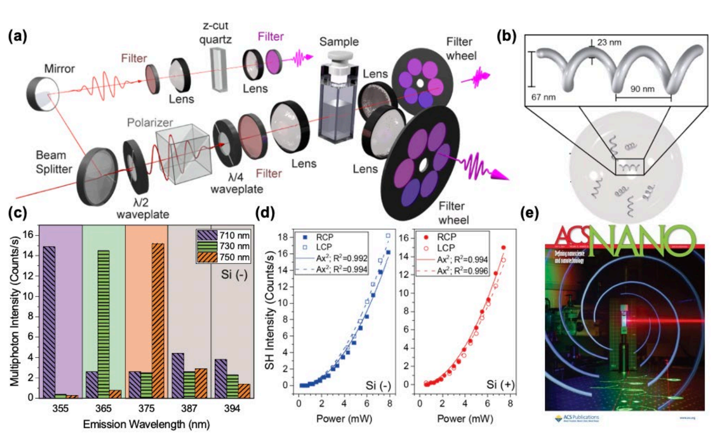

Figure 20: (a) A general overview of the optical setup used to measure the second-harmonic scattering performance of dispersed silicon nanohelices in DI water. (b) A schematic representation of dispersed nanohelices in DI water, along with their corresponding structural parameters. (c) Multiphoton emission intensity measured at five different wavelengths under three distinct laser illumination wavelengths. (d) Second-harmonic (SH) intensity plotted for right circularly polarized (RCP) and left circularly polarized (LCP) light as a function of incident laser power at a wavelength (λ) of 730 nm. The data points represent median values of 90 measurements, and the curve fits follow the equation $y = Ax^2$ and the R^2 values provided. These measurements were conducted in collaboration with Prof. Vensistlav Valev from the University of Bath. (e) An artistic depiction of chiroptical second-harmonic Tyndall scattering from silicon nanohelices, featured as the front cover of *ACS Nano*.

The ability to control second-harmonic scattering through chirality provides opportunities for creating advanced photonic systems, particularly in secure communication systems for quantum cryptography and photonic integration. This collaborative effort not only deepens the fundamental understanding of chiroptical second-harmonic scattering but also paves the way for transformative applications in next-generation photonic technologies. **Kilic** also conducted theoretical investigations into optical chiral second- and third-harmonic generation, analyzing the decomposition of circularly polarized scattering dichroism into its electromagnetic multipole moments. This approach provided a deeper understanding of the primary driving mechanisms behind the remarkably large and controllable nonlinear optical activities observed across diverse nanophotonic platforms, offering valuable insights to ongoing fabrication efforts. The ability to precisely control photon conversion at different frequencies enables the creation of entangled photon pairs, which are critical for quantum key distribution and other quantum communication protocols. This capability is instrumental in developing secure communication systems with applications in quantum cryptography.

Beyond the research, **Kilic, E. Schubert, and M. Schubert** have collectively published several papers in high-impact journals and actively contributed to conferences. Notably, they submitted four abstracts to the APS 2024 March Meeting, two of which were accepted for presentation by UNL graduate students. In collaboration with M. **Ghashami**, they submitted a paper on plasmonically tunable thermal emission properties of Ti mound structures, currently under review in Advanced Energy Materials. Their groundbreaking study on broadband-enhanced chirality from broken L-shaped all-dielectric metamaterial designs was published in Nature Communications. Additionally, their work on the general scaling rules of optical anisotropy in columnar metamaterial platforms appeared in Advanced Optical Materials. Their collaborative efforts also produced a study on the nonlinear second harmonic Tyndall-Rayleigh scattering performance of Si helical metamaterials, published in ACS Nano. In collaboration with Christos **Argyropoulos**, a former EQUATE program SI, the team developed a planar metamaterial system with a checkerboard structure exhibiting topologically protected edge states with high-Q factors and narrow bandwidth. This study, which also explores nonlinear Kerr-induced nonreciprocity, has been submitted to Nanophotonics.

In EQUATE Year 4, this FRG2 team presented their research at prestigious conferences, including the AVS International Symposium and Exhibition (AVS-70), the 50th International Conference on Metallurgical Coatings and Thin Films (ICMCTF 2024), the Conference on Lasers and Electro-Optics (CLEO), and the APS March Meeting. Collectively, they and their students delivered over 15 oral presentations. In 2024, an FRG2 collaboration (**M. Schubert , E. Schubert, and Kilic)** presented their research at several prestigious conferences, including the AVS International Symposium and Exhibition (AVS-70), the 50th International Conference on Metallurgical Coatings and Thin Films (ICMCTF 2024), the Conference on Lasers and Electro-Optics (CLEO), and the APS March Meeting—for a total of more than 15 oral presentations (including SIs and students. Additionally, **Kilic** was invited to give a short course on the introduction to spectroscopic ellipsometry and its applications at ICMCTF 2024.

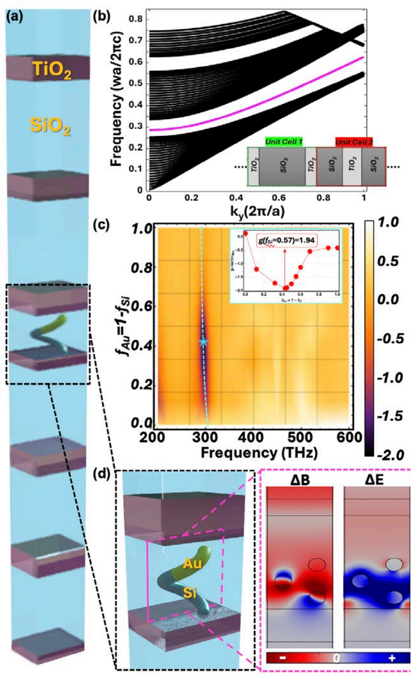

Figure 21: Boosting the Chirality via 1D Photonic Topological Insulator design: (a) Schematic representation of the envisioned structure design consisting of multilayered thin films of TiO_2 and SiO_2, arranged in a repeating ABA-BAB pattern, where A represents TiO_2 and B represents SiO_2. (b) Energy dispersion band diagram of the 1D photonic topological insulator system, with the magenta band highlighting the edge mode. (c) Spectral evolution of Kuhn's dissymmetry factor, defined as g-factor=$2CD/\sum A_i$ where i: LCP and RCP. (d) Central cross-sectional slice (depicted by magenta dashed lines) showing changes in the electric field ($\Delta E=E_{LCP}-E_{RCP}$) and magnetic ($\Delta B=B_{LCP}-B_{RCP}$) fields.

In terms of training and professional development for FRG2 participants during EQUATE Year 4, one student (under the supervision of **M. Schubert , E. Schubert,** and **Kilic**) was trained on performing photo and electron beam lithography for experimentally realizing theoretically optimized structure designs that exhibit topological edge states. Another FRG2 student was trained on scanning electron microscopy imaging as the graduate student who was performing the nanostructure imaging, Shawn Wimer (supervised by **E. Schubert**), graduated with his PhD in August 2024.

For **Objective 2.b Robust Entangled Photon Generation from Nanoscale Structures**, FRG2 has addressed **2.2.1. Achieving Enhanced and Nonreciprocal Chiroptical Response by harnessing Topological edges states** via **Kilic.** In collaboration with **M. Schubert and E. Schubert**, he engineered an all-dielectric planar two-dimensional photonic topological insulator (2D-PTIs) which exhibits nonreciprocal chiral response due to design of an edge with creation of lattice mismatch condition in periodic arrangement of checkerboard structure. The work is currently under submission to the high impact *Nanophotonics* journal. Importantly, such structure designs have garnered attention for their potential applications in quantum information technologies and advanced photonic integrated circuits. Inspired by this concept, the team explored a 1D photonic crystal system combined with a 3D nanohelical metamaterial platform to achieve a large and nonreciprocal chiral response. The optical manifestation of chirality, known as circular dichroism (CD), is defined as the differential absorption (A) of left-handed circularly polarized (LCP) light and right-handed circularly polarized (RCP) light (CD = $A_{LCP} - A_{RCP}$).

In this study, a one-turn nanohelical heterostructure metamaterial platform, comprising alternating Au and Si subsegments, was integrated into a 1D photonic topological structure formed by alternating TiO_2 and SiO_2 thin-film layers. The schematic representation of proposed system is given in **Fig. 21(a).** FEM based systematic calculations revealed the emergence of a strong leak mode within the photonic bandgap region, characterized by perfect transmissivity and strong electric field confinement at the interface of the 1D-PTI. The spectral position of this leak mode aligns precisely with the topological edge mode frequency in the superlattice energy dispersion diagram of the proposed PTI system (**Fig. 21(b)**).

By precisely tuning the layer thicknesses in the 1D photonic crystal (PC) system, we achieved alignment between the nanohelical structure's chirality and the frequency of the topological leaky mode, thereby enhancing the chiroptical response to an impressive value of 1.94 (**Fig. 21(c)**). In this enhancement, one of the key factors was to strategically position at the topological interface, where electric field coupling was maximized (**Fig. 21(d)**).

Furthermore, by leveraging localized field enhancement at the interface and optimizing the placement of the nanohelical structures, we achieved Kerr nonlinearity-induced nonreciprocal chirality from the system. Showcasing both the spectral evolution of nonreciprocal response and the laser input intensity dependency of nonreciprocity in **Fig. 22** summarizes the FEM simulations based theoretical demonstration of nonlinear Kerr effect induced nonreciprocal chiroptical response from the proposed system. In conclusion, our findings demonstrate that integrating nanohelical structures into the PTI system provides a robust approach to generating a strong and nonreciprocal chiroptical response. This study highlights the potential of such hybrid systems in advancing photonic device technologies and exploring transformative nonlinear optical mechanisms. (On schedule/meets metric)

<u>Objective 2.c</u> Plasmonic Nanocavity to Boost Single Photon Emission from Defects in Thin Hexagonal Boron Nitride Recent advancements in nanofabrication have enabled the development of efficient, bright, and ultrafast quantum emitters with high single-photon purity and indistinguishability. Hexagonal boron nitride (hBN) has emerged as a promising platform due to its exceptional quantum properties, chemical stability, and ability to form ultrathin flakes that operate at room temperature. These characteristics make hBN a viable host for single-photon emitters (SPEs) in diverse quantum communication and sensing applications. In this study, deterministic SPEs were created in thin hBN flakes (15–35 nm) deposited on an optically thick gold substrate. This was achieved through a high-temperature annealing process (1100 °C) under oxygen flow, which activated SPEs in the flakes.

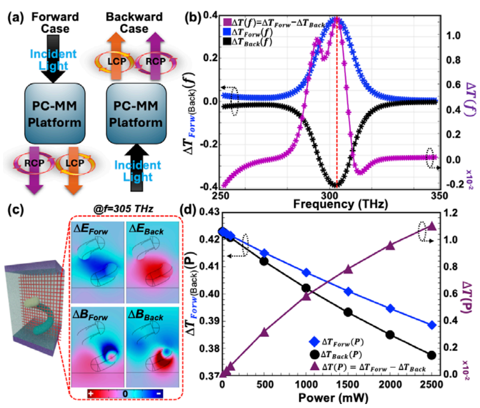

Figure 22: Unraveling Nonlinear Kerr Effect-Induced Nonreciprocity in Chiral Response via Hybrid Helical Metamaterials Integrated into 1D PTI system: (a) Schematic representation of the theoretical framework used to extract non-reciprocal chirality in transmission operation mode. (b) Spectral evolution of chirality in transmission for forward (blue) and backward (black) light illumination, along with their difference, representing nonreciprocity (purple). (c) Corresponding changes in electric ($\Delta E = E_{LCP} - E_{RCP}$) and magnetic ($\Delta B = B_{LCP} - B_{RCP}$) fields shown as color density plots along a central cross-section of the structural design. (d) Power-dependent evolution of the extrema point (f=305 THz) for forward (blue diamonds) and backward (black circles) light illumination, with nonreciprocity quantified as the difference $\Delta f = f$for-$f$back (purple triangles).

Through a joint effort, **Kilic** and **Laraoui** enhanced the quantum properties of SPEs using plasmonic cavity enhancement mechanisms, as illustrated in **Fig. 23(a).** Their findings, recently published in *Laser & Photonics Reviews*, demonstrated that the integration of metallic nanocavities with hBN flakes containing defect-based SPEs substantially improves nonclassical light emission performance. This hybrid nanophotonic structure not only achieves rapid speedup and a large enhancement in single-photon emission at room temperature but also significantly outperforms plain hBN flakes and hBN-on-gold structures without nanocavities. Theoretical calculations further confirmed that the plasmonic nanocavity plays a pivotal role in achieving efficient and compact SPE performance, offering a groundbreaking solution for room-temperature integrated quantum photonic networks.

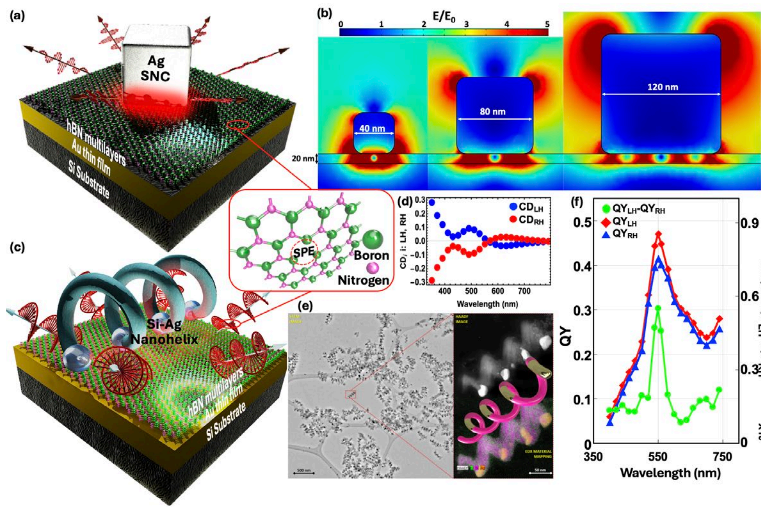

Fig. 23. (a) Schematic of a hybrid nanophotonic cavity, consisting of hBN sandwiched between an Au film and SNCs, designed to enhance the quantum properties of single-photon emitters (SPEs). (b) The confinement of light at the hBN flake interface can be further boosted by adjusting the size of the Ag nanocube. (c) Schematic illustration of SPEs emitted from thin hBN flakes under a SiAg plasmonic heterostructure with a helical structure for circularly polarized emission. (d) Handedness effect from the dispersed helical structure, with left-handed (LH, blue) and right-handed (RH, red) cases. (e) Scanning transmission electron microscopy (STEM) images with energy-dispersive X-ray spectroscopy (EDS) material mapping of dispersed helical heterostructures on a TEM mesh grid system. (f) Quantum yield spectra from LH and RH Ag helical heterostructures, where the difference shows chiral single-photon emission.

The systematic Finite element modeling (FEM) studies confirms that the spatial coupling between plasmonic silver nanocubes (SNCs) and SPEs to achieve further enhncement (**Fig. 23(b)**). This coupling was further exploited to realize chiral single-photon emission (see the structural design in **Fig. 23(c)**). Specifically, single photons emitted from hBN SPEs were filtered through glancing-angle-deposited silicon (Si)-silver(Ag) helical heterstructured metamaterials, enabling SPEs gain circular polarization (**Fig. 23(d)**). FEM revealed that these helical structures function as highly selective chiral filters, significantly improving the signal-to-noise ratio for chiral single photons. The envisioned struture were successfully fabricated usng GLAD technique and using the scanning transmission electron microscopy (STEM) and energy-dispersive X-ray spectroscopy (EDS) material mapping were performed and shown in **Fig. 23(e).** (On schedule/meets metric)

Additionally, the quantum yield spectra from left-handed (LH) and right-handed (RH) silver helical heterostructures demonstrated pronounced chiral selectivity, as illustrated in **Fig. 23(f).** This chiral-SPE platform represents a breakthrough in achieving circularly polarized single-photon emission, with significant implications for quantum encryption and secure communication. This study highlights the integration of plasmonic cavity-enhanced SPE platforms with all-dielectric metamaterial systems, paving the way for compact quantum optical communication technologies.

Kilic modified the previously developed COMSOL model for investigating the enhancement of the quantum properties of single photon emitters by using plasmon metallic nanocavities. Now the model is able to pursue the chiral single photon emission process analysis, as well. **Laraoui** trained an undergraduate student (electrical engineering) in performing quantum optics experiments using single photon emitters in hBN. **Laraoui** will present two oral talks, one as a contributed talk at the APS Global Physics Summit 2025, and the other as invited at the 2025 Boron Nitride Workshop.

In addition to their research, in EQUATE Year 4 several FRG2 SIs made impacts in areas benefiting the project and its participants, including:

- **Laraoui** received an NSF grant ($800k) in collaboration with Paresh Ray from Jackson State University (JSU), MS (an EPSCoR jurisdiction) with an ExpandQISE program Track 1 project: a JSU-UNL Collaboration on Quantum Sensing Research and Education.

- **Laraoui** received an NSF award of $300,000 entitled "EPSCoR Research Fellows: NSF: Plasmonic Cavity Nanostructures to Boost Single Photon Emission from Multilayered Hexagonal Boron Nitride" in collaboration with Prof. Christos Argyropoulos, a previous EQUATE FRG2 SI, now at Pennsylvania State University.
- **Laraoui** shared the syllabus of a new elective MATL- 492/892: Introduction to Quantum Materials and Technologies with science and engineering departments at non-UNL campuses (UNO, UNK, and Creighton University). In the Spring 2024 semester (January- May), 14 students registered for the class comprising 4 graduate students and 10 undergraduate students from UNL's Electrical & Computer Engineering (ECE) and Mechanical & Materials Engineering (MME) departments.
- **M. Schubert** organized a full two-term online lecture series that continued in Spring 2024 (16 lectures total), the Nebraska Ellipsometry Lecture series. Lectures are given by speakers from Europe, Asia, and North America, and attract up to 100 attendees biweekly. The content of the lecture series is related to quantum science and applications of ellipsometry in this field and is directed towards students. **M. Schubert** received a $1 million DURIP award from AFOSR for development and acquisition of a world-unique field-flattened split-coil superconducting magnet to perform THz EPR ellipsometry at field homogeneity of better than 300ppm. **M. Schubert** received a new NSF award with Dr. Shubhendu Bhardwaj from UNL ECE: Investigating Semiconductor-based Terahertz Traveling Wave Amplifiers for Monolithic Integration. As main organizer of the 2025 International Conference on Spectroscopic Ellipsometry, **M. Schubert** had initiated the North American Ellipsometry Association group on LinkedIn, as a platform for professionals in North America's ellipsometry field to connect, share knowledge, discuss trends, and explore collaborative opportunities. The group has 121 members.
- **E. Schubert** and **M. Schubert** are organizing the 10^{th} International Conference on Spectroscopic Ellipsometry to be held in Boulder, Co from June 8-13 2025. The conference is financially supported by an NSF conference grant received in 2024. **E. Schubert** hosted 2 Young Nebraska Scientists high school students in her lab during summer 2024. One high school student developed a motor control to operate optical systems, and a high school student from Texas, under supervision of **Kilic,** developed a python code to simulate the change of optical polarization states upon reflection with different sample systems. The codes will be made available to the public through the NSF funded website Funsize Physics to educate about optical applications for polarized light. **E. Schubert** organized a new monthly ECE graduate student seminar series which highlighted speakers from UNL, Johns Hopkins University, the Army Reserarch Laboratory and advanced ECE graduate students. **E. Schubert** engaged with adults and children from the region in a community outreach event "Sunday With a Scientist" at UNL Morrill Hall Science Museum to teach about physical phenomena in material and nanoscience.
- **Kilic** remodeled and refurbished the ALD and GLAD lab facilities in the new labs at UNL, under the supervision of both **E. Schubert and Kilic**. Importantly, visitors from the Leibniz Institute for Surface Engineering in Leipzig, Germany, actively participated in nanofabrication instruments training and research alongside UNL graduate students.
- **Liou** remodeled the magnetic force microscopy (MFM) setup to measure topological spin textures and trained EQUATE funded students from FRG1 and FRG2 on the setup. **Liou** in collaboration with **Laraoui** supervised a PhD student on aspects of quantum sensing. The student published two high impact papers at ACS Nano (IF = 17.1) and Nano Letters (IF = 10.8).
- **Ghashami** (SEED awardee) received NSF's Early CAREER Award in 2024, before he departed UNL.

FRG3 – Quantum Information Processing (Year 4: June 2024 – May 2025)

Year 4 for EQUATE FRG3 was marked by significant progress in all areas of our focus on quantum emulation and quantum computation. At the same time, our trainees this year include 8 undergraduate students, a masters student, 2 PhD students, a post-masters researcher, and 6 postdoctoral researchers in quantum science techniques. Key personnel are FRG3 leader **Wrubel** (Creighton University), **Armstrong** (UNK), **Wong** (Creighton University), **Mei** and **Sabirianov** (UNO), **Wysocki** (UNK), and **Sinitskii** (UNL).

In **Thrust 1**, a significant new collaboration has developed between seed-awardee Laura **Wang** and FRG3 SI Alexander **Sinitskii**. They have just begun work to produce an exciton-polariton BEC using materials synthesized by Sinitskii and integrated onto a photonic platform developed by Wang. Their work could yield a new class of quantum-simulators using highly-versatile photonic waveguide technology, and complements the experimental cold atom BEC effort by **Wrubel** and the theoretical BEC work of **Armstrong**.

In **Thrust 2**, the work on a next generation qubit is progressing due to collaborations with FRG-1. **Binek** has demonstrated Coulomb blockade in a graphene crosswire and **Sinitskii** has fabricated layered 2D crosswires from transition-metal di(tri)-chalcogenides. **Mei** and **Sabirianov** are working to reproduce the transport measurements and predict the behavior of arrays of crosswire quantum dots.

Similarly, **Wysocki** has continued to explore theoretically the possibility of novel qubit platforms formed from adatoms on 2D surfaces. Fruitful collaborations have involved SIs **Dowben** and **Lai** (FRG1) and **Binek** and **Guo** (FRG1).

Several theoretical results on quantum walk algorithms have been published by SI **Wong** since his return to the project in January 2024 (from leave in Washington D.C.).

Thrust 1. Quantum Emulation.

Objective 1.a: Surpassing the Standard Quantum Limit in a ^{41}K BEC. (in-progress) In year 3 **Wrubel**'s (Creighton University) group demonstrated we could load about 15×10^3 atoms into our crossed optical dipole trap, but light-shifts caused by the trapping laser were limiting the loading process. To overcome this limitation Year 4 had design, construction and implementation of a second laser system to achieve lower temperatures using a "gray-molasses" cooling technique on the D1 atomic transition (**Fig. 24)**.

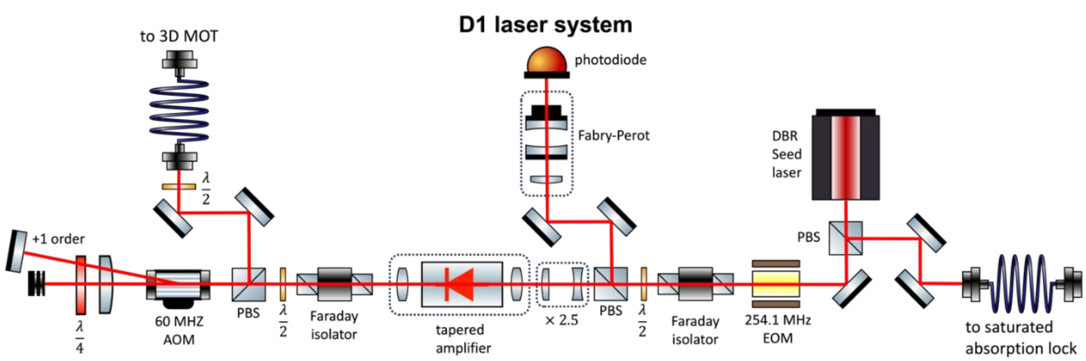

Figure 24. New D1 laser system incorporating a commercial seed laser (distributed Bragg-reflector) with a home-made tapered-amplifier laser for up to 1 W of output power. Coherent sidebands are produced using an electro-optic modulator (EOM) and the power and overall detuning are controlled by an acousto-optic modulator (AOM).

The gray molasses technique reduced the temperature of the atoms from about 60 to about 16 µK when released from the trap, similar to results by other groups. Then, taking advantage of our octupole-symmetry magneto-optical trap, the temperature was further reduced to 4 µK, which is the lowest temperature observed using a gray-molasses technique. We recently demonstrated loading of 7x more atoms (200×10^3) into our optical dipole trap using the novel octupole/gray-molasses technique and we are working to further optimize this process (**Fig. 25**).

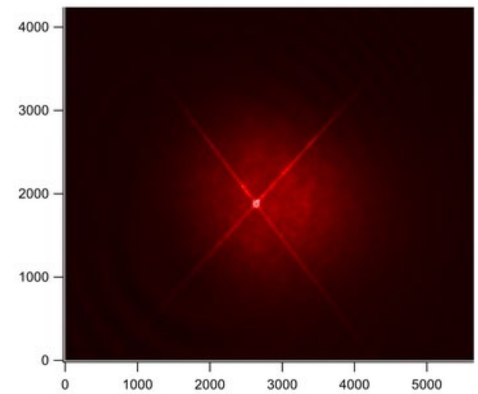

Figure 25. False-color image of loading ^{41}K into the 1550 nm crossed optical dipole trap from the gray-molasses in our octupole-symmetry magneto-optical trap.

This larger and more stable number of trapped atoms will make possible an immediate search for the RF Feshbach resonance (one of our main physics goals). With some modest improvement in total number of atoms, we expect to be able to achieve Bose-Einstein condensation in the optical dipole trap.

A full-time post-masters research associate was hired in December 2024 who has helped to accelerate the pace of research. There are currently 4 undergraduates, 1 masters student and 1 post-masters researcher active in the lab learning laser-cooling techniques. SI **Wrubel** presented the main results on loading the optical dipole trap at the American Physical Society Division of Atomic, Molecular, and Optical Physics (DAMOP) in Ft. Worth, Texas (June 2024). A paper was published with SI **Wong** and M.S. graduate Benjamin DalFavero on our joint work on quantum walk algorithms (PRA, **110**, 052411, 2024).

A research slow-down occurred with the departure of our previous postdoc and absence of masters degree students last year. This has been offset by the hiring of a post-masters researcher in December 2024. The need to develop and implement the gray-molasses technique took extra time, but has paid off in significantly lower temperatures and more atoms in the optical dipole trap.

Objective 1.b: Emulation of Novel Spin Systems (in-progress). The goals of this objective depend in large part upon the completion of the activities described in objective 1a, which continue to be the main focus of research. Progress on the optical lattice will be delayed until year 5.

Objective 1.c: Quantum Emulation with an Exciton-Polariton BEC. (meets metric). The objectives for this work for Years 1-3 were completed by Wei **Bao** (UNL) before his departure from UNL in August 2023.

Objective 1.d: Theory of Polarons in Dipolar and Spinor Gases (in-progress/meets metric). In year four SI **Armstrong**'s group at UNK has extended their calculation of time-dependent densities. These have shown the response of the medium to the implantation of an impurity. We have done these calculations in a variety of systems: In 3D with a strongly interacting, Gaussian impurity, and in 2D with experimentally relevant dipolar impurities with two different trapping orientations. We also expanded on our 2D results from years 2 and 3 to include self-energies for many different dipolar impurities looking at particle number dependence as well as on the strength of the dipolar impurity.

Fig. 26 shows the time evolution of the dipolar gas that has an impurity introduced at the origin at t=0. Here the 1D cross sections along the x-axis at various times are plotted. The repulsive impurity quickly makes a hole in the density in the center of the trap, which ends up bottoming out completely with zero remaining density at some point, before rebounding back up to the original state, and oscillating back.

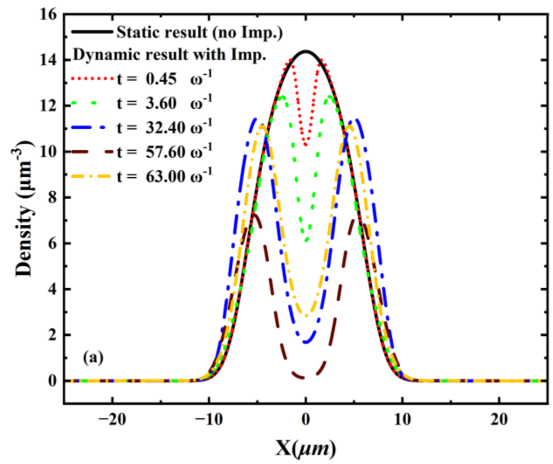

Figure 26. Time evolution of the dipolar gas that has an impurity introduced at the origin at t=0, which we show with 1D cross sections along the x- and z-axes at various times.

We began modifying codes to implement a scissors mode oscillation in Bose-Einstein condensate systems: a pre-cursor to investigating this behavior in so called Lee-Huang-Yang (LHY) liquids, which are more strongly interacting quantum fluids. We are working on matching collaborators' previous results in BECs and will then proceed to the LHY liquids.

We finished our work with a now graduated undergraduate on atomic structure properties of some highly charged tungsten ions which are important for plasmas used in the ITER fusion power project.

The significant result is that an anisotropic medium response for dipolar BECs regardless of the symmetry of the impurity's interactions. The preferred shape of a deformed impurity was identified to be prolate with the long dimension along the dipolar axis.

In 2D trapped dipolar gases, the self-energy of a dipolar impurity is not affected by the deformation of the trap if the trap is perpendicular to the dipolar direction. In contrast if the deformation is parallel to the dipolar axis, then it follows the 3D results in which lengthening the trap along the dipolar direction decreases the self-energy of the impurity.

Our 3D results have been published in Physical Review A: Phys. Rev. A 110, 053317 (2024). A presentation on the above results was presented in Prague in July at the "10th Frontiers of Quantum and Mesoscopic Thermodynamics conference". Our 2D results have been submitted to the journal Atoms. Our tungsten ions results have also been submitted to Atoms.

Thrust 2. Quantum Computation

<u>Objective 2.a:</u> Quantum Walk Algorithms (in-progress/meets-metric). SIs **Wong** and **Wrubel** (Creighton), with EQUATE master's student Benjamin DalFavero, as well as collaborators from UC San Diego, published in Physical Review A an analysis of a quantum algorithm on an effectively nonlinear many-body quantum system that was able to search a "database" more quickly than standard quantum algorithms by utilizing parallel queries.

In collaboration with David Meyer from UC San Diego, SI Wong met an EQUATE Year-4 milestone by determining conserved quantities related to energy for nonlinear quantum search algorithms, whose effective Hamiltonians are time-dependent. The results are being prepared for publication.

Explorations of quantum walk algorithms have opened new areas of interest. With EQUATE-funded Creighton undergraduate Jonas Duda, SI Wong published a paper in Physical Review A demonstrating that different types of continuous-time quantum walks, a form of analog quantum computing that is analogous to continuous-time random walks, can lead to different behaviors when searching a network consisting of two fully connected cliques connected by a single weighted bridge (**Fig. 27**). This work was presented in a talk at the American Mathematical Society (AMS) 2024 Fall Eastern Sectional Meeting, as well as through a poster at the 2024 Southwest Quantum Information and Technology (SQuInT) workshop.

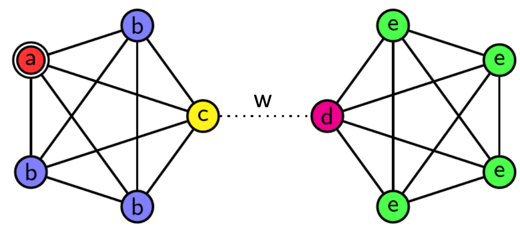

Figure 27. Barbell graph of weakly connected cliques. Quantum walks tend to get stuck in cliques that have a limited number of edges leaving the clique.

SI Wong and EQUATE-funded Creighton undergraduate Molly McLaughlin have conducted the first algorithmic study of a third kind of continuous-time quantum walk, showing that it behaves differently from the previous two established kinds of continuous-time quantum walks when searching a particular kind of database, and in some cases, it searches more quickly. This raises the potential for new quantum algorithms based on this third kind of quantum walk. The results are being prepared for publication.

SI Wong submitted for publication the results of a study of 107 public high school students on how their self-efficacy in quantum computing was affected by playing a football-themed quantum computing board game and learning the game's connections with quantum computing. The study showed that self-efficacy improved by 33.4%, which was a very statistically significant shift of 7 standard deviations. This work was conducted in collaboration with a local high school physics teacher, Kristina Armbruster, as well as a physics education research (PER) expert at Creighton, Gintaras Duda.

Wong partially returned to academia in January 2024 after two years in-person at the White House Office of Science and Technology Policy (OSTP) National Quantum Coordination Office (NQCO), as well as the Department of Energy. He spent an additional year, until December 2024, serving part-time and remotely for OSTP/NQCO.

<u>**Objective 2.b:**</u> **Crosswire Quantum Dots for Quantum Computing (in-progress).** SIs **Mei and Sabirianov** (UNO) are in the process of calculating the energy states of a 2D array of crosswire quantum dots with graphene and TMD. We are studying the decay rate in this system. Mei and Sabirianov have also studied the anomalous Hall effect in Cr_2Te_3.

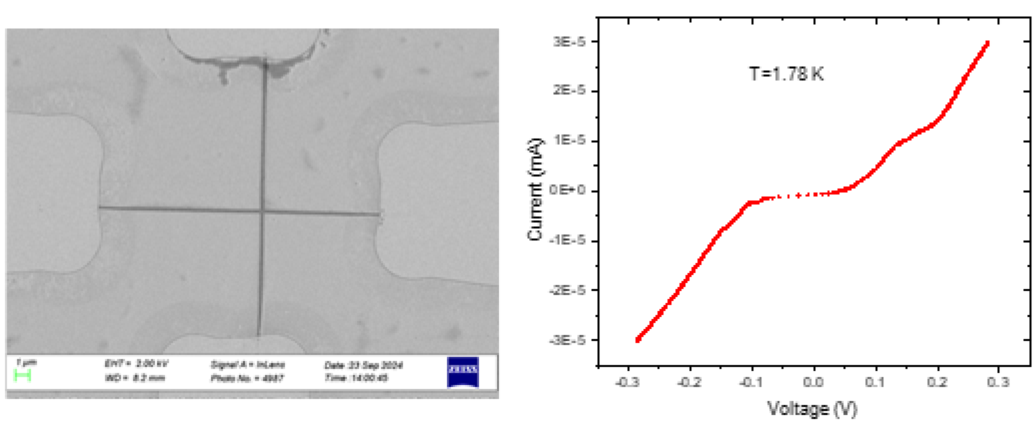

Figure 28. Image of graphene crosswire (left) and transport measurements showing Coulomb blockade at 1.78 K (right).

The experimental work on crosswire quantum dots has made significant progress with the demonstration of Coulomb Blockade for a crosswire of graphene (**Fig. 28** left) nanofabricated by SI **Binek**'s group (UNL, FRG1). The Coulomb blockade effect (**Fig. 28** right) was shown to go away with increased temperature as expected for localized electronic states.

Mei and Sabirianov discovered the temperature-induced reversal of the sign of the anomalous Hall effect in Cr_2Te_3 (**Fig. 29**). They also discovered a proximity effect in chiral h-BCN molecule on the WSe_2 substrate, an optically active system which is in-preparation for submission. They initiated a machine learning project towards designing novel magnetic material, and started analysis of the transport properties of graphene crosswire quantum dots in support of the experimental work by **Binek** and **Sinitskii**.

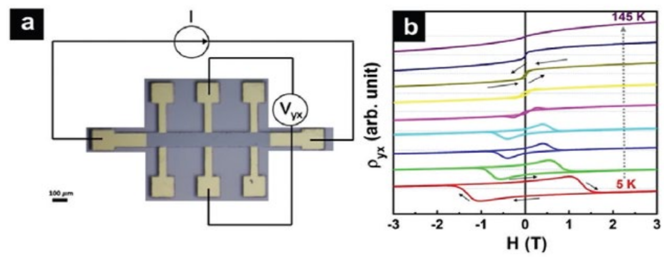

Figure 29. Hall effect measurements and two interpretations of the observed unconventional anomalous Hall effect (AHE) in Cr_2Te_3. a) A schematic of the Hall bar device used for Hall effect measurements. b) Shown from bottom to top are the magnetic field-dependent Hall resistivity ρ_{yx} measured at temperatures of 5, 25, 45, 65, 75, 85, 105, 125, and 145 K, respectively. The solid arrows indicate the looping directions, showing a change of polarity of the measured Hall resistivity with changing temperature. Published in *Adv. Sci.* **2407625**, 2024.

Mei and Sabirianov trained several researchers in computational physics methods. Two students (Trevor Gibbons, Aaron Franz) started working on the modeling and DFT calculations of graphene on WSe_2 and graphene based QDs. Postdoctoral fellow (Yogesh Khatri) worked on a high-throughput search of novel quantum materials. Postdoctoral fellow (Jaeil Bai) worked on analysis of novel quantum materials, and machine learning towards analysis of nanoparticle synthesis. Supervised/discussed postdoctoral fellow (Dmitri Bednik) in analysis of twisted bilayer graphene.

Objective 2.c: **Computational design of new spin-qubit materials (in-progress).** SI **Wysocki** (UNK) computed the low-energy spectrum for lanthanides (Tb, Dy, Ho) adatoms on graphene for different adatom oxidation states. Crystal field parameters and the effective magnetic anisotropy barriers were then determined. The intra-site exchange coupling between 4f and 6s/5d electrons was found to be much stronger than the spin-orbit coupling.

The trivalent 4f occupation was found for all oxidation states, but the sign of the magnetic anisotropy barrier (uniaxial vs. in-plane) depends on the occupation of the 6s5d orbitals and thus can be controlled by gating.

Hyperfine coupling and nuclear quadrupole interaction parameters were calculated for Sm adatoms on MgO (001) surface. A very large Fermi contact contribution is obtained for adatoms with an unpaired 6s orbital. The electronic-nuclear spectrum was computed. The electric field dependence of the hyperfine and quadrupole interaction parameters was calculated.

Wysocki demonstrated efficient Rabi oscillations between nuclear spin levels induced by a time dependent electric field for a Sm adatom on MgO (**Fig. 30**). The Rabi frequency for nuclear transition is shown to be linearly dependent on the resonant electric field amplitude.

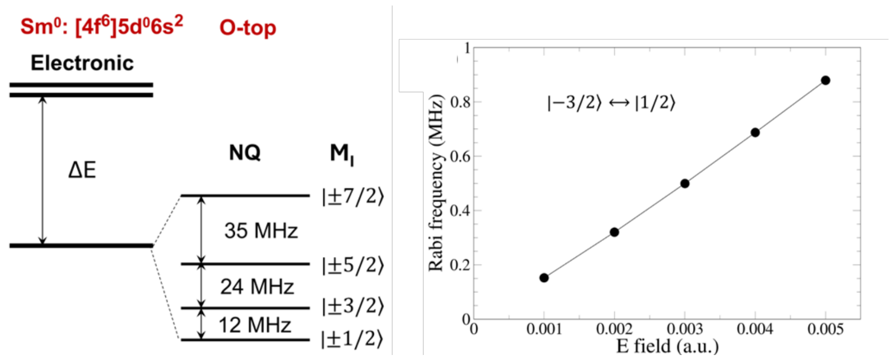

Figure 30. Electronic-nuclear spectrum of a neutral Sm adatom on MgO (left). Calculated Rabi frequency as a function of an electric field amplitude for resonant time-dependent electric field induced transition between a pair of nuclear spin levels (right).

Electronic structure, magnetic moments, and exchange coupling were calculated for a $[Fe(qsal)_2][Ni(dmit)_2]$ spin-crossover molecular crystal. This work is progressing in collaboration with SIs **Dowben and Lai** from FRG-1.

Magneto-structural properties of B-doped Cr_2O_3 were studied from first principles. We found that O-substitution, Cr, substitution, and interstitial doping configurations can all be realized. We found that the interstitial B doping induces symmetry breaking distortions, which produce an electric dipole, and can be responsible for formation of experimentally observed polar nanoregions. This work is in collaboration with SIs **Binek** and **Guo** from FRG-1.

SI **Wysocki** trained an undergraduate student in using VASP code for electronic structure calculations, trained a postdoctoral researcher in using the Molcas and Orca quantum chemistry codes, trained a postdoctoral researcher in microscopic magnetic anisotropy model based on the Green's function theory, and trained an RET researcher (Kearney High School science teacher) in fundamentals of quantum information science. Since Monirul Shaikh left UNK, a new postdoc is being hired.

<u>Objective 2.d:</u> Experimental Realization of Crosswire Quantum Dots in Transition Metal Di(Tri)chalcogenides (in-progress). SI **Sinitskii** (UNL) continued work on the synthesis and characterization of 2D materials of interest for quantum applications. These materials included graphene, transition metal dichalcogenides (TMDs, such as MoS_2, WSe_2, and SnS_2), trichalcogenides (TMTs, such as TiS_3, ZrS_3, and HfS_3), and carbides (MXenes, such as $Ti_3C_2T_x$). These materials were provided to investigators from all three FRGs.

The group also patterned sub-20-nm strips of TMDs, TMTs, and 2D ferromagnetic materials and demonstrated their stacking into crosswire QD junctions. This provides an alternative possible platform for crosswire quantum dots compared to the graphene wires fabricated by **Binek**.

Sinitskii's group developed a procedure for the synthesis of a new 2D MXene material, $Cr_2TiC_2T_x$, and demonstrated that this is the first known MXene with p-type properties (**Fig. 31**). This material will be combined with the n-type 2D materials available to the investigators for creation of nanoscale p-n junctions. The procedure was reported in a high-impact-factor journal Matter (S. Bagheri, et al., *Matter* **2024**, *7*, 4281) and covered by Nebraska Today.

While working with nanoscale MXene devices, discovered layer-dependent gas sensing properties of 2D titanium carbide ($Ti_3C_2T_x$) MXene (*ACS Nano* **2024,** *18*, 26251) and demonstrated its metallic conductivity (*ACS Materials Letters* **2024,** *6*, 298).

Two graduate students, Jehad Abourahma and Michael Loes, who were partially supported by EQUATE, graduated with PhD degrees in Chemistry. Jehad Abourahma is now working in a quantum-computing company, IonQ, that is developing a trapped ion quantum computer and software to generate, optimize, and execute quantum circuits. Michael Loes is now working in NuTech Ventures. Rashmeet Khurana (primary support from the EQUATE project) continues working in my lab toward her PhD degree.

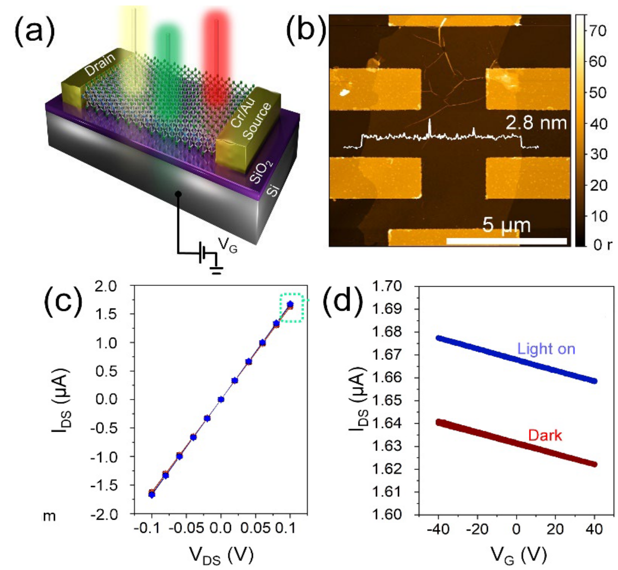

Figure 31. Electronic and optoelectronic properties of $Cr_2TiC_2T_x$. (a) Scheme of a two-terminal $Cr_2TiC_2T_x$ FET device under illumination with different lasers. (b) AFM image of a six-terminal $Cr_2TiC_2T_x$ device. The MXene flake shows no signs of structural degradation after the device fabrication. (c) I_D-V_{DS} curves obtained from the device shown in (b) at V_G = -40, -20, 0, 20, and 40 V, in the dark and under illumination with white light. (d) I_D-V_G dependence for the same device measured at V_{DS} = 0.1 V.

In Fall 2024 Sinitskii taught a senior-level chemistry laboratory class (Chem 443 Inorganic Materials Chemistry), which exposed approximately 20 students to some of the EQUATE-supported research through laboratory experiments on synthesis and characterization of 2D materials (graphene, TMDs, 2D hybrid perovskites).

Sinitskii's group also presented three oral presentations on the above EQUATE-supported papers at the 2024 MRS Spring meeting. SI Sinitskii presented invited seminars on the above papers at UNL Department of Mechanical & Materials Engineering and the University of Waterloo, Canada.

SOLICITATION-SPECIFIC PROJECT ELEMENTS:
Education, Outreach and Workforce Development (Year 4: June 2024 – May 2025)

The goal of the EQUATE Workforce Development portfolio is to prepare the next generation of highly qualified and motivated students, educators, and researchers through comprehensive programs, activities, and mentoring through the duration of the grant.

For **Objective 4.1: Equip Nebraska students (grades 6-12) with resources for success in STEM workforce**, Year 4 showed an increased interest in ***Young Nebraska Scientists (YNS) Summer Camps*** with 10 faculty-led camps, most reaching participation capacity. Three new camps were offered directly through YNS including *The Science of Cookies* and *The Science of Ice Cream* camps for both middle and high school students. At the University of Nebraska-Lincoln (UNL), High School Research in Molecular Engineering (HiRe-ME), a camp hosted by EQUATE seed grant awardee, S. **Nejati**, brought 29 students to UNL for one week to learn about molecular engineering and related careers. This camp was unique in that participants submitted competitive applications and were paid to attend if selected. Additionally, YNS supported M. Long, a new faculty member at Creighton University (CU), in the development of a new camp about Quantum and Nanoscience. Students were recruited from Omaha schools to learn laboratory techniques and help develop effective course materials. The students will work as teaching assistants (TAs) at future camps to leverage near peer learning and gain valuable internship experience in STEM. In EQUATE's Year 4 (Summer 2024) YNS summer camps were attended by 181 students. Fifty-six campers learned EQUATE-specific topics. **Meets metrics: Yr 1 development, Yrs 2-5, 85 participants (30 at EQUATE-specific summer camps) annually.**

YNS, with Nebraska Center for Materials and Nanoscience (NCMN) and the JA Woollam Foundation, hosted 18 **YNS High School Researchers** in laboratories at UNL (**Fig. 32**). The students were hosted by EQUATE researchers including **Lai, Laraoui, Streubel, Guo, Xu, E.Schubert, Hong, and Alexandrov**. Two students participated in the program as part of the Wong Laboratory and for the first time, Biomechanics researchers hosted two student researchers on the University of Nebraska – Omaha campus. Twenty-two students presented posters at the UNL Summer Research Fair. **Meets metric: Yrs 1-5, 8 students annually.**

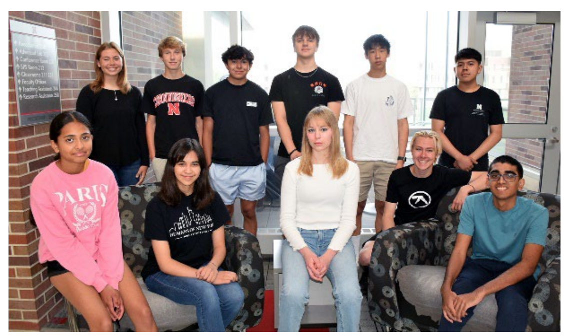

Figure 32: YNS High School Researchers, funded by NSF via Nebraska's EQUATE collaboration, gather at UNL Jorgensen Hall for their training in Summer 2024.

Three quantum-themed YNS **mobile labs** were deployed, providing hands-on activities and education materials to teachers throughout Nebraska. The EQUATE kits were created to work at both the middle and high school level; the kits include topics such as spectral analysis, tribo-electric series, and photoelectric effect. An additional module using a cloud chamber is being developed that will not need dry ice to function making it easier for rural schools to use. The molecular biology for secondary classrooms (MBSC) mobile labs (pGlo Bacterial Transformation, Restriction Enzyme Digestion of Lambda DNA, and PV92 PCR) continued to enhance secondary educational curriculum. There is ongoing work to transition a dog genetics citizen science project to the mobile labs program and expand state-wide. This project was designed by faculty at Southeast Community College and Neogen, an animal genetics company, to get students interested in biotechnology while testing their dogs for genes that are thought to correlate to behavior. In the 2024-2025 school year, mobile labs have reached over 800 students so far. **Metric: 1,000 students/yr with 3 EQUATE- specific kits offered during YRS 2-5.**

Teacher Programs

Teacher development is an important part of equipping Nebraska's students for STEM success. Beyond the mobile labs program, additional opportunities are included within EQUATE to provide teachers with the knowledge and skills necessary to prepare the next generation of STEM professionals.

Research Experience for Teachers (RET). Due to unexpected opportunities, Nebraska EPSCoR and NCMN staff hosted two national conferences in 2024. The added events reduced the amount of time we were able to dedicate to recruiting and mentoring RET participants at UNL. Allison Klein, a science teacher from Kearney High School, continued work started with **Wysocki** during the previous summer. The two submitted a journal article for publication and created a quantum computing curriculum module for high schoolers. They presented their module at Nebraska Association of Teachers of Science (NATS) conference held in Grand Island, NE. Klein has applied to present at the National Science Teacher Association (NSTA) conference. **Metrics: Yrs 1-5, 5 participants annually in EQUATE labs.**

Summer Institute for Middle School Teachers (SIMST). Nine teachers participated in the 2024 SIMST bringing the total to 32 during EQUATE. Curriculum includes both nanoscience and quantum related topics and activities teachers can implement in their classrooms. This has become a popular program with recruitment progressing by referrals from past participants. This year, two participants shared how they incorporate knowledge and activities into their classrooms with colleagues from all over Nebraska at the NATS conference. **Metrics: Yr 1 development; Yrs 2-5 10 participants annually.**

Objective 4.2: Continue influencing the STEM pipeline through programs for undergraduate and graduate students, and postdoctoral researchers.

Postdoctoral Scientist Mentoring Program. There were 15 EQUATE postdoctoral fellows working on the project in the first year. **Metrics: 35 postdoctoral scientists, (7 per year).**

Graduate and Undergraduate Student Mentoring. Thirty-seven graduate students and 17 undergraduate students in Year 4. Meets metrics: 16 grad, 17 undergrad (cumulative 90 undergrad and 80 grad).

Student Seminar Series. This monthly seminar series brings together all EQUATE participants to hear short, informal presentations from postdoctoral researchers, graduate, and undergraduate students. It provides an opportunity for EQUATE trainees to improve their presentation and science communication skills. It aims at informing participants of the ongoing research within each FRG, as well as stimulating inter- and cross-FRG collaboration. Additionally, speakers from Sandia National Laboratories, University of Washington, and University of New Mexico shared their work during the series providing new ideas to faculty and students alike. **Metrics: 12 meetings per year.**

Nanoscience/Quantum Class, Minicourses, and Training. Introduction to Quantum Materials and Technologies (MATL 492/892) continues to be a popular offering for both undergraduate and graduate students. Spring 2025 registration includes 19 students (9 undergraduate, 10 graduate) from Chemical Engineering, Electrical & Computer Engineering, and Materials & Mechanical Engineering departments. **Metric: Cumulative 35 grad students, 250 participants (in progress).**

Objective 4.3 Provide professional development opportunities for faculty across Nebraska's colleges.

FIRST Award Program. Nebraska EPSCoR's annual **FIRST Awards** program provides assistance to this state's early-career, tenure-track faculty in the amount of $25,000 (with match required from each recipient's academic department). The grants are designed to help early career faculty initiate their research programs and compete more effectively for NSF CAREER Awards. In 2024, Nebraska EPSCoR awarded 6 recipients. The 2024 proposals were reviewed on November 4 by Nebraska's State Committee for final selection of funding. **Metrics: 6 awards annually.**

Broadening Participation

Objective 4.4: Increase the number of participants in STEM programs.

In the summer of 2024, Nebraska EPSCoR provided scholarships for 60 students attending **Loper Launch Summer Camps** at UNK, formerly known as PAWS University. Students in this program attend a variety of STEM-focused workshops over the summer to combat the inevitable summer slide. Additionally, Nebraska EPSCoR was able to work with **Aim for the Stars** summer program located at UNO to host a satellite camp in South Omaha.

A **2024 UNL Science Conference** engaged high school students in a wide variety of science-related fields and encourage them to pursue majors and careers in science, technology, engineering, and mathematics. Participants explored UNL's campus, met with student groups, and experience different STEM fields through hands-on activities in research labs. The conference will return in April 2025. **Metric: 90 students and 10 teachers.**

New this year, Nebraska EPSCoR was able to work with other UNL departments to bring **Dr. Raven the Science Maven** to campus for an evening of fun and impactful conversations about science communication, higher education, and her career. The 30 students, faculty, and staff attending found her talk to be inspirational and enjoyed Dr. Raven's ability to combine science and music.

Chemistry Professor **Mark Griep** has been working with two community colleges in Northeast Nebraska to increase research opportunities for faculty and engagement with the surrounding rural communities. Within the past year, one community college sponsored two outreach events: one was a public gardening event, and the other was an open house for middle and high school students. Another community college also sponsored two events: one was targeted to local high school students and the other was their annual online graduation celebration event. Griep and Hank Miller at the latter site created the online event during the remote Covid year to provide an event where undergraduates could describe their research. However, it has become an event that focuses on all graduating students and not just for researchers only.

College prep groups. Meets metric: 100 students/yr.

Nebraska EPSCoR and NCMN continue to host activities for middle and high school visitors to UNL campus. Students engage in tours and hands-on activities designed to help them learn about STEM careers. This year, two students who participated in the program during prior years became High School Researchers working in EQUATE labs.

Wignall, **Sangster**, and NCMN's **Huttenmaier** participated in a repeating afterschool program held at five middle schools in Lincoln, Nebraska. EQUATE staff spend time with students, teaching them about quantum topics and doing hands-on activities. Through this program, outreach staff impacts 75+ students several times per year. Additionally, the students visit UNL during the summer for hands-on activities and tours. This spring, one of the middle schools is planning a Family Science Night where EQUATE members will host activities.

The UNL College of Engineering's **Discover Engineering Days (DED)** introduce middle school students (grades 6-8) and their teachers to topics in engineering, physics, and the science programs offered at the University of Nebraska-Lincoln. The event is hosted by the college's outreach organization and is filled with hands-on activities that advance engineering habits such as collaboration, problem solving, creativity, and critical thinking skills. The DED offers 7 workshops over the year, averaging 100-150 students at each meeting. EQUATE Outreach is involved with this program throughout the year, teaching students about Triboelectric Energy and how it relates to Quantum. Students attending DED come from both rural and urban schools.

Communication and Dissemination

Objective 4.5 Increase public awareness of EQUATE

Tours, museum exhibits and public event participation were used to share EQUATE topics throughout the state. One museum exhibit is at the Elkhorn Valley Museum in Norfolk, NE; another, space-themed exhibit is at the Nebraska State Museum in Lincoln, NE. These exhibits bring quantum topics to thousands of people during Year 4. EQUATE representatives led activities at public events including Family Science Nights (Lincoln and Beatrice, NE), Astronomy Night (Lincoln, NE), and Forest Fest (near Plattsmouth, NE). Of special note, EQUATE SIs, graduate students, and staff joined forces to host hands-on activities for **Sunday With a Scientist** (**Fig. 33**)at the Nebraska State Museum (Streubel, Lai, Griep, E. Schubert, Wignall, Sangster, and Allen). Spring 2025 adds a new event: EQUATE's Omaha-based SIs, students, and staff (Wong, Wrubel, Wignall, and Sangster) share quantum activities at the Arbor Day celebration in Lauritzen Gardens. (meets metric)

The 2025 **Nebraska Research and Innovation Conference (NRIC)** is set for Friday, March 28 at the Graduate Hotel in Lincoln, NE. The slate of speakers for this year's public event was arranged by **FRG3 leader Jonathan Wrubel** with the event's theme: Quantum Computation and Quantum Simulation. Approximately 100 attendees, including 40 student poster presenters, are expected based on prior years' outcomes. (meets metric)

Figure 33: From Nebraska EPSCoR's 2024 annual report publication: EQUATE team members lead hands-on quantum activities with approximately 200 guests who visited Sunday With a Scientist in November 2024.

Dissemination of EQUATE research continues to be strong, with Web of Science showing 186 papers attributed to OIA-2044049 (Emergent Quantum Materials and Technologies/EQUATE, funded by NSF EPSCoR) at this writing, eight months into Year 4. This count is an 80% increase over the Year 3 number of 104 journal publications, and meets the goal metric of an average of four papers per SI.

EQUATE Management Team (MT) Meetings took place monthly in Year 4 (meets metric); the interaction helps coordinate project endeavors such as the statewide annual conference ("NRIC"), external review panel visits, external evaluation participation, and budget updates. Nebraska EPSCoR's **annual PR report publication** continues to share EQUATE accomplishments to a state-and-national mailing list of 800, plus online (PDF) views at the Nebraska EPSCoR website (meets metric).

Social media trends have shifted since EQUATE's Strategic Plan was set. The goal of 10% year-over-year increase for #NebEQUATE is on track to reach 84 mentions in Year 4 (ending in May 2025), rising from 76 in Year 3. EQUATE's website visits were not available at the time of this report's writing, due to long illness of the site's webmaster. (on track to meet metric)

Emerging Areas and Seed Funding

EQUATE's ***Faculty Mentoring through EQUATE Seed Grants*** program solicits seed proposals requesting one year of funding through a call for proposals. Seed proposals should be tightly focused on a particular research topic in quantum science and technologies, and typically involve one or two PIs at the tenure-track assistant, associate, and full professor levels. Projects that address quantum phenomena relevant to the current EQUATE FRG research themes are especially welcome. Funding for seed projects is limited to $56K/year (total cost).

Unlike previous years, in Year 4 the proposal call was announced to all six EQUATE-participating universities and colleges, including UNL, UNO, UNK, Creighton University, and the project's two Nebraska community colleges. Three proposals were submitted for consideration, and one was selected for funding in November 2024. The proposal chosen was from **Yanan "Laura" Wang** of UNL Electrical and Computer Engineering, who proposed "Van der Waals Heterostructures Toward Exciton-Polariton Quantum Simulators." She will work with Alexander Sinitskii, EQUATE FRG3 SI, on this research.

Dr. Wang's Year 4 Seed Award will continue into Year 5 and will expire when EQUATE program funding is scheduled to end on May 31, 2026. Despite the availability of EQUATE-related seed funding to all six of EQUATE's participating institutions, the only applicants were from UNL. When EQUATE faculty from the other participating institutions were asked why there were no seed applicants, the unanimous response was that any researchers working on quantum materials and technologies at those institutions were already receiving EQUATE funds as Senior Investigators with the project.

Metric: Yrs 1 and 2: 2 awards annually, Yrs 3 and 4: 1 award annually.

Table 1.

Seed Grant Recipient Name	Project Year	Title of Funded Seed Project
Yanan "Laura" Wang	1	Dynamic Control of 2D Single-Photo Quantum Emitters via Strain Engineering
Siamak Nejati Alexander Sinitskii	1	Heterostructures of 2D vdW and Porphyrin-Based Covalent Organic Frameworks as a Tunable Device Platform for Quantum Technologies
Martin Centurion	2	Characterization of the Ultrafast Structural Response in Photoexcited Materials
Mohammad Ghashami	2	Quantum Size Effect on Radiative and Electronic Transport
Yanan "Laura" Wang	4	Van der Waals Heterostructures Toward Exciton-Polariton Quantum Simulators

It is important to note that when rare departures of the project's Senior Investigators (SIs) occur, EQUATE has benefited from this pool of seed recipients (**Table 1**) who may merit elevation into the project as SIs. This was the case in Year 3 when **Wei Bao** moved to another state; **Alex Sinitskii** was a willing and capable addition to the FRG3 team, and he was readily approved in a vote by EQUATE's FRG leaders.

Partnerships and Collaborations

In addition to the typical types of higher education research collaborations (see EQUATE's list of collaborators in its Year 3 EDOCS report input), EQUATE continued to serve as a resource for the state of Nebraska and the U.S. Department of Defense on quantum topics. The project is frequently consulted through in-person visits of high-ranking leadership representatives of the U.S. Strategic Command (STRATCOM), associated with the National Strategic Research Institute (NSRI). The meetings are organized by Allen Geist, the director of the Electromagnetic Spectrum Operations (EMSO) Programs at the NSRI which is a DOD-designated University Affiliated Research Center sponsored by STRATCOM.

In addition to meetings with EMSO, the EQUATE scientific director Binek is now regularly consulted by Marty Sikes, Associate Executive Director of the Chemical and Biological Defense Program at NSRI. In Year 4, SI **Binek** became an NSRI Fellow, following EQUATE PI **Andrews** and EQUATE Associate Director Rebecca **Lai**, who had both previously attained NSRI Fellow status.

EQUATE continues to play a pivotal role in the second quantum revolution, driving discoveries, innovation, and workforce development. The Year 4 results highlight the success of the center's interdisciplinary, multi-campus collaboration. EQUATE remains honored to serve the nation as a trusted knowledge resource for STRATCOM.

Sustainability

In Year 4, EQUATE is intensifying its efforts to ensure long-term sustainability. In line with its strategic plan, the research and partnerships pursued by EQUATE are paving the way for proposals that will extend beyond the organization's lifespan.

A significant sustainability milestone is the Catalyst Award from UNL's Grand Challenges initiative. UNL is offering a total of $40 million over five years across seven areas identified as key Grand Challenges themes. EQUATE played a crucial role in advancing for Quantum Science and Engineering as one of these themes. Scientific Director **Binek**, a central figure in shaping the theme, was also appointed to the steering committee approved by the Chancellor's executive leadership team. In collaboration with Dr. Susan Hermiller (UNL Mathematics), Binek and a team of 21 UNL faculty members which include many EQUATE SIs and leaders, resubmitted a Catalyst proposal titled *Quantum Approaches Addressing Global Threats*, which was funded for five years with $4.7M. This highly interdisciplinary and expansive quantum research initiative strengthens EQUATE's sustainability and significantly expands quantum research participation beyond the traditional STEM fields by including the Arts and Humanities.

Another notable achievement includes an $800k grant secured by FRG2 leader **Laraoui** and collaborators from Jackson State University in Mississippi (an EPSCoR jurisdiction). This grant, running from 08/2024 to 09/2027, is titled *ExpandQISE: Track 1: JSU-UNL Collaboration on Quantum Sensing Research and Education … .* Additionally, PI Laraoui obtained a $300k single-investigator grant, from November 2024 to December 2025, titled *EPSCoR Research Fellows: NSF: Plasmonic Cavity Nanostructures to Enhance Single Photon Emission from Multilayered Hexagonal Boron Nitride*.

The EQUATE team is thrilled to announce that our non-R1 institutions, UNO and UNK, have secured a significant $2.8M DOE-EPSCoR 2023-2025 grant, led by SIs **Sabirianov** (UNO) and **Wysocki** (UNK). This grant is titled *A High-Throughput Computational and Experimental Approach to the Design of Unconventional Magnets*.

These early successes are strengthened by ongoing efforts to secure continued funding for collaborative interdisciplinary research. One such initiative is a proposal for a *Quantum Leap Challenge Institute (QLCI) titled Advances in Materials Science for Quantum Technologies* (AMSQuT). If funded, this six-year award will provide between $2M and $7M per year for a large interdisciplinary group of quantum researchers.

Scientific Director **Binek** is also a co-PI in an NSF Engine proposal led by Iowa State, titled *RuralSTAMINA: Ascending Rural Communities through Sustainable, Transformative Advanced Manufacturing Innovations and Alliances*. This proposal offers potential funding for up to 10 years, with a progressive budget starting at $7M in year 1 and reaching a maximum of $20M by year 10.

FRG1 leader **Hong** leads a DOE proposal titled *DoE EPSCoR Implementation: Emergent Interface Phenomena Enabled by Ferroelectric Oxide Thin Films and Membranes*. If funded, this two-year award will provide $1.5M per year for Hong and co-PIs **Dowben, Tsymbal, Zhang, and Xu**, who are EQUATE SIs.

Furthermore, **Binek** and selected EQUATE SIs are involved in a proposal led by the University of New Mexico, in collaboration with the University of Delaware, University of Arkansas, and MIT, to attract an NSF Engineering Research Center for Next-Generation Sustainable CMOS+X Technologies. If successful, this proposal will provide 5 years of support, with EQUATE PIs receiving a share of $2.25M.

Finally, under the leadership of Scientific Director **Binek**, a UNL team of approximately 25 PIs from physics, chemistry, mechanical and materials engineering, and electrical and computer engineering—including many EQUATE SIs—will compete for a new NSF-funded Materials Research Science and Engineering Center (MRSEC). The preliminary title of the proposal is *Atomically Engineered Materials* (AtEM). If funded, the MRSEC will provide six years of support with an annual budget of around $3M.

Management, Evaluation and Assessment

Each EQUATE FRG leader—as well the project's PI, Co-PI, Outreach team co-leads, and Nebraska EPSCoR staff—attends the project's monthly management team meetings (meets metric). The meetings are a well-regarded resource for project coordination, with a structured agenda shaped to address upcoming activities as well as recap recent initiatives. PI **Andrews** leads the discussions with foresight on lead times necessary ahead of initiatives, as well as follow-up on prior tasks assigned. The annual statewide research symposium, known as the Nebraska Research & Innovation Conference (NRIC), is an important topic for the EQUATE Management Team as the slate of speakers is arranged and event logistics are solidified. Annual project reporting to NSF is another extensive topic of preparation at these meetings of EQUATE leaders. Outreach occasions are also discussed with regard to volunteers needed for summer STEM placements of project-funded REUs and Young Nebraska Scientists camps in EQUATE research labs.

Also in attendance at these meetings is a representative from EQUATE's external evaluator, the Office of Educational Innovation and Evaluation (OEIE), participating remotely from Kansas State University. OEIE provides services contracted, including data collection and analysis of project outputs; annual evaluation reports are shared with the EQUATE Management Team and uploaded to EDOCS ahead of annual reporting deadlines. Their reviews of project interactions and bibliometrics are especially popular during OEIE presentations at each month's meeting.

In Year 4, EQUATE had a very thorough interaction with the NSF Site Visit Panel in mid-January 2025. NSF Program Officers Jose Colóm and Pinhas Ben-Tzvi facilitated the day-long review of FRG and Outreach presentations, and a half-day inspection of EQUATE facilities in Lincoln. Key points are represented in the Site Visit Panel's report and in the EQUATE response document, provided with this Year 4 reporting.

Expenditures and Unobligated Funds

As of this reporting period (June 1, 2024 – May 31, 2025), 86.23% of EQUATE Year 4 funds have been either spent or are committed to cover the current project year's salaries for researchers and staff participating in this Track-1 project. Regarding fund liquidation, 74.52% of the Year 4 funds have been drawn from NSF as of February 27, 2025. However, we anticipate that approximately $468,279.64 will soon be liquidated, given the monthly salary spending rate and the fact that the University of Nebraska System typically requires over a month after incurrence to complete the draw to cover actual expenditures posted in our accounting system.

Additionally, we expect to receive more invoices from our partnering institutions and sub-awardees (Creighton University, University of Nebraska at Omaha, University of Nebraska at Kearney, LPTC, NICC, University of Nebraska Medical Center, and Chadron State College) for expenditures anticipated in the remaining months of EQUATE Year 4 (February, March, April, and May).

Once these commitments are met, EQUATE spending will exceed 90% for the current reporting year, ensuring compliance with the EQUATE Cooperative Agreement's Programmatic Terms and Conditions.

Regarding the 60.57% increase in indirect costs in the expenditures table, this change is due to the recategorization of indirect costs associated with EQUATE researcher Salaries & Benefits. Previously, these indirect costs were included within Salaries & Benefits in the Expenditures table, following the same approach as the Salary Support table. Now, they have been separately categorized and added to the indirect costs row in the Expenditures table, while the Salary Support table continues to follow the previous format of including Salaries, Benefits, and other Indirect Costs.

Special Conditions

NSF conducted its Site Visit on EQUATE, with a panel meeting in Lincoln, Nebraska: Jan. 13-15, 2025. On Feb. 4, the Site Visit Report was provided to EQUATE's Principal Investigator, Matt Andrews, who shared it with the project's Management Team. On Feb. 17, EQUATE's Site Visit Report Response was provided by PI Andrews to NSF Program Officers Pinhas Ben-Tzvi and José Colom. These PDF documents have been uploaded with EQUATE's Year 4 Report materials via NSF's EDOCS website.

TABULAR/GRAPHIC REPRESENTATION OF PROGRESS TO DATE

The following table, from the most recent (Year 4) update of EQUATE's Strategic Plan, shows progress along the project commitments over time. (Please note, color-coded highlighting for annual EQUATE progress tracking: Green = task/s accomplished; Yellow = task/s in progress; Red = task/s behind schedule; underline indicates metric and bold text indicates milestone.) Also, this Year 4 representation includes "Tracked Changes" edits (text in red ink) and, upon approval by the cognizant Program Officer, these adjustments will be accepted as the official Strategic Plan version for EQUATE until further notice. Please note: a PDF version of this Year 4 edition of EQUATE's Strategic Plan is uploaded at the NSF reporting tool, EDOCS.

Table A1: FRG1 - Quantum Materials

FRG1 Goal: Gain understanding and control of a range of emerging quantum phenomena driven by correlation, topology, spin orbit coupling, and ferroic switching.						
Thrust 1: Topology, SOC, and Correlation-Driven Phenomena in Emergent Ferroic Materials Goal: Realize a range of emergent topology, spin, and correlation phenomena in novel ferroic materials, including topological antiferromagnets, 2D vdW magnets, and correlated oxides.						
Objective 1a: Explore quantum materials for antiferromagnetic spintronics.						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Characterize magnetic order and spin dynamics in B-doped chromia	Investigate the diffusion mechanism of boron in chromia	Characterize the ME response **Identify AFM order parameter and boundary magnetization** <u>Metrics: Extract the Néel temperature, magnitude of boundary magnetization, or direction of the Néel vector</u>	Probe spin structure and canting of boundary magnetization Explore 90-degree AFM DWs	Investigate switching dynamics **Achieve electrical rotation of Néel vector** <u>Metrics: Demonstrate via magnetic, magneto-optical, or NV center microscopy measure-ments</u>	Pump-probe dynamic investigation of Néel vector rotation	Binek, Laraoui
Characterize magnetic state of chromia heterostruc-	Characterize the electronic structure of Pd on	**Identify ferromagnetism in Pd induced by interfacial**	Investigate exchange coupling of Pd on chromia	**Fabricate 2D TMTC, such as TiS_3 and HfS_3, on chromia**	**Identify induced polarization in TiS_3 and HfS_3 on**	Dowben, Binek

tures	chromia	**chromia** Metrics: Extract the Curie temperature or the magnitude of magnetization		Metrics: Demonstrate via electrical and chemical techniques	**chromia** Metrics: Extract the magnetization via magnetic or spectroscopy techniques	
Explore the topological effect and spin transport in novel AFM thin films	**Synthesis of AFM thin films, such as 2D vdW $CrCl_3$.** Metrics: Demonstrate via electron microscopy/ spectroscopy techniques. Characterize the properties of the AFM films.	Synthesis of AFM thin films, such as $MnPd_x$. Establish theoretical model of the AFMs.	Examine electric, magnetic, and transport properties. Model the magneto-transport results.	Use Néel SOT to probe topological properties. **Theoretical search of other AFM candidates**. Metrics: Predict specific AFM materials.	**Achieve electrical control of topological properties.** Metrics: Demonstrate via electrical, transport, or magneto-optical techniques. Theoretical modeling of properties of the new AFM candidates.	Binek, Hong, Tsymbal
Objective 1b: Probe and control topological spin textures in ferroic oxides.						
Fabrication and characterization of ferroelectric oxides that can host persistent spin texture	Theoretical search of PST candidates Examine $EuO/BaTi_2O_5$ heterostructures Set up low frequency Raman spectroscopy	**Epitaxial growth of ferroelectric thin films potentially hosting PST** Metrics: Structural and surface characterization of the thin film samples Study the magneto-capacitive effects in Ni on $BiInO_3$	**Ferroic domain imaging** Metrics: Identify the domain structure via PFM or MFM imaging **Raman studies of collective local structural and polar fluctuations in complex**	Raman studies of spatial inhomogeneity and local structural dynamics. **Theoretical search of other PST candidates.** Metrics: Predict specific PST materials. Characterize the ME coupling in	Synthesis/ investigate new PST materials. Theoretical modeling of new PST materials. Raman studies of spin/carrier relaxation	Guo, Hong, Streubel, Tsymbal

			oxide films Metrics: Identify the associated Raman peaks	heterostructures based on antiferroelec-trics and ferromagnets, i.e., Ni/$BiInO_3$. Metrics: Quantify magnetic field-controlled current-voltage curves and anticipated capacitive behavior.		
Fabrication and characterization of PST tunnel junction devices		**Fabrication of tunnel junction** Metrics: Demonstrate the device layout and fabrication flow via optical image and AFM Develop first-principles approaches to calculate anomalous and spin Hall effects	**Characterize tunneling resistance** Metrics: Demonstrate the I-V characteristic of tunneling behavior Theoretical modeling of tunneling results	**Imaging tunnel current** Metrics: Demonstrate via conductive probe AFM imaging or NV center microscopy Theoretical modeling of tunneling anomalous Hall/spin Hall effects	**Characterize tunneling anomalous Hall/spin Hall effects** Metrics: Demon-strate via magneto-transport measure-ments Study thickness dependence of tunneling effects	Binek, Hong, Laraoui, Tsymbal
Explore topological Hall effect (THE) in magnetic oxide thin films	**Thin film growth of $NiCo_2O_4$, $CoFe_2O_4$ and rare earth garnet** Metrics: Structural and surface characterization of the thin film	**Resolve magnetic state via anomalous Hall effect and THE** Metrics: Demonstrate via magnetotransport measurements	Charac-terize the magnetic properties of strain-free $NiCo_2O_4$ films via magnetometry. Metrics: Determine	**Imaging of magnetic structures** Metrics: Demonstrate via MFM/ MOKE/XPM/ NV center microscopy Theoretical studies of Berry phase	Theoretical modeling of transport signatures due to appearance of meron, bimeron, or anti-meron in in-plane magnetic system	Hong, Kovalev, Streubel, Xu

	samples Develop micro-magnetic theory approaches for modeling THE	Fabricate yttrium iron garnet films via metal-organic decomposition epitaxy	the magnetic Curie tempera-ture and suscep-tibility.	due to quantum-spin fluctuations		
Achieve strain and field effect control of THE		Probe the surface to bulk core level shift	**Achieve strain control of THE** Metrics: Demonstrate via magnetotransport measurements	**Fabricate field effect devices with dielectric and ferroelectric gates** Metrics: Document the device layout and fabrication flow via optical image and AFM	**Achieve field effect control of THE** Metrics: Demonstrate via magnetotransport measurements Correlate magnetic imaging with spin transport studies	Hong, Laraoui, Xu
Objective 1c: Probe entanglement and correlation effect.						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Achieve voltage-controlled entanglement in B-chromia	Establish NV imaging condition in magnetic oxides	**Probe 90 degree switching of surface spin of B-chromia and its interaction with NV center spin** Metrics: Demonstrate via NV center measurements	Probe voltage-controlled surface/NV spin-spin interaction	**Achieve chromia magnetization/NV center spin entanglement via voltage-controlled exchange interaction** Metrics: Demonstrate via NV center measurements	**Achieve oxide/NV center spin entangle-ment via ferroelectric polarization control** Metrics: Demonstrate via NV center measurements	Binek, Laraoui,

Theoretical understanding of entanglement and correlation effects	Modeling of cubic AFMs with reduced magnetic point-group symmetry					
Develop new solid state schemes and platforms for quantum information control and protection		**Identify new solid state platforms for realizing bosonic error correction, e.g., magnons, phonons, plasmons, polaritons, etc.** Metrics: Identify the relevant parameters for realizing bosonic error correction	Develop new quantum information protection schemes and platforms, e.g., skyrmions for majorana modes	**Develop new experimental proposals for realizing bosonic error correction** Metrics: Propose specific experimental setup and parameters	**Develop new experiment-tal proposals for realizing novel majorana modes based on skyrmions** Metrics: Propose specific experimental setup and parameters Identify best schemes for quantum information control and protection	Kovalev
Thrust 2: Magnetoelectric and Valley Control of Layered Two-Dimensional Materials						
Goal: achieve ME and valley control of layered 2D vdW materials.						
Objective 2a: Achieve magnetoelectric control of topological states in graphene.						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Investigate SOC effects in graphene/chromia heterostructure	Use spin transport to evaluate SOC in graphene induced by chromia	**Investigate quantum interference effects in graphene on chromia** Metrics:	Explore effects of sublattice symmetry breaking and magnetic interaction	Investigate spin transport in graphene on B-chromia, focusing on 90-degree	Investigate quantum interference effects in graphene on B-chromia Metrics:	Binek, Dowben, Kovalev , Streubel

		Demonstrate via magnetotrans-port measurements **Establish the characterization capability for ferromagnetic resonances in magnetic thin films.** Metrics: Determine the ferromagnetic resonances and magnetic homogeneity of YIG films.	on spin lifetime in graphene **Theoretical modeling of spin transport** Metrics: Extract spin relaxation time	rotation Utilize x-ray magnetic linear dichroism and x-ray magnetic circular dichroism to probe the Néel vector orientation and general spin structures and spin switching in chromia.	Extract spin relaxation time Utilize ferromagnetic resonance spectroscopy to probe the Néel vector orientation and general spin structures and spin switching in chromia. Modeling of experimental data	
Predict ME effect in novel 2D ferroics		**Theoretical prediction of ME effect in designed ferroelectric 2D magnets** Metrics: Extract ME coupling coefficient	Predict electronic and magnetic properties of novel 2D ME materials	**Design novel 2D ME materials and structures** Metrics: Predict specific candidate materials and structures	Explore 2D ME AFMs	Tsymbal
Objective 2b: Explore emergent 2D materials for designing valley spin valves.							
Investigate valley spin valves based on 2D vdW materials	Examine chiral effects in TiS_3 **Theoretical search of 2D materials for realizing VSV**	**Probe electronic structures of TiS_3, ZrS_3** Fabricate vdW heterostructures for constructing the VSVs **Theoretical search of 2D materials for realizing nonvolatile VSV**	**Search for FM in Pd on MoS_2** Magnetotransport characterizations of vdW heterostructures	Study electronic structure of Au on MoS_2 **Identify transport and MOKE signatures of VSV effect in vdW heterostructures**	Investigate charge density wave effects in $TiTe_3$ **Optimized the material design of nonvolatile VSV** Metrics: Identify optimized material parameters **Demonstrate**	Dowben, Hong, Tsymbal, Zhang

					control of valley and spin degrees of freedom by using magneto-optical spectroscopy. Metric: Quantify the valley lifetime across multiple devices under different vertical electric fields.	
Probe dynamic Coulomb screening in 2D vdW interfaced with halide perovskites and ferroelectric oxides	Demonstrate dynamic emission Stokes shift in halide perovskites as tunable substrates	**Set up low temperature confocal microspectroscopy** Metrics: Perform low temperature measurements	**Extract coupling strength between band edge transition in TMDC and substrate dielectric screening** Metrics: Identify the magnitude of coupling strength Modulating of TMDC edge transitions	**Spatially resolve domain structures in ferroelectrics or defects in halide perovskite** Metrics: Demonstrate via optical spectra mapping Assess local variations of carrier dynamics modulated by substrate Coulomb screening or ferroelectric polarization	Probe the modulation of carrier and valley populations via Coulomb screening/ polarization effects of the substrate	Guo
Thrust 3: New Materials for Spin-Qubit Systems						
Goal: explore the material design of ferroic molecules and metal-organic frameworks as new platforms for constructing spin-qubit.						
Objective 3: Explore molecular system as materials platforms for spin-qubit systems.						
Realize electric control of	**Fabricate SCO molecular**	**Study effect of dielectrics on the spin state**	**Fabricate SCO/ ferroelectri**	**Study SCO properties in heterostruct**	**Identify effect of ferroelectric**	**Dowben, Lai, Xu , Streubel**

molecular spin state	**crystal thin films on dielectric substrates** Metrics: Demonstrate via AFM, electric, or spectroscopy characterizations **Build $Fe(trz)_2$-based light polarization phototransistors** Metrics: Demonstrate via electric measurements	**of SCO** **Thin film deposition and device fabrication of $Co^{2+/3+}$ SCO molecules** Metrics: Demonstrate via AFM, electric, or spectroscopy characterizations	**c heterostructures** Metrics: Demonstrate via AFM, electric, or spectroscopy characterizations **Build transistors/phototransistors based on $Co^{2+/3+}$ SCO molecular and $Fe(HB(tz)_3)_2$** **Determine spin precession in SCO molecular transistors using FMR** **Demonstrate magnetic field-controlled electronic transport in spin-crossover molecular films**	**ures in response to heat and light stimuli** **Extract exchange coupling in SCO molecular bilayer systems** Metrics: Identify the magnitude of exchange coupling strength	**polarization on the SCO transition in heterostructures** Metrics: Extract the transition temperature or order parameter as a function of ferroelectric polarization **Demonstrate the magnetic field-driven and voltage-controlled excitation of ferromagnetic resonances in spin-crossover molecules**	
Build a Zener - Mach solid state interferometer as a logic gate		**Establish the group theory of a Zener - Mach solid state inferometer as a logic gate** Metrics: Propose the operation			**Build a Zener - Mach solid state interferometer from spin crossover molecules** Metrics:	Dowben

		scheme			Demonstrate the logic operation	
Develop MOF for scalable quantum information	**Fabricate [Fe-(pyrazine){Pd(CN)$_4$}] thin films using layer-by-layer assembly approach** Metrics: Demonstrate via SQUID, XPS, XAS, XRD, UV-Vis, or electro-chemistry charac-terizations	Synthesis and characterization of [Fe(Htrz)$_2$(trz)](BF$_4$), polyaniline, and Fe_3O_4 nanocomposites	**Design, synthesis, and characterization of Fe/Ni SCO complexes** Metrics: Demonstrate via SQUID, VSM, XAS, XRD, SEM, mass spec, NMR, UV-Vis, Raman or IR	**Fabrication of devices with improved device character-istics** Metrics: Demonstrate via SQUID, VSM, SEM, TEM, transport or AC conductivity measure-ments	**Fabrication and characterization of voltage-controlled devices with Fe, Fe/Ni, Fe/Pd SCO complexes** Metrics: Demonstrate via SQUID, VSM, transport measure-ments	Lai
Characterize framework phonon modes in MOF	**Set up low frequency Raman spectroscopy for measuring collective framework phonon modes** Metrics: Demonstrate the performance on calibration samples	Spectroscopic characterization of [Fe(Htrz)2(trz)](BF4)	**Identify vibrational signatures of spin states in SCO complexes using Raman spectroscopy.** Metrics: Measure Raman spectra of SCO complexes as optical readout of its spin state	Tune the structure and structural dynamics of SCO complexes using high pressure conditions generated inside a diamond anvil cell (DAC).	**Achieve modulation of spin crossover transitions under high pressure** Metrics: Identify optical signatures of high-pressure modulation of spin crossover transitions	Guo, Lai
New tenure-track hire process (UNL)	**Select short list** Metrics: Send out interview	**Interview candidates** Metrics: Arrange	Ensure new hire connects with FRG leader and	Welcome new hire to campus and introduce them to	Continue new hire's mentoring from FRG leader/team	Binek, Laraoui, Hong, Tsymbal, Streubel

	invitations	interview visits **Make offer** Metrics: Provide a startup package	project science director for effective mentoring.	EQUATE team		
Outputs for FRG1	Metrics: publish 10 peer-reviewed papers per year (total: 50 papers/5y), present 20 conference presentations per year (total: 100 presentations/5yr), submit 4 external proposals per year (total: 20/5yr), and graduate 5 PhD students over 5 years.					

Table A2: FRG2 - Quantum Technology

FRG2 Goal: explore different quantum technologies based on solid-state spin qubits for quantum sensing and metrology, and photons for ultrafast, compact, and low-power quantum communication nanophotonic devices.						
Thrust 1, Objective 1.a: Probing Spin-Magnon Interactions in Ferromagnetic (FM) Waveguides						
Goal: Study spin-magnon interactions in a hybrid system composed of NV spin qubits coupled with ferromagnetic (FM) waveguides.						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Fabrication and integration of FM waveguides to NV centers in diamond	Grow YIG, CoFeB films/Nanowires. Make devices (electrodes) to control the magnon modes. **Make FM waveguides to study effect of sample on magnon modes** METRICS: made CoFeB and YIG waveguides integrated with MW stripelines.	Grow CoxFe1-x (x=0-1) thin films and waveguides. METRICS: made CoxFe1-x (x=0-1) waveguides integrated with MW stripelines.		Engineer single NVs to FM waveguides (nanowires) for distant NV spin coupling using magnons as quantum buses.	Check other defects in SiC for better integration/ Fabrication of FM waveguides on SiC .	Laraoui, Liou
Setup development	Integrate cryostat (3.5 - 350 K) and electro-magnet to the NV setup. METRICS: built the cryogenic NV setup				Modify the setup to accommodate SiC spin characterization and sensing.	Laraoui
Quantum sensing microscopy of magnons in FM waveguides	Perform NV microscopy of FMR modes in CoFeB and YIG waveguides. METRICS: characterized CoFeB and YIG samples	Study the effect of film thickness and waveguide geometry on the magnon frequency and linewidth (damping) as function of	Determine spin-magnon coupling coefficients and type of magnon proposes relevant in YIG METRICS: determined	**Study spin-magnon interactions in other FM insulators such TmIG** METRICS: Optimized the hybrid diamond-FM	**Explore magnons as quantum buses and understand effect of magnetic noise on spin coherence**	Laraoui

		temperature and magnetic field in YIG, CoFeB METRICS: understood effects of thickness of CoFeB and YIG on magnon modes (frequency, linewidth, damping).	the NV-spin magnon coupling coefficients in YIG	waveguide for single NV spin qubits-magnon coupling.	**lifetime T2 of single NVs** METRICS: determined the feasibility of using magnons as quantum busses to couple distant spin qubits.	
Equipment	Purchase equipment: cryostat 3-400 K, electromagnet (up to 3T), single photon detectors, MW and optical equipment METRICS: by end of year 1 most of the equipment is purchased and installed.					Laraoui
Thrust 1, Objective 1.b: Quantum Sensors for Low Field Magnetic Resonance Spectroscopy						
Goal: Develop low field magnetic resonance microscopy using diamond quantum sensors integrated with hyperpolarization schemes and FMN nanoparticles as spin amplifiers/contrast agents.						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Setup develop-ment	**Build and optimize NV setup for low-field (LF) - magnetic resonance (MR) imaging.** METRICS: by end of year NV-LF-MR setup is ready for	Integrate hyperpolarization protocols based on solid state effect and double spin resonance to NV- LF-MR setup		Enhance the NV magnetic sensitivity using hybrid NV-FMN nanoparticles		Liou, Laraoui

	measurements.					
Nanofabrication and integration	Fabricate diamond membranes /thin films to optimize NV layer for low magnetic resonance spectroscopy	**Make grating on top of diamond for better control of density and NV-distance of the target samples.** METRICS: optimized grating nanofabrication on top of diamond substrates and tested on iron-containing biomolecules	Optimize and integrate microfluidic chips to diamond chips for NV-LF- MR setup	Fabricate FMN to amplify weak magnetic fields generated from external target spin molecules		Liou
Quantum sensing and NV-LF MR imaging			**Improve the sensitivity and spectral resolution of NV-LF-MR system using hyperpolarization schemes.** METRICS: optimized the sensitivity and spectral resolution of LF-NV MR imaging by using hyperpolarization schemes	**Improve sensitivity of NV-LF-MR using FMN as spin amplifiers.** METRICS: improved the sensitivity and spectral resolution of LF-NV MR imaging setup by using FMN	**Perform LF - MR imaging of different solid and liquid samples.** METRICS: understood of the local spin environment of the solid and liquid target samples	Liou, Laraoui
Equipment	Purchase of equipment: single photon detectors for single NV NMR, MW and optical equipment, NMR magnets					Laraoui, Liou

	METRICS: By end of year 1 the equipment is integrated to the NF-LF-MR setup.					
Thrust 1, Objective 1.c: Characterizing new solid-state Qubits in Ultrawide Band Gap semiconductors						
Goal: develop THz-EPR-Ellipsometry as a novel tool for identification and characterization of solid-state qubits in UWBG heterostructures and vdW materials. Superior to conventional, absorption-based EPR, THz-EPR-E measures the complex-valued dielectric function tensor including anisotropy in thin layers and heterostructures.						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
THz-EPR Setup development and improve-ment	**Develop high-frequency scanning high-field (7 Tesla) Terahertz electron paramagnetic resonance ellipsometry (THz EPR-E) instrumentation using free electron laser sources** Metrics: built and optimized high-field THz-EPR-E system	Develop THz-EPR-E instrumentation using solid state synthesizer sources	Develop THz-EPR-E electron nuclear double resonance instrumentation (THz-EPR-E-ENDOR) using solid state synthesizer sources	Develop photo modulation THz-EPR-E using tunable near-infrared - ultraviolet photoexcitation sources	Develop photo modulation THz-EPR-E-ENDOR using tunable near infrared-ultraviolet photoexcitation sources	M. Schubert
Spectro-scopy of color centers in UWBG semicon-ductors	Test THz-EPR on diamond NV centers to check the sensitivity.	**Demon-strate THz-EPR-E on defect spin systems in Gallium Oxide bulk crystals.** Metrics: demonstrated THZ-EPR-E	**Demonstrate characterization of spin dynamics in SiC and Ga_2O_3 single crystals.** Metrics: demonstrated THZ-EPR-E single of defect spin systems in Ga_2O_3 and SiC	**Demon-strate charac-terization of photo-ionization and carrier excitation dynamics of potential quantum emitters in**	**Demon-strate time evolution of characterization of photoionization of quantum emitters in SiC, Ga_2O_3 and AlN**	M. Schubert

		single of defect spin systems in Ga_2O_3 bulk crystals	single crystals	**SiC, Ga_2O_3 and AlN** Metrics: demon-strated photoionization and carrier excitation dynamics of quantum emitters in Ga_2O_3, SiC, and AlN.	Metrics: demon-strated time evolution of photoionization of quantum emitters in Ga_2O_3, SiC, and AlN.	
Thrust 2, Objective 2.a: Enhanced Nonlinear Optical Effects at the Nanoscale						
Goal: Design new nanocomposite nonlinear nanostructures to substantially enhance the nonlinear optical effects efficiency						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Develop nonlinear optics simulations and theory	Theoretically design new chiral nanostructures to substantially enhance the nonlinear optical effects efficiency.	**Determine the best and most realistic ultrathin nanostructure that can achieve maximum nonlinearity enhance-ment** Metrics: optimized ultrathin nanostructures for enhanced nonlinear optical properties.		Design chiral quantum optical devices based on the fabricated structures.		Kilic
Fabrication and Epitaxial growth of optical	Fabricate new anisotropic and chiral	Develop new ALD epitaxial growth techniques		**Obtain circular polarized high**	Use TiN, and lattice resonances in the	E. Schubert, M. Schubert

nanostructures	nonlinear structures using iGLAD bottom-up growing technique. **Nanofabrication system optimized.** Metrics: Fabricated anisotropic chiral nonlinear structures.	to design nonlinear optical structures		**harmonic generated waves from the fabricated helical structures** Metrics: demonstrated circular polarized harmonic generation form the fabricated chiral structures	nanophotonic structures to achieve stronger and tunable nonlinear responses.	
Measurement setup development	Implement g(2)(t) mapping, photon statistics and life-time measurements to study of chiral nanostructures.	Perform ellipsometry on chiral optical nanostructures.	Measure various enhanced nonlinear optical effects from the fabricated structures at multiple and single photon level.	**Optical nonlinear measurement setup optimized.** Metrics: built and optimized the nonlinear optical measurement setup.		M. Schubert, Laraoui
Thrust 2, Objective 2.b: Robust Entangled Photon Generation from Nanoscale Structures						
Goal: Produce enhanced and robust entangled photons that will carry the quantum optical information in a secure way.						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Simulate processes that can generate entangled photons.	Theoretically design ultrathin nanocomposite nanostructures to enhance the	Optimize and determine ultrathin nanostructure that can achieve maximum SPDC leading			Measure various quantum optical effects, such as photon statistics and inter-	Kilic

	nonlinear process of SPDC. **Model the SPDC process.** Metrics: modeled the SPDC process in different ultrathin nanocomposite structures	to a strong entangled photon pair generation.			ference.	
Fabricate entangled photon sources.			Fabricate nonlinear metasurfaces and integrate them with conventional BBO nonlinear crystals to enhance the SPDC efficiency.	**Fabrication of SPDC meta-surfaces** Metrics: Fabricated SPDC metasurfaces		E. Schubert, M. Schubert
Develop experimental setup for quantum photon statistics measurements.	Develop experiment-tal set-up to produce and measure SPDC two-photon entangled pairs.	**Optimize SPDC efficiency.** Metrics: Optimized the SPDC processes	Implement g(2)(t) mapping, photon statistics of entangled photon-pairs.			Bao left UNL; his tasks in Years 4 and 5 are discontinued
Equipment	Purchase of equipment: tunable femtosecond laser, single photon detectors, MW and optical equipment. Metrics: By end of year 1 the equipment is integrated to					Laraoui

	the SPDC setup.					

Thrust 2, Objective 2.c: Efficient Single Photon Generation from Nanoscale Structures						
Goal: Produce single-photon quantum optical sources operating at room temperature with high fidelity, indistinguishability, and brightness that will carry the quantum optical information in an efficient way.						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Simulations and theoretical design of single-photon sources			Theoretically design single-photon optical sources compatible with CMOS chips operating at room temperature.	**Simulate the single-photon emission and other photon statistics quantum optical processes.** Metrics: theoretically understood single-photon emission related to quantum optical processes	**Optimize and determine the best and most realistic single-photon quantum sources.** Metrics: determined the best config-uration for single-photon quantum sources	Kilic
Fabrication of single-photon sources.			Fabricate single-photon optical sources, e.g. hBN, SiC, AlN integrated with novel composite structures	**Optimize the fabrication of efficient single-photon quantum optical sources from nanoscale structures.** Metrics: fabricated photonic nanoscale		E. Schubert

				structures with enhanced single-photon emission properties		
Develop experimental setup to measure single photons.			Develop experimental set-up to characterize single photon emission by measuring the photon correlation function mapping.	**Measure the single photon emission from various nanostructures.** Metrics: measured single-photon emission from various photonics structures.	**Charac-terize single photon emission by measuring the photon correlation function mapping.** Metrics: characterized single photon emission by using photon correlation mapping	Laraoui
Equipment	**Purchase of equipment:** tunable pulsed picosecond laser, single photon detectors, and optical equipment Metrics: By end of year 1 the equipment is integrated to the optical setup for single-photon characteriz-ation.					Laraoui
Outputs for FRG2	Metrics: published 6 peer-reviewed papers per year (total: 30 papers/5y), presented 12 conference presentations per year (total: 60/5y) , submitted 3 external proposals per year (total: 15/5y) , and graduated 5 PhD students graduated over 5 years.					

Table A3: FRG3 - Quantum Information Processing

FRG3 Goal: To identify and emulate novel many-body quantum systems capable of expanding the horizon of quantum material technologies and quantum computation						
Thrust 1, Objective 1.a: Surpassing the Standard Quantum Limit in a ^{41}K BEC						
Goal: Exploit spin-dependent control of a spinor potassium BEC using radio-frequency Feshbach resonance to demonstrate interferometer precision beyond the standard quantum limit						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Develop-ment of RF Feshbach Resonance	Capital equipment purchases of cooling laser and dipole trap laser Produce 41-K BEC Install hardware and computer control needed to produce RF-FR	Capital equipment purchase of imaging camera Install magnetic field noise cancellation system Measure lifetime of atoms in the presence of the RF-FR	**Measure the spin-dependent scattering lengths in a BEC using the RF-FR** Metric: measured spin-dependent scattering length versus RF power and frequency			Wrubel
Spin-Interferometry beyond the standard quantum limit		Install hardware for hyperfine ac Stark shift of atoms	Measure the spin-dependent interaction energy from the spin-mixing dynamics	Measure magnetization spin-noise and quantify spin-correlations resulting from parametric down-conversion	**Measure the maximum fraction of atoms for which entanglement can be reversed using the RF-FR** Metric: measured maximum fraction of atoms for which entanglement can be reversed using the RF-	Wrubel

					Fr	

Thrust 1, Objective 1.b: Emulation of Novel Spin Systems						
Goal: Use the RF Feshbach resonance to emulate novel spin systems and quantum walks						
Activities	Checkpoints and **Milestones (bold)**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Complex phases in 2D optical lattices	Capital equipment purchase of laser for 2D optical lattice	Install lasers and optics for 2D optical lattice	Demonstrate momentum-space crystal structure in 1D and 2D optical lattices	**Determine the ground-state of a magnetic phase made possible by the RF-FR** Metric: Measurement of spinor diffraction after time-of-flight release from the 2D lattice versus RF-FR modulation.		Wrubel
Emulation of quantum walks with a spinor BEC				Implement hardware control techniques needed to emulate quantum walks	**Emulate a 1D quantum walk in a spinor BEC** Metric: Measurement of the fidelity of a quantum walk in a spinor BEC	Wrubel

Thrust 1, Objective 1.c: Quantum Emulation with an Exciton-Polariton BEC						
Goal: Develop a room-temperature quantum emulation system using an exciton-polariton BEC						
Activities	Checkpoints and **Milestones in bold**					
	Year 1	Year 2	Year3	Year 4	Year 5	Responsible
Demonstrate old landmark	Build the full sample preparations and	**Demonstrate the old landmark**				Bao left UNL after Year 2

experiments, previously only possible with cold atom or GaAs	photoluminescence capability in exciton polaritons	**superfluidity Cerenkov experiments previously only possible with cold atom or GaAs** Metric: Measurement of Cerenkov wave pattern as a hallmark of superfluidity in halide perovskite exciton-polariton BEC				
Explore unique experiments at room temperature with perovskites, such as spin-orbital physics, best only possible or impossible with cold atom			Demonstrate spin-orbital physics in perovskite microcavity at room temperature perovskites			Bao
Thrust 1, Objective 1.d: Theory of Polarons in Dipolar and Spinor Gases						
Goal: Theoretically predict the behavior and measurable effects of dipolar polarons in Bose-Einstein condensates						
Activities	Checkpoints and **Milestones in bold**					
	Year 1	Year 2	Year 3	Year 4	Year 4	Responsible

Develop a theory based on a modified Gross-Pitaevskii equation for analysis of dipolar polarons and other experimentally relevant systems with impurities	Create and adapt codes for standard and dipolar GPE equation	**Produce a code/solver for the static properties (such as self-energy and effective mass) of dipolar polarons using the developed theory** Metric: Computer code solving for the static properties of dipolar polarons				Armstrong
Develop codes for various dipolar polaron systems and relevant spinor optical lattice systems			Develop/extend code(s) for more properties of polarons such as induced polaron-polaron interactions and the time-dependent properties of the quasi-particle	Modify codes as necessary to calculate time dependent densities of dipolar and Gaussian impurities. Modify or create codes to calculate scissors-mode oscillations in BECs to use in Lee-Huang-Yang (LHY) liquids.	**Complete computer codes for structural polaron properties and polaron-polaron interactions in different interaction regimes** Metric: Computer code solving for structural polaron properties and polaron-polaron interactions **Adapt optical lattice codes for 2D to calculate energies and**	Armstrong

					heat capacities. Metric: Computer code calculating energies and heat capacities in 2D optical lattices	
Thrust 2, Objective 2.a: Quantum Walk Algorithms						
Goal: Determine the consequences for computational efficiency of nonlinear search algorithms						
Activities	Checkpoints and **Milestones in bold**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Determine the general properties of nonlinear search algorithms			**Calculate the computational efficiency of nonlinear search algorithms with multiple correct answers** Metric: Calculated computational efficiency of nonlinear search algorithms with multiple correct answers	**Determine the correct Hamiltonians for nonlinear search algorithms** Metric: Hamiltonian for nonlinear search algorithms		Wong
Evaluate computation speed up for nonlinear quantum walks in realistic systems				**Determine the distribution of 1D nonlinear quantum walks** Metric: Predicted distribution	**Predict computational efficiency of nonlinear search algorithms on networks that are highly connected***	Wong

				of 1D nonlinear quantum walks	**Predict computational efficiency of nonlinear search algorithms on periodic lattices in 1D, 2D, and 3D*** ***both milestone & metric**	
Evaluate performance of quantum search algorithms				**Determine how a bottleneck affects quantum search on the barbell graph** **Calculate the speed of a quantum search algorithm governed by the signless Laplacian**		Wong
Thrust 2., Objective 2.b: Crosswire Quantum Dots for Quantum Computing						
Goal: Investigate crosswire quantum dots as possible qubits for quantum computation						
Activities	Checkpoints and **Milestones in bold**					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Theoretical analysis of sub- and super-radiant spaces created by the coherent interaction	Develop a code (Matlab) computing quantum states in cross-road QD, interaction	Construct effective Hamiltonian of the quadratic spin-spin interaction with long-range force	**Calculate the decay rates of a single QD and finite-size array of QDs coupled to the resonant**			Mei and Sabirianov

of N interacting qubits in 1D (or possibly 2D) finite lattices.	between qubits and their dynamics (code for numeric simulation of time evolution of QD arrays)	and strong correlation	**waveguide mode** Metric: Predicted decay rates of single QD and finite-size array of Qds coupled to the resonant waveguide mode.			
DFT analysis of 2D materials to characterize the properties of proposed crosswire QD applications including graphene-based systems, TMDs, and thin film ferromagnetic systems.				Calculate energy states of 2D array of cross-road quantum dots with materials of promise (target for fabrication with our collaborators)	**Based on the DFT modeling, compute configurations for semiconducting QDs with long lifetime of the bound state and design a prototype application for quantum computing** Metric: Predicted configurations of QDs with long lifetime of the bound state Metric: Design of a prototype application for quantum computing	Mei and Sabirianov

Thrust 2., Objective 2.c: Computational Design of New Spin-Qubit Materials
Goal: Investigate novel spin-qubit materials theoretically
Activities (Checkpoints and **Milestones in bold)**

Activities	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Magnetic adatoms as spin-qubit materials		Identify promising adatom type and surface combinations. Determine preferred adsorption sites. Perform atomic relaxations.	**Compute the low-energy electronic spectrum** Metric: Calculate magnetic anisotropy and hyperfine coupling parameters	Study exchange coupling between adatom pairs **Construct spin Hamiltonian and investigate spin dynamics** Metric: Compute electric field dependence of magnetic interactions	Study the effect of atomic structure and vibrational modes on magnetic interactions Metric: Predict adatom spin-qubit systems that satisfy the DiVincenzo's criteria	Wysocki
Thrust 2., Objective 2.d: Experimental Realization of Crosswire Quantum Dots in Transition Metal Di(Tri)chalcogenides						
Goal: Produce and test crosswire quantum dot structures						
Activities (checkpoints, **Milestones in bold)**	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Experimental realization of crosswire QD structures based on graphene-based systems, TMDs, and thin film ferromagnetic systems.			Growth of high-quality graphene, TMDs and 2D ferromagnetic materials (such as CrI_3) for the fabrication of crosswire QD structures.	Patterning of sub-20-nm strips of TMDs, TMTs, and 2D ferromagnetic materials and their stacking into crosswire QD junctions. Metric: Demonstration of crosswire QD structures with a control over the width of wires and the twist angle.	**Measure transport properties of crosswire QD structures** Metric: Demonstration of QD properties in crosswire QD structures	Sinitskii

New Faculty Hire in FRG3 at the University of Nebraska at Kearney

New tenure-track hire	Applicant screening;	New incumbent begins work;	Ensure new hire connects with FRG leader and	TBD	TBD	Department of

process (UNK)	offer/s made and accepted	meets EQUATE team	project science director for effective mentoring.			Physics, UNK
Outputs for FRG3	Metrics: publish 6 peer-reviewed papers per year (total: 30 papers/5y), present 12 conference presentations per year (total: 60/5y), submitted 2 external proposals per year (total: 10/5y), and graduate 4 Masters students and 1 PhD students over 5 years.					

Table A4: Outreach and Workforce Development

Goal: Create/continue programs that encourage youth to pursue further STEM education.						
Objective 4.1: Equip Nebraska students (grades 6-12) with resources for success in the STEM workforce.						
Young Nebraska Scientists Activities	Checkpoints / Milestones					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Young Nebraska Scientists Camp Development	Camp curriculum development	**1 new camp/yr**	**1 new camp/yr**	**1 new camp/yr**	**1 new camp/yr**	NE EPSCoR
YNS Middle School & High School Camps	Development	**85 (Total) with 30 EQUATE participants /yr**	**85 (Total) with 30 EQUATE participants /yr**	**85 (Total) with 30 EQUATE participants /yr**	**85 (Total) with 30 EQUATE participants /yr**	NE EPSCoR
YNS HS Researchers	8/yr	8/yr	8/yr	8/yr	8/yr	NE EPSCoR
YNS Mobile Labs: Molecular Bio (existing) & add STEM/Quantum	Development	**3 EQUATE-specific kits released**	3 EQUATE specific kits in operation	3 EQUATE specific kits in operation	3 EQUATE specifics kits in operation / yr	NE EPSCoR
Remotely Accessible INstrument prog	Development	**Made available to 200 teachers/yr with minimum of 5 experiences/ yr**	**Made available to 200 teachers/yr with minimum of 5 experiences/ yr**	**Made available to 200 teachers/yr with minimum of 5 experiences/ yr**	**Made available to 200 teachers/year with minimum of 5 experiences/ yr**	NCMN
Objective 4.2 Continue influencing the STEM pipeline through programs for undergraduate and graduate students, and postdoctoral researchers.						
Activities	Checkpoints / Milestones					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible

Postdoctoral scientists & student mentoring programs	**7 postdocs**	**7 postdocs**	**7 postdocs**	**7 postdocs**	**Cumulative: 35 person-years**	Lai and FRG leaders
Graduate, Undergraduate Students	**16 grad** **18 undergrad**	**16 grad** **18 undergrad**	**16 grad** **18 undergrad**	**16 grad** **18 undergrad**	**Cumulative: grad students (16x5) = 80** **Undergrad (18x5) = 90**	FRG leaders
Student Seminar Series	**12 mtgs/yr**	**12 mtgs/yr**	**12 mtgs/yr**	**12 mtgs/yr**	**12 mtgs/yr**	FRG leaders
Nano-Quantum Mini-course (PHYS 891 Tools & Methods in Nano)	**50 total (7 grad) / yr**	**50 total (7 grad) / yr**	**50 total (7 grad) / yr**	**50 total (7 grad) / yr**	**Cumulative 35 grad students/ 250 total participants**	Andrei Sokolov (NCMN+NNF)
Host REUs	**3 /yr; 1 Community College /yr**	**3 /yr; 1 Community College /yr**	**3 /yr; 1 Community College /yr**	**3 /yr; 1 Community College /yr**	**3 /yr; 1 Community College /yr**	EQUATE SIs = hosts, NCMN+NE EPSCoR help recruit via UNL Grad Studies office

Objective 4.3: Provide professional development opportunities for faculty across Nebraska's colleges.						
Activities	Specific accomplishments, milestones, and/or outputs					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
FIRST Award program helps early-career faculty prepare to pursue CAREER Awards	**6 FIRST awards**	**6 FIRST awards**	**6 FIRST awards**	**6 FIRST awards**	**6 FIRST awards** (Cumulative: 30 FIRST Awards issued)	NE EPSCoR
Faculty Mentoring	**Align for early-career faculty**	**New hires (EQUATE-funded) arrive at**			**Cumulative: 5 early-career faculty**	Binek, Wrubel

		UNK, UNL			**mentored**	
Objective 4.4: Increase the number of participants in the STEM field.						
Activities	Specific accomplishments, milestones, and/or outputs					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Sponsor Community College student researchers	**5 students present at annual Neb Acad Sciences**	**5 students present at annual Neb Acad Sciences**	Public event at community colleges	Public event at community colleges	**5 students present at annual Neb Acad Sciences** **Cumulative: 30 students supported**	NE EPSCoR
Sponsor annual Women in Science conference	**90 students & 10 teachers**	**90 students & 10 teachers**	**90 students & 10 teachers**	**90 students & 10 teachers**	**90 students & 10 teachers (cumulative: 500 participants supported)**	NE EPSCoR
College prep groups (ETS, Upward Bound, Girls Inc.)	**100 URM/yr: low-income / first-gen**	**100 URM/yr: low-income / first-gen**	**100 URM/yr: low-income / first-gen**	**100 URM/yr: low-income / first-gen**	**100 URM/yr: low-income / first-gen**	NCMN
Objective 4.5 Increase public awareness of EQUATE progress.						
Activities	Specific accomplishments, milestones, and/or outputs					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
EQUATE Management Team meetings	**monthly**	**monthly**	**monthly**	**monthly**	**monthly**	EQUATE Mgt Team
Journals/ Presentations	**4 per SI, per yr**	**4 per SI, per yr**	**4 per SI, per yr**	**4 per SI, per yr**	**4 per SI, per yr**	Each SI
Annual "NRIC" (conference)	**60 attendees**	**70 attendees**	**80 attendees**	**90 attendees**	**100 attendees**	NE EPSCoR + EQUATE MT
EQUATE website	**Development; Establish baseline #**	+ 10% year-over-year	+ 10% year-over-year	+ 10% year-over-year	+ 10% year-over-year	NCMN's Behrendt, w/input via

	views per year					Allen
Social media: #NebEQUATE (Twitter hashtag)	**Establish Baseline # of #NebEQUATE mentions/ retweets per yr**	+ 10% year-over-year	+ 10% year-over-year	+ 10% year-over-year	+ 10% year-over-year	Allen
Annual "PR" report	Mail to 800 recipients + online views	Mail to 800 recipients + online views	Mail to 800 recipients + online views	Mail to 800 recipients + online views	Mail to 800 recipients + online views	Allen
Facility tours at NCMN/Jorgensen *DEPENDENT ON COVID-19 PROTOCOLS*	200 (150 virtual, 50 in-person)	200 (150 virtual, 50 in-person)	200 (150 virtual, 50 in-person)	200 (150 virtual, 50 in-person)	200 (150 virtual, 50 in-person)	Wignall
Traveling museum exhibit *DEPENDENT ON COVID-19 PROTOCOLS*	**2 exhibits, 2 placements per year**	**2 exhibits, 2 placements per year**	**2 exhibits, 2 placements per year**	**2 exhibits, 2 placements per year**	**2 exhibits, 2 placements per year**	Wignall
EQUATE presence at Public Events *DEPENDENT ON COVID-19 PROTOCOLS*	**2/yr, e.g. Nebraska Science Fest, STEM Ecosystem Mtgs, etc.**	**2/yr, e.g. Nebraska Science Fest, STEM Ecosystem Mtgs, etc.**	**2/yr, e.g. Nebraska Science Fest, STEM Ecosystem Mtgs, etc.**	**2/yr, e.g. Nebraska Science Fest, STEM Ecosystem Mtgs, etc.**	**2/yr, e.g. Nebraska Science Fest, STEM Ecosystem Mtgs, etc.**	Sangster + Wignall