Emergent QUAntum materials and TEchnologies (EQUATE)
NSF EPSCoR RII Track-1 Project #OIA-2044049
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REVISED

Year 3 Narrative Report – February 2024
(Y3: 6/1/2023 – 5/31/2024)

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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 today's progress in science and technology happens at the interface between disciplines. Emergent Quantum Materials and Technologies (EQUATE)--a multicampus research cluster--involves 20 investigators from University of Nebraska campuses at Lincoln, Omaha, and Kearney, plus Creighton University; the project also supports undergraduate learning in STEM (science, technology, engineering, and math) at Nebraska's two tribal colleges.

Materials science is amid a second quantum revolution. Quantum phenomena are often introduced via the properties of matter at the scale of atoms and below. Here the fundamental laws of nature are the laws of quantum physics. An essential insight from the first quantum revolution is the fact that electrons can manifest as particles and waves alike, a phenomenon known as wave-particle duality. EQUATE's interdisciplinary research has three interacting focused research groups (FRGs)—each with thrust areas for a collective theoretical, experimental, and engineering effort:

FRG1 (Quantum Materials) creates the project foundation in basic materials science. New quantum materials are designed and guided by theory. Quantum materials are grown, nanofabricated into hybrid structures and prototype device structures, characterized, and modeled. The process includes continuous feedback between theory and experiment.

Some of the provided material platforms can potentially be applied in FRG2 (Quantum Technologies) and FRG3 (Quantum Information Processing). FRG1 searches for quantum materials where new quantum phenomena emerge from non-trivial topologies, spin ordering, and strong correlation (Thrust 1); exploits magnetoelectric coupling and valley degree of freedom in low dimensional systems and at interfaces (Thrust 2); and focuses on novel molecular platforms for spin quantum bit systems (Thrust 3). FRG2 focuses on sensing and metrology utilizing the extreme sensitivity of various quantum systems (Thrust 1) and on quantum communication emphasizing photons as quantum information carriers (Thrust 2).

FRG3 tops this hierarchy, aiming at quantum information processing via implementation of quantum emulation (Thrust 1) and general quantum computing (Thrust 2) as a vision with critical components in development. Across the FRG teams, senior investigators (SIs) from UNL, UNO, UNK and CU bring expertise in physics, chemistry, materials science, mechanical engineering, electrical engineering, and computer science. A particular strength is the well-established collaboration and feedback between theory and experiment, which promotes inter-institution exchange and is based on past success expediting theory-guided discoveries.

Development and application of quantum materials into quantum technologies in the state of Nebraska benefits from the internationally-renowned Nebraska Center for Materials and Nanoscience (NCMN). Coupled with faculty expertise at EQUATE's participating campuses, Nebraska gains a head start in the fierce and economically decisive race for leadership in quantum technologies.

As the next big leap, quantum technologies can play a key role in securing Nebraska's future economic well-being. EQUATE has the potential to bring University of Nebraska institutions and the state to the forefront of research, development, and education efforts in quantum materials and technologies to establish a well-trained workforce for the American Midwest.

Executive Summary

The success of the first two years of EQUATE allowed the motivated team of researchers, collaborators, advisors, external partners, administrators, and education/outreach coordinators to build up the strong momentum that carries the center forward into Year 3. As a result, Year 3 advances in accordance with the forward-looking statements expressed in the project's strategic plan. At the same time, new opportunities emerge which are largely enabled through the hire of senior investigator and theorist Dr. **Aleksander Wysocki** at the University of Nebraska at Kearney (UNK) and through the recent hire of Dr. **Zuocheng Zhang**. Dr. Zhang joins the Department of Physics and Astronomy at the University of Nebraska-Lincoln (UNL) in summer 2024. He brings scientific background in two-dimensional materials and topological insulators to EQUATE experience; he acquired this expertise in part as a postdoctoral researcher at UC Berkeley. Dr. Zhang will become an integral part of EQUATE's experimental work and virtually immediately start collaborations within FRG1 and FRG2.

Figure A: NSF EPSCoR workshop on Quantum Computing, Information, Science, and Engineering, Alexandria, VA March 23-24, 2023. EQUATE scientific director Binek was part of the Academic Panel that took place on the gathering's first day.

An additional change in the structure of EQUATE's senior investigator team happened through the recent departure of Dr. **Wei Bao**. He moved 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. As an EQUATE senior investigator Dr. Bao contributed to FRG2 and FRG3 with work on parametric down conversion for the creation of entangled photon pairs and non-equilibrium Bose-Einstein condensates (BECs) in condensed matter systems with application in quantum emulation. The vacancy he left in the FRGs has been filled by EQUATE seed awardee and senior physical chemist Dr. **Alexander Sinitskii** who will further strengthen and diversify the work done in FRG3. Dr. Sinitskii is a UNL chemist and an internationally renowned expert in graphene and two-dimensional quantum materials. Dr. Sinitskii synthesizes and grows 2D materials and nanoribbons for applications in quantum devices which he nanofabricates and characterizes. His strength in synthesis allows EQUATE to explore avenues toward BECs in condensed matter systems which Dr. Bao did not. Currently, plans are evolving to utilize the expertise of former EQUATE seed awardee Dr. **Laura Wang** to bring the work on BECs to a new level which allows for advances in quantum emulation approaches complementary to the ultra-cold atom approach by FRG3 leader Dr. **Jonathan Wrubel**.

Strengthened by the strategic innovations outlined above, EQUATE continues to position itself as a leading center in quantum materials science and technologies. This is evidenced for example by the fact that the EQUATE scientific director Dr. **Christian Binek** served as panel member and advisor for the workshop on quantum computing, Information, Science and Engineering at NSF, Alexandria, VA in March 2023 (**Fig. A**). Similarly, EQUATE 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 the DOD-designated University Affiliated Research Center sponsored by STRATCOM. Al Geist has been accompanied by highest ranking military representatives such as Dr. James L. Stewart, Spectrum Warfare Systems Department Chief Scientist who also serves as the NATO Chairman for the Suppression of Enemy Air defense. In January 2023, EQUATE educated Brigadier General AnnMarie K. Anthony from the Joint Electromagnetic Spectrum Operations Center and Mr. Pedro Ramirez, Technical Director of the Nuclear Command, Control, and Communications (NC3) Enterprise Center about work done by EQUATE researchers on quantum materials and quantum technologies. EQUATE scientific director Binek was accompanied by FRG2 leader Dr. **Abdelghani Laraoui** who supported the conversation on FRG2 related work on quantum communication, specifically the creation and transmission of identical and entangled photons. EQUATE is proud to serve the country as a recognized knowledge resource for STRATCOM.

EQUATE continues to be recognized as a driving force in the second quantum revolution: enabling discoveries, innovation, and workforce development. The Year 3 results are a testimony to the effectiveness of the center's interdisciplinary multi-campus-based collaborative approach.

FRG1’s focus on quantum materials continues to reach new milestones in Year 3 with breakthroughs in fundamental quantum materials science for applications in quantum and spintronic devices based on quantum materials. Highly collaborative work within and across FRGs and between experimentalists and theorists continues to be a hallmark of EQUATE. The field of magnetoelectric antiferromagentic oxides with Néel vector rotation by pure electric means is an example where senior investigators from physics, engineering, chemistry and national labs collaborate and break new ground. Topological spin textures with device applications enabled through the topological Hall effect are another prospering field of collaborative FRG1 research where theory and experiment advance through synergy.

Remarkable progress is also reported from FRG2 where for example the periodic modulation of magnetization created by a particular type of spin wave excitation (Damon-Eshbach mode) could be mapped in real space with the help of the quantum meteorological approach utilizing FRG1 expertise in materials growth and FRG 2 expertise in NV-center microscopy. The work highlights collaborative work between senior investigators across FRGs and across physics and engineering.

FRG3 can report the return of Dr. **Tom Wong** (Creighton University) who served for three years at the National Quantum Coordination Office in Washington D.C.. The fact that an EQUATE senior investigator has been selected for this prestigious position speaks volumes for the reputation of senior investigators and their work done in EQUATE and FRG3 in particular. Dr. Wong’s return will boost FRG3’s work on quantum computing algorithms which he leads in collaboration with FRG3 leader Dr. Wrubel. FRG3’s work on BECs from ultra-cold atoms is on schedule with the successful setup of an optical dipole trap while, at the same time, the complementary work on condensed matter BECs has the potential to expand into a new direction with the help of Dr. Sinitskii. The first graphene-based crosswire quantum qubits have been fabricated in 2024 by the Binek group in a cross-FRG collaboration where experience in e-beam lithography from FRG1 meets the theoretical guidance in the physics of quantum crosswires by FRG3. The devices fabrication approaches the mature stage where characterization by electric transport measurements can start. The work of Binek's group will be complemented by Sinitskii's group who employs alternative 2D materials with theoretical guidance from Drs. **Sabirianov** (UNO), **Mei** (UNO) and **Wysocki** (UNK).

The Education and Outreach activities of EQUATE continue to be exceptional in numbers and breadth of the program, with our unique relationship to Tribal colleges being just one example of this remarkable effort. Details are in this document's Solicitation-Specific Project Elements section, expanding from the project's vigorous Education and Workforce Development work.

RESEARCH AND CAPACITY BUILDING

FRG1 – Quantum Materials (2023-2024)

In EQUATE Year 3, FRG1 continued its progress in gaining understanding and control of a range of emerging quantum phenomena driven by correlation, topology, spin-orbit coupling (SOC), and ferroic switching by combining sample synthesis (Binek, Hong, Lai, Xu) and material characterization (Binek, Dowben, Guo, Hong, Xu) with theoretical studies (Kovalev, Streubel, Tsymbal).

Among FRG1's three research thrusts, the goal of Thrust 1 is to realize a range of emergent topology, spin, and correlation phenomena in novel ferroic materials, including topological antiferromagnets, two-dimensional (2D) van der Waals (vdW) magnets, and correlated oxides.

Thrust 1, Objective 1a aims to explore quantum materials for antiferromagnetic (AFM) spintronics. In Year 3, SI **Binek**'s group continued the collaboration with Dr. Jeffrey Lynn and Dr. Jamie Weaver from NIST, utilizing their cold neutron depth profiling (cNDP) capabilities to resolve the effects of B-doping on magnetoelectric (ME) properties of Cr_2O_3 (chromia) thin films. Combined cNDP and magnetotransport studies show that annealing a homogeneously B-doped chromia film gives rise to a B-concentration gradient, reflecting a thermodynamically driven surface segregation process. **Fig. 1a** shows the depth resolved x-ray photoemission spectroscopy (XPS) data taken after multiple annealing temperatures, which reveals the formation of a ~50 nm thick surface segregation layer. This layer is thermodynamically stable and has an increased Néel temperature (T_N) of >400K (meets metrics), which is beneficial for device functionality, *i.e.*, voltage controlled nonvolatile rotation of the Néel vector for antiferromagnetic spintronics. This work is published in *Adv. Physics Res.* and selected as the cover (**Fig. 1b**) for the journal (Issue 1, 2024). PI Binek gave a well-received invited talk at the 2023 *MRS Fall Meeting* about these results.

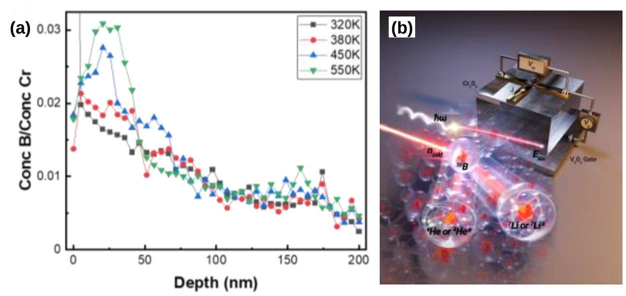

Figure 1. (a) B-concentration depth profiles of sapphire (0001)/V_2O_3 (25 nm)/B:Cr_2O_3 (200 nm) measured via XPS after annealing at various temperatures. Spectra are taken at 300 K upon subsequent local Ar-ion etching. (b) Cover page depicting the interrogation of a memory device based on a B-doped Cr_2O_3 thin film with voltage controlled Néel vector.

Canting of boundary magnetization has been revealed via spin resolved XPS and exchange bias studies in collaboration with SI **Peter Dowben**. There is non-zero exchange bias for in-plane anisotropic exchange bias heterostructures but virtually no exchange bias in perpendicular anisotropic exchange bias heterostructures based on B:Cr_2O_3 pinning layers, a strong indication for canting of boundary magnetization away from the surface normal. The team also investigated spin canting in Pt/B:Cr_2O_3 heterostructures and identified a substrate induced magnetization in Pt. Spin resolved XPS determined its orientation relative to the normal of the sample plane. The investigation of exchange bias in these systems is on schedule.

In collaboration with experimentalists at Stanford, SI **Tsymbal** provided theoretical insights into the unconventional spin–orbit torques (SOTs) generated by AFM $MnPd_3$ thin films interfaced with a CoFeB ferromagnet. While conventional SOTs require an external bias magnetic field to generate magnetization switching in ferromagnets with perpendicular anisotropy, the unconventional SOTs enable magnetization switching with no external fields. The team observed the presence of out-of-plane anti-damping-like torques originated from the out-to-plane polarization of the spin current generated by the spin Hall effect. This leads to complete field-free switching of perpendicular magnetization of the CoFeB ferromagnet. Our density functional theory calculations showed that the observed unconventional torques are due to the AFM structure and low symmetry of the (114)-oriented $MnPd_3$ films (meets metrics). This result provides a path toward the realization of a practical spin channel for ultrafast magnetic memory and logic devices. This work is published in *Nat. Mater.* (2023).

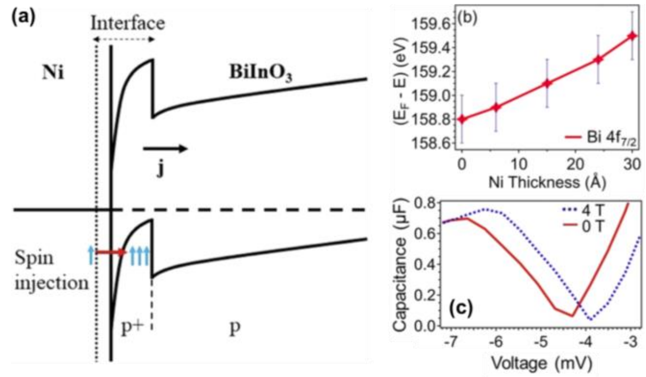

Figure 2. (a) Schematic energy level diagram at the Ni to $BiInO_3$ interface. (b) Binding energy of Bi^{3+} $4f_{7/2}$ photoemission core levels as a function of Ni overlayer thickness on $BiInO_3$. (c) Room-temperature capacitance vs voltage with and without a perpendicular magnetic field applied.

Thrust 1, Objective 1b 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 assess the polar/magnetic properties of epitaxial $BiInO_3$ thin films deposited on $(Ba,Sr)RuO_3$ buffered $NdScO_3(110)$ substrates. Structural characterizations show that strained $BiInO_3$ films are in the non-ferroelectric Pnma phase, similar to the literature reports. This result is also consistent with the literature reports. This is consistent with the piezoresponse force microscopy (PFM) imaging results (meets metrics), which reveals an absence of retention in the domain structure written with conductive AFM. The team observed the formation of a p-type Schottky barrier (**Fig. 2a**) and successfully demonstrated a magneto-capacitance effect at the interface between Ni and epitaxial non-polar $BiInO_3$ thin films at room temperature (meets metrics). XPS studies reveal the formation of an intermetallic Ni–Bi alloy at the Ni/$BiInO_3$ interface and a shift in the Bi 4f and In 3d core levels to higher binding energies with increasing Ni thickness (**Fig. 2b**). The current–voltage characteristics of the Ni/$BiInO_3$ heterostructure on $(Ba,Sr)RuO_3/NdScO_3(110)$ show a significant dependence on the applied magnetic field and voltage cycling (Fig. 2c), which can be attributed to voltage-controlled band bending and spin-polarized charge accumulation in the vicinity of the Ni/$BiInO_3$ interface. The result is significant because it demonstrates a significant magneto-capacitance effect at room temperature without involving multiferroic materials. This work is accepted for publication in *ACS Appl. Mater. & Interfaces* (2024).

SI **Xu** successfully modeled the topological spin structure and topological Hall effect (THE) in centrosymmetric magnetic nanoparticles. Topological spin structures are generally not expected in centrosymmetric systems, while the noncoplanar monodomain magnetic states such as flower and curling states do emerge due to the contribution of surfaces and edges in nanoparticles. The team calculated the topological charges *Q* associated with these intriguing noncoplanar and the corresponding THE as a manifestation of the Berry phase accumulation. We assessed these spin textures across various particle sizes and along magnetic hysteresis loops and mapped the spin structures in confined geometries using magnetic force microscopy. We showed that *Q*, as a fractional number, increases with particle size and saturates as the system transits from the flower state to the curling state. Along magnetic hysteresis loops, smaller particles that show flower states in zero field exhibit a peak in *Q* near the coercive field (**Fig. 3**), a signature of the THE demonstrated in other systems. In contrast, larger particles that show curling states during the magnetization reversal, exhibit transitions between the homogeneous state, flower state, and curling state, which generates jumps in *Q* and the THE response. These results reveal the rich topological nature of centrosymmetric magnetic nanoparticles, offer control using magnetic field and probe using electric transport, suggesting promising potential applications.

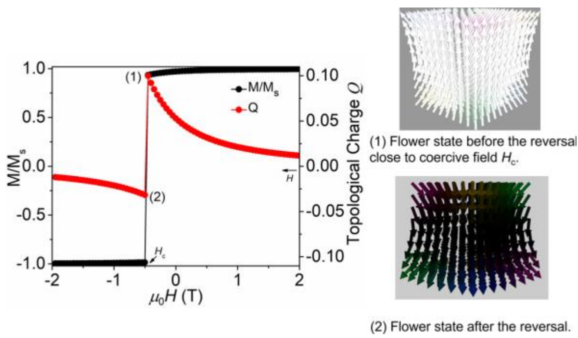

Figure 3. Micromagnetic simulations of *M* and *Q* for a cubic ferromagnetic particle with a radius showing (left) field dependence of *M* and *Q* along half of the hysteresis loop, where *Q* reaches the maximum values near the coercive field *H*c, and (right) spin structures for the two points in the left figure.

To generalize the observation and understanding of anharmonic collective lattice dynamics in a perovskite lattice, SI **Guo** identified the lattice modes of oxide perovskite using $SrTiO_3$ (STO) via Raman spectroscopy. **Fig. 4** shows the Raman scattering from different surfaces of single crystal STO (meets metrics), which confirms the consistency of their spectral response. Complex oxide heterostructures based on STO can host a range of quantum phenomena, including the two-dimensional electron gas at the $LaAlO_3$/STO interface and the interface induced/enhanced T_c for high temperature superconductivity in the FeSe/STO systems, indicating the critical role of STO lattice responses. The measurement of the STO phonon spectrum serves as a benchmark for investigating dielectric solvation behaviors across the interface.

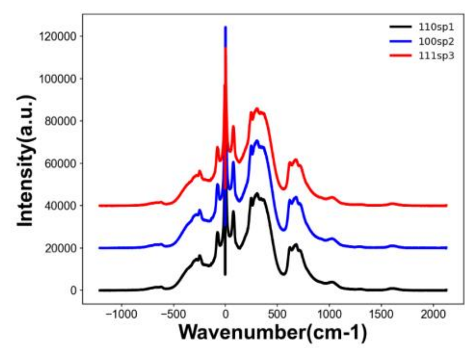

Figure 4. Raman spectra of $SrTiO_3$ crystals from different crystal faces.

SI **Hong** group fabricated ferroelectric tunnel junction (FTJ) composed of 4 nm PZT tunnel barrier $LaNiO_3$ electrodes and successfully quantified the tunneling electroresistance (TER). Switching the polarization of the tunnel barrier induces nonvolatile modulation of the tunneling current, with a TER of ~400% achieved at 300 K (**Fig. 5a**). The tunneling *I-V* characteristics can be well described with direct tunneling in the on state and Glazman-Matveev inelastic tunneling model in the off state (**Fig. 5b**), reflecting enhanced contribution from defect states when itinerant charges are depleted from the interface (meets metrics).

SI **Hong** fabricated strain-free $NiCo_2O_4$ (NCO) membranes with high crystallinity by depositing epitaxial thin films on water soluble $Sr_3Al_2O_6$ buffered $LaAlO_3$ substrates followed by water etching. Hong collaborated with SI Streubel to carry out magnetometry studies on the suspended membranes samples. The characterizations of magnetization and T_C are on schedule. SI **Hong** also used epitaxial strain to engineer the THE response in epitaxial $NiCo_2O_4$ thin films. Magnetotransport studies reveal emergent THE response in thick (110) $NiCo_2O_4$ films and ultrathin (001) $NiCo_2O_4$ films (meets metrics). These results show that crystalline orientation and film thickness can be utilized to engineer the THE response, providing critical material information for developing $NiCo_2O_4$-based topological devices.

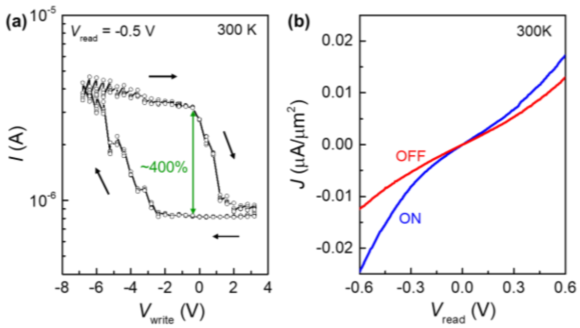

Figure 5. (a) Tunneling current vs. writing voltage hysteresis, and (b) tunneling current density vs. reading voltage for the on and off states taken on a $LaNiO_3$/4 nm PZT/$LaNiO_3$ FTJ at 300 K.

SI **Xu** collaborated with SI **Dowben** to characterize the magnetic state of NCO films grown on $MgAl_2O_4$ (001) substrates using magnetometry, x-ray magnetic circular dichroism (XMCD) based on x-ray absorption spectroscopy (XAS), and spin-polarized inverse photoemission spectroscopy (SPIPE). Studies of films with various thicknesses down to 1.6 nm reveal a layer of optimal NCO and an interfacial layer (1.2 ± 0.1 nm), with a small canting of magnetization at the surface. The thickness dependence of the optimal layer can be described by the finite-scaling theory with a critical exponent consistent with the high perpendicular magnetic anisotropy. The magnetization hysteresis measured using XMCD for an ultrathin 1.6 nm film show the exchange-spring style with a step of magnetization near zero field, suggesting two components coupled antiferromagnetically (**Fig. 6**). The proportion of the two features changes with temperature: while the soft feature (1) vanishes at about 150 K, the hard feature (2) persists up to room temperature, corresponding to the optimal and interfacial layers, respectively. The magnetic properties of the interfacial layer are also measurement-speed dependent, suggesting substantial interfacial diffusion between the substrate and the film. Non-zero in-plane polarization of the unoccupied states above the Fermi level was observed using SPIPE, indicating that magnetic moments are canted near the surface region. These results reveal fundamental parameters of NCO magnetism as well as the possible disordered nature of the $NCO/MgAl_2O_4$ interface, which is critical for the application of ultrathin films.

Thrust 1, Objective 1c aims to probe entanglement and correlation effect. SI **Binek** collaborated with FRG2 SI **Laraoui** to image the antiferromagnetic domains in the B:Cr_2O_3 using NV-microscopy. The team compared the domain structures in B-doped chromia with domains in pure Cr_2O_3 (meets metrics). The study of antiferromagnetic domains in epitaxial Cr_2O_3 films via scanning diamond magnetic probe microscopy is published in *RSC Adv.* (2023). There is evidence that the domains in B:Cr_2O_3 are strongly affected by confinement effects and change in contrast on voltage application. The NV-microscopy results are consistent with the micro-Raman investigation by SI **Guo**, which identified the characteristic magnon and phonon behaviors in boron doped chromia and demonstrated voltage dependent switching of the two-magnon mode (meets metrics). These results provide important insight into the voltage-controlled surface spin switching in B:Cr_2O_3, an important magnetoelectric quantum material, paving the path for developing high speed, energy efficient antiferromagnetic spintronics. Collaborating with FRG3 SIs **Wysocki, Mei, and Sabirianov**, the team developed theoretical models to describe the magnon spectrum of the boron doped chromia. The numerical model being developed incorporates magnon-magnon and magnon-phonon interactions and will elucidate the interplay between magnon and lattice degrees of freedom and reveal the voltage control mechanism.

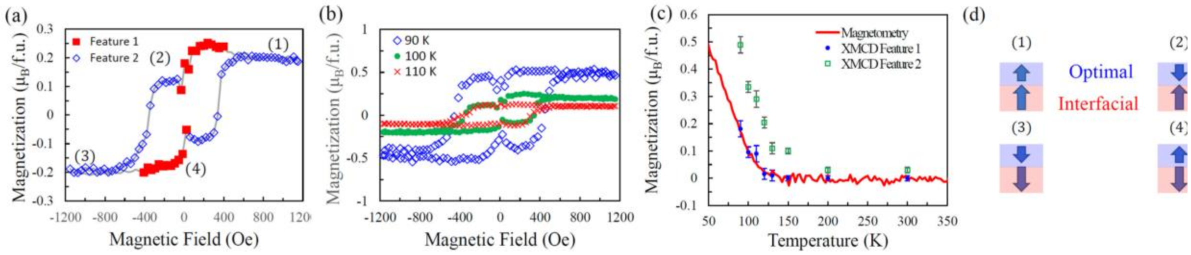

Figure 6. (a) Magnetization hysteresis loops measured using the Ni L3 edge at 100 K and (b) different temperatures, and (c) T-dependence of magnetization and two features from XMCD for 1.6 nm NCO on $MgAl_2O_4$ (001). (d) Schematic illustration of exchange spring behavior for two antiferromagnetic coupled layers corresponding to the states labelled in (a).

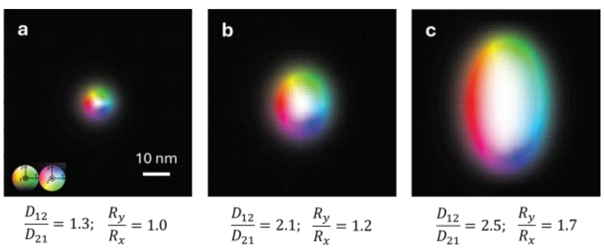

Figure 7. Simulated magnetic antiskyrmions of different radii and aspect ratios for different DMI parameters.

SIs **Kovalev** collaborated with SI **Tsymbal** to develop new quantum information protection platforms based on skyrmion. The team proposed exploiting stacked 2D vdW heterostructures that break inversion symmetry to create anisotropic Dzyaloshinskii-Moriya interaction (DMI). Using the material parameters obtained in *ab initio* studies, the team used micromagnetics and analytical descriptions to predict the emergence of elliptical magnetic skyrmions and antiskyrmions in 2D van der Waals (vdW) magnets and derived analytical results for the shape and radius of skyrmions and antiskyrmions (**Fig. 7**). Our results based on the Harmonic Transition State Theory demonstrate the stability of elongated skyrmions and antiskyrmions at finite temperatures in bilayer CrI_3. This work is accepted for publication in *Phys. Rev. B* as Editor's suggestion. We have also studied spin-orbit torques that can be used to manipulate skyrmions and antiskyrmions. These results can be important for realizations of computing and logic devices relying on skyrmions and antiskyrmions.

SI **Kovalev** also predicted a diode effect in a phase-controlled planar Josephson junction comprising a two-dimensional electron gas with strong spin-orbit coupling and *d*-wave superconductors, which originates from mirror and time-reversal symmetry breaking. Josephson's current is calculated analytically and numerically for different pairing orientations using Matsubara Green's function approach, concentrating on *d*+i*d*', *d*+i*s* pairings realizable in twisted cuprate bilayers. Nonreciprocity has been studied for different system parameters, including the Zeeman-field, spin-orbit coupling, pairing orientation, and gate bias. We have tried to differentiate between the super-current that arises due to the presence of edge states and the bulk states. Furthermore, we have assessed the relevance of Majorana-bound states and how they influence the observed nonreciprocity. Our results on the *d*-wave superconductor Josephson junctions can facilitate the realization of Majorana bound states for quantum computing.

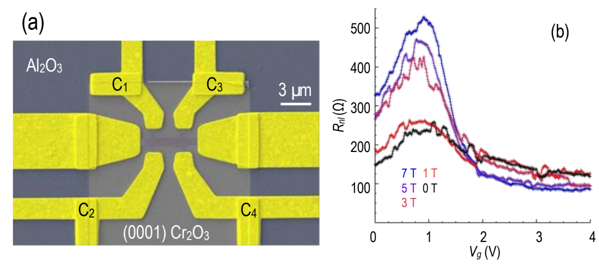

Figure 8. (a) Colorized scanning electron micrograph of a graphene Hall bar device on chromia. (b) Variation of R_{nl} at 290 K in various out-of-plane magnetic fields.

Thrust 2, Objective 2a aims to achieve magnetoelectric control of topological states in graphene. SIs Binek and Dowben used spin transport in a non-local geometry to assess effects of sublattice symmetry breaking and magnetic interaction on spin lifetime in graphene on chromia. The team demonstrated evidence of robust induced spin-orbit coupling in graphene placed in proximity with the magnetic surface of the Cr_2O_3. With current (I_d) driven between one pair of Hall probes (C_1 & C_2 in **Fig. 8a**), non-local voltage (V_{nl}) develops across probes C_3 & C_4 located several microns away. The dependences of non-local resistance $R_{nl} \equiv V_{nl}/I_{nl}$ on gate voltage (**Fig. 8b**), magnetic field, and temperature provide insights into the spin-dependent transport. The magnitude of R_{nl} increases substantially with increasing magnetic field strength, the expected behavior for the spin-Hall signal, and is inversely proportional to the charge conductivity of graphene. Our results point to the presence of an extrinsic spin-orbit coupling in the graphene that arises from its contact with the chromia, representing an important step forward for the realization of graphene-based 2D spintronics. This work is published in *IEEE ExPlore* (2023). Theoretical modeling of the spin relaxation time in graphene on chromia and prediction of other ME 2D systems are on schedule.

Thrust 2, Objective 2b aims to explore emergent 2D materials for designing valley spin valves. In collaboration with researchers from Chinese Academy of Sciences, SI **Tsymbal** predicted the emergence of a tunneling valley Hall effect (TVHE) driven by tilted Dirac fermions. Using a representative model for an all-in-one tunnel junction based on a 2D valley material, the team showed these junctions exhibit momentum filtering of the tunneling Dirac fermions, generating a strong transverse valley Hall current dependent on the Dirac-cone tilting. Importantly, the predicted TVHE occurs even in the absence of the Berry curvature and can result in a giant valley Hall angle. This work opens a new approach to generate valley polarization in realistic valleytronic systems. This result is published in *Phys. Rev. Lett.* (2023). The theoretical search of 2D materials to realize a nonvolatile valley spin valve effect is on schedule.

SI **Dowben** mapped out the band structure of the transition metal dichalcogenides 2H-MoS_2(0001) with Pd overlayer via low energy electron diffraction (LEED) and high-resolution angle resolved photoemission (ARPES). The Palladium overlayer is in registry with the MoS_2(0001) substrate, as seen in LEED and the band structure (**Fig. 9**). Palladium adsorption on 2H-MoS_2(0001) results in significant band shifts than that for Pd on 2H-WSe_2(0001), indicating charge donations from the MoS_2(0001) to Pd (meets metrics). Photoemission and inverse photoemission (IPES) reveal an increase in the MoS_2(0001) substrate band gap with palladium adsorption. The modulation of MoS_2 edge transitions is on schedule.

Seed project recipient **Martin Centurion** implemented a new setup to characterize material response to optical excitation using ultrafast electron diffraction. In collaboration with SI **Hong** and FRG 2 SI **Sinitskii**, Centurion's group carried out ultrafast electron diffraction experiments to investigate ultrafast dynamics in $NbOI_2$, a monoclinic low-symmetry ferroelectric vdW material. The team captured changes in the polarization on the picosecond scale that are triggered by laser excitation and observed the formation of coherent and acoustic phonon comprising both longitudinal and shear waves. This work provides a new capability to characterize the ultrafast polarization and structural changes in material after optical excitation.

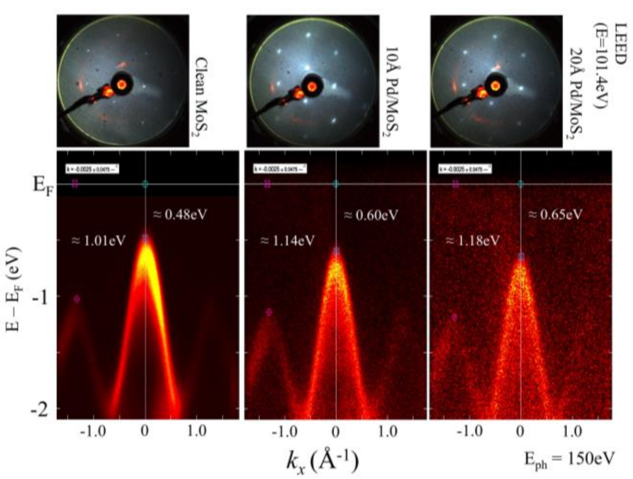

Figure 9. LEED image of MoS_2(0001) with increasing Pd overlayer coverages on surface. The shift to higher binding energy with increasing Pd coverage is seen in the band structures (bottom).

Thrust 3, Objective 3 aims to develop molecular system-based materials platforms for spin-qubit systems. SI **Dowben** developed transistors and phototransistors based on Co2+/3+ spin crossover (SCO) molecules. A metal-ligand unoccupied state has been identified in $[Co(SQ)(Cat)(3\text{-}tpp)_2]/[Co(SQ)_2(3\text{-}tpp)_2]$ through density functional theory and the combination of XPS, XAS, and inverse photoemission spectroscopy experiments. The team discovered interesting fluctuation of the spin state and associated conductance near the phase transition and/or at critical gate voltages (**Fig. 10**). This result provides important information for designing molecular electronics and modeling their fidelity and control characteristics. This work is published in *Nanoscale* (2023). SI **Streubel** collaborated with SI **Dowben** to study the ferromagnetic resonances (FMR) in SCO films to determine structural and magnetic homogeneity and quantify magnetic materials parameters. The determination of spin precession via FMR hinges on the improved sample quality and is on schedule).

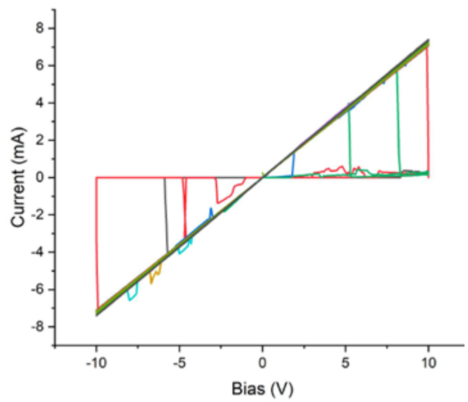

Figure 10. Fluctuations between the high-spin high-conductance state and low-spin low-conductance state in a [Co(SQ)(Cat)(3-tpp)$_2$]/[Co(SQ)$_2$(3-tpp)$_2$] thin film transistor, with the applied V_g reaching the critical value for spin state switching (-16 V).

In collaboration with SIs **Dowben** and **La**i and Talat S. Rahman (UCF), SI **Streubel** examined the impact of adding magnetic nanoparticles to SCO polymer films to control the electronic transport properties. The team studied the magnetic order in dilanthanide SCO polymers. Joint studies of ab initio calculations (Rahman) and XPS, XAS, and magnetometry measurements reveal the dominance of spin-orbit coupling over j–J coupling due to the inversion symmetry-breaking ligand field and antiferromagnetic alignment of the Gd_2 dimers. The antiferromagnetic exchange coupling within the molecule was identified via DC magnetic susceptibility and density functional theory. The electronic transport properties in dinuclear molecular magnets are governed by the intermolecular and intramolecular exchange interactions. The latter is set by the chemistry of the molecule, the former is strongly dependent on the structural short-range order. Hence, understanding the magnetic order and electronic transport through these films will benefit molecular microelectronics. This work is published in *Phys. Chem. Chem. Phys.* (2023).

SI **Lai** carried out the design, synthesis, and characterization of Fe/Ni SCO complexes, such as Fe(qsal)$_2$Cl (qsal: N-(8-quinolyl)salicylaldimine), and further coupled Fe(qsal)$_2$Cl with Ni(dmit)$_2$ (dmit: 1,3-dithiole-2-thione-4,5-dithiolato), a complex well known for its conductive properties when in a fractional oxidation state. An overall yield of ~60% was achieved, which is considered high for this class of organometallic complexes. The samples have been characterized via scanning electron microscopy (SEM), infrared spectroscopy (IR), Raman spectroscopy, nuclear magnetic resonance spectroscopy (NMR), and mass spectrometry (MS) (meets metrics). The resulting crystals are very large and suitable for single crystal analysis (**Fig. 11a**). The IR and NMR results confirm the expected molecular structure, with the molecular weight close to the theoretical value. SQUID studies of temperature-dependent magnetic susceptibility during both warming and cooling processes show gradual transition between the high spin (HS) and low spin (LS) states with negligible hysteresis (**Fig. 11b**), consistent with previously published works. The results established reproducible protocols for the synthesis of Fe(qsal)$_2$Cl and [Fe(qsal)$_2$][Ni(dmit)$_2$], paving the way

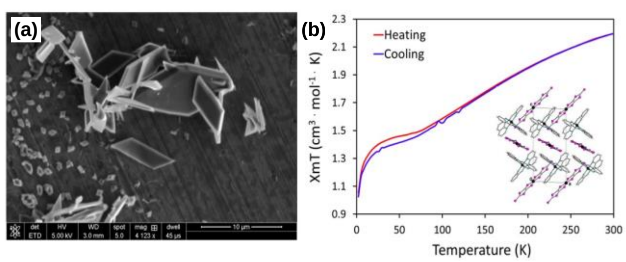

Figure 11. (a) SEM image of [Fe(qsal)$_2$][Ni(dmit)$_2$] crystals. (b) SQUID data showing T-dependent magnetic susceptibility for [Fe(qsal)$_2$][Ni(dmit)$_2$] during warming and cooling segments. Inset: Structural arrangement of the crystal showing mixed layers of $[Fe(qsal)_2]^+$ and [Ni(dmit)$_2$].

for developing bimetallic SCO systems with unique physical properties due to the synergy between each building block.

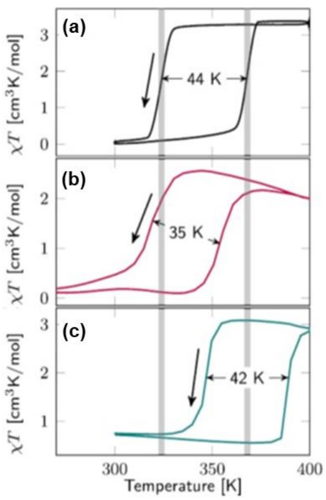

Figure 12. *T*-dependent magnetic susceptibility of (a) $[Fe(Htrz)_2(trz)](BF_4)$, and its composites with (b) PANI and (c) PANI/Fe_3O_4 demonstrating shifted SCO transition temperature and restoration of cooperative effects after the addition of Fe_3O_4.

SI **Lai** also achieved the synthesis and characterization of $[Fe(Htrz)_2(trz)](BF_4)$, polyaniline (PANI), and Fe_3O_4 nanocomposites. $[Fe(Htrz)_2(trz)](BF_4)$ is an Fe(II) SCO polymer that shows a well-defined and reversible LS to HS transition with hysteresis at temperatures slightly above room temperature, *i.e.*, 330-380 K (**Fig. 12a**), making this polymer attractive for building nonvolatile voltage-controlled memory devices. The high resistance of this SCO thin film has been a key impediment to creating a competitive memory device. The team focused on addressing this constraint by incorporating the conducting polymer PANI and successfully fabricated PANI-based two-component composites and PANI/Fe_3O_4-based three-component composites. As shown in **Fig. 12a**, $[Fe(Htrz)_2(trz)](BF_4)$ possesses a thermal hysteresis with a width of 44 K, corroborating cooperative effects due to significant intermolecular interaction. The addition of PANI reduces the warming transition temperature (smaller hysteresis) and causes an overall less steep transition (**Fig. 12b**), which can be explained by the increased separation of individual $[Fe(Htrz)_2(trz)](BF_4)$ molecules due to intermixing with PANI. Using state-of-the-art ptychographic imaging at the Advanced Light Source, SI **Streubel** revealed a phase separation of $[Fe(Htrz)_2(trz)](BF_4)$ and PANI due to the addition of Fe_3O_4 nanoparticles that restores cooperative effects between the SCO molecules, resulting in a thermal hysteresis comparable to the pure $[Fe(Htrz)_2(trz)](BF_4)$ (**Fig. 12c**). The team further observed ferromagnetic exchange coupling between $[Fe(Htrz)_2(trz)](BF_4)$ and Fe_3O_4 nanoparticles by means of XMCD spectroscopy at the Advanced Light Source. Electronic transport measurements with and without external magnetic field reveal that the addition of Fe_3O_4 nanoparticles increases the on-off ratio of DC conductivity by enlarging the resistivity of the high-spin state (off state) and leads to an AC conductivity of the on state that is 20 times larger than the DC on state. No sizeable influence of the external magnetic field on resistivity was observed. This work points to an effective strategy to tune the intermolecular coupling and control spin states in SCO. Manipulating cooperative effects through the presence of superparamagnetic nanoparticles opens a new avenue for tailoring electronic transport properties of spin-crossover systems for microelectronics. This work is accepted for publication in *Journal of Physics: Materials* (2024).

In collaboration with SI **Lai** and FRG 2 SIs **Laraoui** and **Liou**, SI **Guo** performed Raman spectroscopy measurements on iron triazole SCO molecules. Samples were prepared on diamond substrates with well-defined spin states. Raman response of high spin and low spin states of the SCO molecules were measured (meets metrics). This work is published in *ACS Nano* (2023). Further, the team observed spin crossovers induced by high power excitation laser and investigated their switching mechanisms. Power dependent *in situ* Raman observations under different temperatures ranging from 10K to 300K showed evidence of a non-thermal behavior of spin crossover, contrary to recent literature discussions. Our low frequency Raman capability enabled us to measure external lattice vibrations of the iron triazole crystals and uncovered spectral evolution dependent on crystal domain size.

The UNL Physics Department has successfully recruited a new faculty as part of EQUATE FRG 1. **Dr. Zuocheng Zhang** specializes in the synthesis of novel 2D vdW heterostructures and transport and optical characterization. His effort can contribute to Thrust 1, Objective 1a and Thrust 2, Objective 2a. He will start in Aug. 2024 and has made campus visits to discuss collaboration opportunities with EQUATE SIs (meets metrics).

For **Changes/Problems** in Year 3, FRG1's collaborations by SIs **Dowben** and **Streubel**, and SIs **Lai** and **Guo** have made critical progress in the study of spin crossover molecules. To sustain momentum and facilitate the teamwork, SIs **Lai** and **Guo** have reallocated their research efforts on the spin crossover molecule project and suspended the effort on the metal organic framework (MOF) composites; the film quality of molecular magnets has been insufficient to perform reliable electronic transport and ferromagnetic resonance spectroscopy measurements. Spin coating and other chemicals will be used to circumvent this problem.

In terms of **Other Accomplishments**, FRG1 is proud to share that graduate **students Kai Huang, Esha Mishra, Ahsan Ullah, Jia Wang, Kun Wang, and Detian Yang** graduated with Ph.D. degrees. Approximately 20 FRG1 graduate students 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. In addition:

- REU undergraduate students Amaya Street (Augustana University), Kyle Lockwood (student, Wartburg College), and **Nina Raghavan** (University of Maryland-College Park) participated in EQUATE research and presented posters at the Nebraska Summer Research Symposium on August 3, 2023. Kyle Lockwood won the Chemistry Travel Award for his summer research and poster presentation.
- Over the past year, the FRG1 research has been disseminated through over 30 peer-reviewed papers, 1 book chapter, and over 30 conference presentations (including 9 invited talks) (meets metrics).

FRG2 – Quantum Technologies (2023-2024)

FRG2's goals 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. This 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**, and formerly **Bao**) explores hybrid nanoscale optical nanostructures for generating single photon sources and entangled photon pairs. During Year 3, FRG2 investigators collaborated extensively with investigators from other thrusts in FRG2 and FRG1 (**Binek**, **Xu**, **Lai**, **Guo**, **Kovalev**). The scientific and educational achievements of this FRG are detailed below.

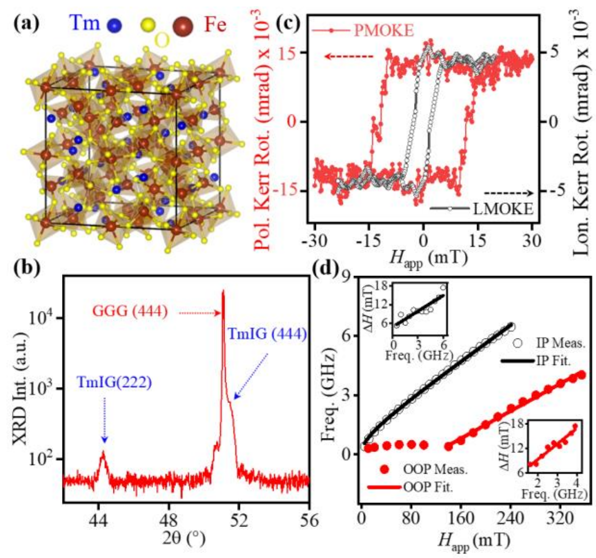

Figure 13. (a) Crystal Structure of TmIG. (b) Measured XRD spectrum of 34 nm thick TmIG film grown on 0.5mm thick GGG substrate showing both TmIG and GGG peaks. (c) Polar MOKE (filled-circle-scattered lines) curves vs. applied magnetic field of TmIG (34nm)/GGG. (d) in plane (IP, open circles) and out of plane (OOP, filled circles) FMR measurements on TmIG (34nm)/GGG. Black and red solid lines are fits to the IP and OOP measurements respectively. Insets of (d): FMR linewidth of IP (open circles) and OOP (filled circles) FMR spectra vs MW frequency. The experimental values are fitted with black and red solid lines for IP and OOP FMR measurements.

For Thrust 1: Quantum Sensing and Metrology, **Objective 1.a - Probing Spin-Magnon Interactions in Ferromagnetic (FM) Waveguides (meets metric), i**n Year 3 **Laraoui** collaborated with **Xu** (FRG1) to study spin wave (SW) transport properties in Thulium Iron Garnet ($Tm_3Fe_5O_{12}$:TmIG, see **Fig. 13(a**) thin films on garnet substrate $Gd_3Ga_5O_{12}$ (GGG) (111) using pulsed laser deposition (PLD) monitored by in-situ reflection high energy electron diffraction (RHEED). TmIG with perpendicular magnetic anisotropy (PMA). PMA have garnered significant interest due to the observation of spin orbit torque-induced switching effects, relevant to spintronics. As shown in **Fig. 13(a)**, the x-ray diffraction (XRD) spectra indicate epitaxial growth with a smooth surface. The (444) TmIG diffraction peak is merged with GGG peak (**Fig 13b**). The Atomic force microscopy (AFM) topography map confirms the smoothness of the grown film with a root mean square (RMS) surface roughness value ~ 0.25 ± 0.5 nm over a 20 μm × 20 μm scan. The magnetic properties of the 34 nm thick TmIG/GGG film have been examined using magneto-optical Kerr effect (MOKE). As shown in **Fig. 13c** for polar MOKE (PMOKE, filled-circle-scattered line) and longitudinal MOKE (LMOKE, open-circle-scattered line) configurations, near-square-shaped hysteresis loops are observed with coercive field H_c of 2.3 mT and 11.8 mT for LMOKE and PMOKE respectively. As shown in **Fig. 13c**, the polar Kerr rotation is ~ four times larger than the longitudinal values indicating a slightly out-of-plane (OOP) magnetic anisotropy. The weaker PMA in 34 nm thick TmIG appears to correlate with the smaller lattice mismatch between TmIG and GGG.

Ferromagnetic resonance (FMR) spectroscopy is used to measure magnetic anisotropy, gyromagnetic ratio γ, and damping constant α values. **Fig. 14a** shows FMR frequency dependence with applied magnetic field H_{app} curves for IP (open circles) and OOP (filled circles) configurations. The solid lines in **Fig. 14d** are fits based on the equations of IP and OOP measurements. To investigate the effect of the propagating microwave (MW) excited surface spin waves on the nitrogen-vacancy (NV) spins, we conducted optical detected magnetic resonance (ODMR, **Fig. 14a**) measurement and obtained an ODMR map of the NV-doped diamond in contact with the TmIG film (**Fig. 14b**). We apply a microwave (MW1) to excite spin waves (above the FMR mode, **Fig. 14d**) for different values of Happ.

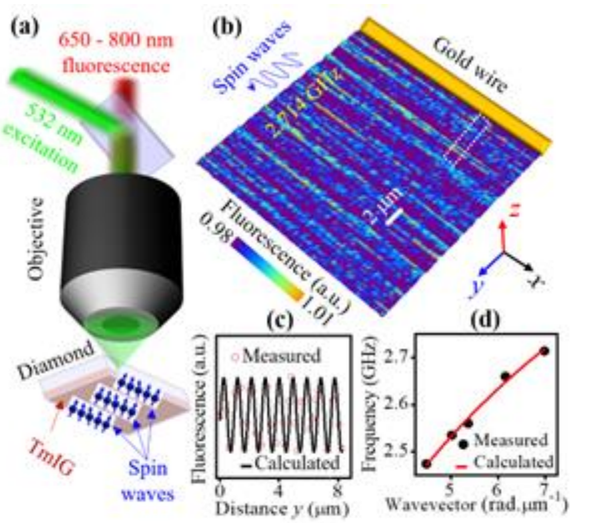

Figure 14. A schematic of the ODMR microscope in confocal geometry used to map SWs in TmIG/GGG. A green laser (532 nm) initializes the NV center spin and results in fluorescence in wavelength range of 650 – 800 nm. The diamond face with doped NV layer is in contact with the TmIG film. A permanent magnet is aligned along the [111] axis of the (100) diamond to generate a magnetic field H_{app}, applied with an angle of 35° relative to the TmIG plane. **(b)** Spatial map of the normalized ODMR contrast while driving spin waves in TmIG at f_{-} of 2.714 GHz at H_{app} = 5.57 mT. **(c)** Horizontal cross-sections of the ODMR map integrated in the dashed rectangle in **b** (open circles) and calculated (solid line) plotted vs distance *y* from the Au wire. **(e)** Measured (filled circles) and calculated (solid line) spin-wave dispersion curve.

To enhance the SW phase sensitivity of NV magnetometry we apply another microwave (MW2) at the same MW frequency into a Cu wire (diameter of 25 µm) placed on top (~ 100 µm) of the diamond substrate and aligned perpendicularly to the Au wire. In **Fig. 14b** we plot the 2D (x-y) NV normalized fluorescence intensity FL/FL0 map at a frequency f of 2.714 GHz (H_{app} = 5.57 mT. FL (FL0) is the fluorescence intensity with (without) MW excitation. **Fig. 14c** shows the integrated (over 10 lines) fluorescence intensity cross section as function of y distance in the dashed rectangle in **Fig. 14b**. Clear oscillations are observed in the curves in **Fig. 14c** explained by the interference of the propagating spin waves excited by MW1 with the uniform reference MW field (MW2). The solid line curve in **Fig. 14c** is a sinewave function fit with the interference between the stray-field induced by spin waves in TmIG and the MW field. The period of the oscillations corresponds to the wavelength λ of the excited SWs. The FFT of the measured normalized fluorescence vs distance curves gives the wavevector ky value associated with the corresponding SW excitation MW frequency at given applied magnetic field. By plotting the frequency of the excited spin waves as function of the wavevector ky one can obtain the measured SW dispersion curve from the NV fluorescence spatial maps, **Fig. 14d**. The SW wavelength (0.8 – 2 µm) and wavevector (4 – 7 rad.µm-1) depend on the amplitude of the applied magnetic field and fits well with the dispersion curve of Damon–Eshbach surface spin waves (solid line in **Fig. 14d**). The spin waves last for distances up to 80 µm with a decay length ld ~ 50 ± 5 μm, much larger than the values measured in earlier studies, opening new applications for using TmIG in magnonic spintronics and quantum magnonics.

Laraoui, in collaboration with **Xu** (FRG1), developed a NV imaging platform to map dynamic magnetic excitations in magnetic materials.

Laraoui trained a high school student from Lincoln, NE on cryogenic NV experiments, and an REU student from Alfred University, NY on modeling the FMR measurements in **Fig. 13**. Laraoui's third-year PhD student built a cryogenic optical microscope with assist from a high school student to study the coupling between NV spin qubits and magnons in magnetic thin films. UNL media coverage of the development is published here: https://engineering.unl.edu/news/231019/mme/laraoui_expandqise/

Laraoui and his students (PhD, high-school, and undergraduate) gave multiple contributed talks and posters at local workshops and national meetings, including the Annual Conference on Magnetism and Magnetic Materials (MMM) and 2024 APS March meeting (details are provided in EDOCS). Laraoui also gave two invited talks on studying Nanoscale Magnetic Phenomena in Magnetic Materials Using Diamond Quantum Sensing Microscopy at the Gordon Research Conference in quantum sensing at the MMM conference in Dallas, TX.

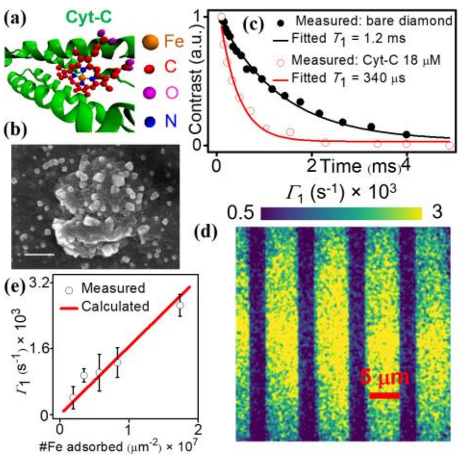

Figure 15. (a) Molecular structure of Cyt-C complex. (b) SEM image of 18 μM Cyt-C drop-casted on a carbon tape to prevent charging effect. (c) T_1 curve measured on a bare diamond (filled circles) and after drop-casting 18 □M Cyt-C solution on diamond (open circles). The black and red solid lines are exponential decay function fits of the measured T_1 relaxation curves. (d) G_1 map acquired by pixelwise exponential fitting of series of maps of the ODMR contrast decays for Cyt-C with a concentration of 54 □M drop-casted on the diamond with SiN grating. (e) Measured (open circles) and calculated (solid line) relaxation rate $\Gamma_1 = \Gamma_{ext}$ of NV spins as function of the density of Fe spins adsorbed on the diamond substrate over 1 mm^2 area. (a) Molecular structure of Cyt-C complex. (b) SEM image of 18 μM Cyt-C drop-casted on a carbon tape to prevent charging effect. (c) T_1 curve measured on a bare diamond (filled circles) and after drop-casting 18 mM Cyt-C solution on diamond (open circles). The black and red solid lines are exponential decay function fits of the measured T_1 relaxation curves. **(d)** G_1 map acquired by pixelwise exponential fitting of series of maps of the ODMR contrast decays for Cyt-C with a concentration of 54 mM drop-casted on the diamond with SiN grating. **(e)** Measured (open circles) and calculated (solid line) relaxation rate $\Gamma_1 = \Gamma_{ext}$ of NV spins as function of the density of Fe spins adsorbed on the diamond substrate over 1 mm^2 area.

FRG2 also published a paper in *Advanced Electronic Materials* (IF = 7.65), entitled "Mapping of Spin-Wave Transport in Thulium Iron Garnet Thin Films Using Diamond Quantum Microscopy."

For **Objective 1.b - Quantum Sensors for Low Field Magnetic Resonance Spectroscopy (on schedule/meets metric)**, in EQUATE's Year 3 **Laraoui** and **Liou** used NV-low field magnetic resonance (LFMR) spectroscopy to study nanoclustered cytochrome C (Cyt-C, **Fig. 15a**) proteins synthesized by **Lai** (FRG1). Cyt-C is a water-soluble protein with a molecular weight of 13 kDa typically located in the inter-mitochondrial membrane, that serves as an intermediate electron receptor during respiration, facilitating the transfer of electrons between Complex III and Complex IV in the electron transport chain. The electron transfer involves the reduction of the oxidized Cyt-C (Fe^{+3}) heme group to Fe^{+2} by an electron from Complex III. Subsequently, Cyt-C releases the electron to Complex IV, and the Fe center returns to the oxidized Fe^{+3} state at room temperature.

Figure 15b shows the scanning electron microscope (SEM) image of nanoclustered Cyt-C proteins on carbon tape with an aggregated diameter that varies from 30 nm to 150 nm. The diameter of a single monomer of Cyt-C is reported to be ~ 3.4 nm. However, due to surface interactions, when Cyt-C is drop-casted on the diamond surfaces, it tends to agglomerate, resulting in larger nanoclusters.

We used NV spin lattice relaxation time T_1 based relaxometry to detect the concentration variations in Cyt-C nanoclusters through the paramagnetic Fe^{+3} centers. **Figure 15c** shows preliminary measurements of the ODMR contrast *vs* the measurement time *t* on bare diamond (filled circles) and after drop-casting 18 μM Cyt-C solution on diamond (open circles). The NV measurements are integrated over an area of 1296 mm^2, fitted with one exponential decay function to extract T_1. A reduction of T_1 from ~ 1.2 ms for the bare diamond to 340 ms after adding 18 μM Cyt-C is obtained and attributed to the spin-noise originating from Fe^{+3} spins present within the Cyt-C proteins. **Figure 15d** shows Γ_1 (= 1/ T_1) image of diamond with SiN and Cyt-C with a concentration of 54 μM. The Γ_1 image is obtained from a series of contrast decay images by pixel-by-pixel fitting with a single exponential function. The relaxation rate G_{sig} in the presence of Cyt-C nanoclusters with a concentration of 54 μM is (2.8 ± 0.2) × $10^{3\ S-1}$ (**Figure 15d**). Note that the relaxation rate G_s of our specific diamond sensor with very shallow NV centers is the sum of the intrinsic relaxation (Γ_{int}) and the relaxation due to surface spin noise (Γ_{sur}), which accounted for almost half of the relaxation of G_s. However, the NV relaxation rate in the presence of Cyt-C is $G_{sig} = \Gamma_{int} + \Gamma_{sur} + \Gamma_{ext}$. From the measurements with very low concentrations of Cyt-C proteins (Figure **15e**), we found that Γ_{sur} is significantly suppressed by Cyt-C and could be neglected, so that $G_{ext} \approx \Gamma_{sig} - \Gamma_{int}$. For instance, 4 mL of 54 mM Cyt-C was drop-casted on the diamond surface (**Figure 15d**) for which we obtained a spin density of ~ 1.7 × 10^7 adsorbed Fe/μm^2. This value agrees well with the calculated Fe^{+3} spin density value based on the NV imaged area of Cyt-C nanoclusters (36 μm × 36 μm).

Laraoui in collaboration with **Liou** (FRG2) and **Lai** (FRG1) submitted an abstract on NV sensing of Cyt-C nanoclusters for oral presentation (accepted) to be presented by a female graduate student at APS 2024 March Meeting. The NV-T1 relaxometry of Cyt-C results is published in the high impact factor (10.8) journal *Nano Letters*.

Laraoui trained a Hispanic REU student from Central Community College in Columbus, NE in the summer of 2023 on the aspects of scanning electron microscopy and NV magnetometry. **Laraoui** held weekly group meetings jointly with **Liou** group where students (4 graduates, 4 undergraduates, and one high school) student) and a postdoc learn new aspects of quantum sensing technologies every week.

Laraoui in collaboration with **Liou** (FRG2) and **Guo**, **Lai** (FRG1) presented two oral talks (one invited) on NV imaging of Cyt-C nanoclusters at Photonics SPIE West 2024, held in San Francisco, CA in January 29 - February 2, 2024, and at MRS Spring Meeting to be held in Seattle, WA in April 22-26, 2024. A female PhD student will present an oral talk at the 2024 APS March Meeting to be held in Minneapolis, MN on March 4-8, 2024. A paper titled "Nitrogen-Vacancy Magnetic Relaxometry of Nanoclustered Cytochrome C Proteins" is just published to the high impact journal *Nano Letters*.

For FRG2's **Objective 1.c, Characterizing new solid-state Qubits in Ultrawide Band Gap semiconductors (on schedule/meets metric)**, 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. Another investigation was performed on Fe^{3+} defects in GaN. There, we were able to measure both the frequency response of the 2 quintuplet spin transitions split by spin-spin (zero-field) interactions and the associated zero-frequency (DC) magnetization using SQUID magnetometry. Then, using the fundamental Bloch equations for the

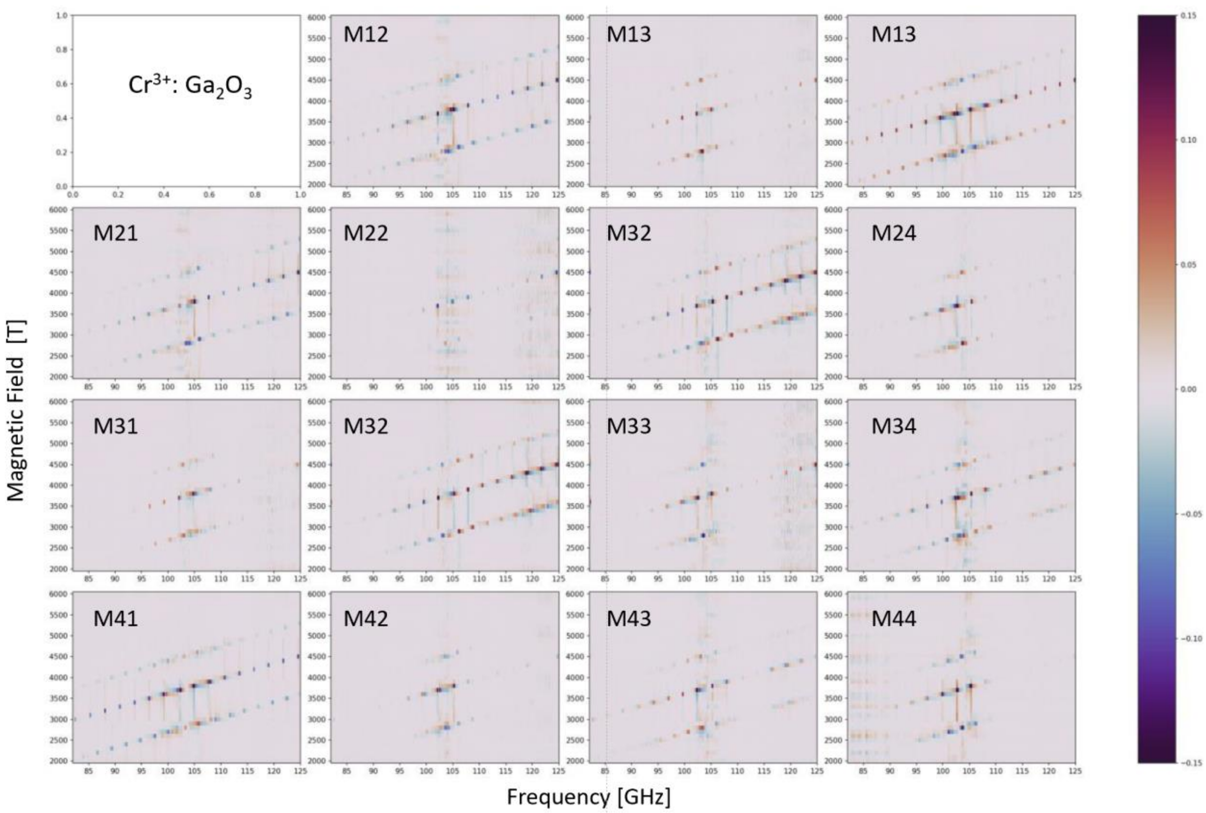

Figure 16. First-ever reported frequency-field map of the full polarization resolved response of a magnetic resonance experiment in terms of the Mueller matrix elements for the Cr^{3+} EPR signal in monoclinic structure Ga_2O_3. The EPR spectra in the THz range obtained by ellipsometry are repeatedly scanned with shifted magnetic field. The spectra are plotted in a heat map and precisely line out the transition shifts. Note that strongest signatures are in the anti-diagonal elements (41, 32, 23, 14) which are related to the circular dichroism and circular birefringence, here caused the magnetic susceptibility function due to changes of the nuclear magnetic moments.

time and field response of nuclear magnetic moments, the **Schubert** group for the first time derived and demonstrate the analogue of the Lyddane-Sachs-Teller relationship for magnetic materials. Due to the unique position to be able to measure the frequency and field dependent complex valued magnetic susceptibility (the analogue of the dielectric susceptibility for dielectric polarization), the Schubert group could demonstrate that integral calculations over the measured EPR frequency response indeed precisely yields the corresponding DC magnetization. A paper for publication in Nature Physics is under preparation. Furthermore, the **Schubert** group investigated potential quantum emitters in UWBG metal oxides. **Fig. 16** depicts the first ever reported frequency-field maps of an EPR transition, he re for the Cr^{3+} in Ga_2O_3. Quantitative analysis of the Hamiltonian parameters and identification of their monoclinic distortion is underway. 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.

Achieving FRG2's Year 3 milestone, we successfully demonstrated frequency-field scanning THz-EPR ellipsometry on EPR transitions in UWBG semiconductors.

Our prototype frequency-scanning THz-EPR ellipsometer setup can be explored for further use time-resolved THz EPR mode using photo-induced EPR signatures detecting decay times with time resolution of 8 microseconds. 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.

Mathias Schubert has become a founding member of the AVS technical group Spectroscopic Ellipsometry at AVS 69 International Symposium and Exhibition (AVS-69) in Portland, OR during November 2023. He was reappointed Commissioning Editor for Applied Physics Letters, and was named guest professor for one year in NanoLund at the Physics Department in Lund University, Sweden starting August 2023.

Graduate student **Alexander Ruder** developed the THz EPR ellipsometry instrumentation and graduated with a PhD in Electrical Engineering from UNL in **M. Schubert**'s group in December 2023, then joined Onto Innovation for continued industrial research. **M. Schubert** visited Linkoping University in Sweden, and the Leibniz Institute for Polymer Research in Dresden, Germany, where he presented seminars on THz EPR methods for quantum defect characterization. In EQUATE Year 3, the **Schubert** group trained new graduate student **Ian Green** and new African-American graduate student **Ray Smith** together with undergraduate student **Preston Sorenson** (ECE, UNL) in ellipsometry basics, basic instrumentation design, and fundamentals of quantum material engineering.

The **Schubert** group published two papers in the journal *Advanced Materials* (IF 29.4): Quantum Composites with Charge-Density-Wave Fillers (doi.org/10.1002/adma.202209708) and The Role of Optical Phonon Confinement in the Infrared Dielectric Response of III–V Superlattices (doi.org/10.1002/adma.202305106). The **Schubert** group presented 20 scientific talks at various in-person and online events at national and international conferences, including invited and plenary talks-- for example, at the Workshop Ellipsometry in Prague, Czech Republic. Undergraduate student **Preston Sorensen** won Best Student Poster Award Paper and graduate student **Alexander Ruder** won best Student Paper Award at the Spectroscopic Ellipsometry Group Meeting at AVS-69. **M. Schubert** was invited to speak at the 2024 Henri Poincaré Webinar Series on Optical Polarization and Related Phenomena organized by the International Society for Optics and Photonics SPIE and hosted by the National Institute of Standards and Technology. The **Schubert** group published 10 peer-reviewed papers. Further, the **Schubert** group presented an invited talk on Strain and defects in Gallium Oxide and related compounds at the 6th U.S. Workshop on Gallium Oxide (GOX 2023) in Buffalo, NY, during August 2023. The team also presented on THz Spectroscopic Electron Paramagnetic Resonance Of The Fe^{3+} Defect In GaN at the 48th International Conference on Infrared, Millimeter and Terahertz Waves in Montreal, Canada, September 2023.

FRG2's **Thrust 2: Quantum Communication: Transmitting Data with Single or Entangled Photons, Objective 2.a Enhanced Nonlinear Optical Effects at the Nanoscale (on schedule)** includes the following achievements:

With **2.1.1 Linear Chiroptical response of Broken L-shape Metamaterials,** in EQUATE Year 3 **Eva Schubert**, **M. Schubert**, and **Ufuk Kilic** played a pivotal role in advancing the field of chiroptically active nanostructure designs. Their collaborative efforts focused on the design, theoretical and experimental optimization, as well as the fabrication of nanostructures using the innovative glancing angle deposition technique. In the new proposed nanostructure design, they fabricated broken L-shaped metamaterial platform, which is axially and spatially coherently defined, relatively well-ordered, three-dimensional, and continuous nanostructure, made out of size-controllable-nano-columnar segments. Hence, they reported the ability to fully control the length of nanocolumns which induces a unique control to the strong chirality spectral location and amplitude. Based on this very simplistic chirality design, they experimentally observed and theoretically verified one of the largest, broadest, and spectrally controllable chirality responses (see **Fig. 17**).

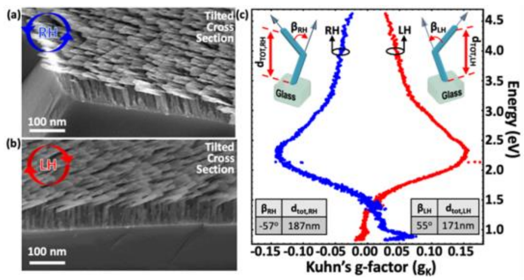

Figure 17. High-resolution titled cross section scanning electron microscopy (SEM) images of left-handed (LH) and right-handed (RH) broken L-shape metamaterial platform. Mueller matrix generalized spectroscopic ellipsometry based measured chiroptical response in terms of Kuhn's dissymmetry factor which is given as circular dichroism ($CD = A_{LCP}-A_{RCP}$) normalized to total absorption ($g_k = 2CD/(A_{LCP}+A_{RCP})$).

Recently, there has been a paradigm shift in the engineering of optical materials from single material building blocks to the hybridized metamaterial platforms which can unlock new possibilities in the manipulation of chiral light-matter interactions at nano scale (see **Fig. 17**). **Figs. 17a** and **17b** show HR-SEM from the tilted cross section of the SiAg broken L-shape metamaterial sample together with the top view SEM image and the scanning-transmission electron microscopy image with atomic resolution energy-dispersive X-ray spectroscopy-based material mapping as insets.

For **2*.1.2 Upconversion performance of Broken L-shape Metamaterial Platforms at second harmonic frequency:*** Beyond the linear chiroptical response, the collaboration among **E. Schubert, M. Schubert, and U. Kilic** explored the nonlinear photon upconversion performance of these metamaterial designs (see **Fig. 18**). Photon upconversion, briefly described, involves the sequential absorption of low-energy photons, such as those from the infrared spectrum, transforming them into higher-energy photons, typically in the visible or ultraviolet range (see **Fig. 18a**).

Remarkably, this FRG2 team showcased that the newly-proposed metamaterial platform exhibits chiral photon upconversion at the second harmonic frequency and is effectively controllable by varying the distortion angle (β). The asymmetry in the transmitted signal between left-hand (LH) and right-hand (RH) circular polarization was notably pronounced at a 45° distortion angle, as depicted in **Fig. 18c.**

The importance of this work extends to diverse applications, particularly in the realms of energy harvesting, quantum communication, and photonic integrated circuit devices. **Kilic** also theoretically investigated optical harmonic generation and up-conversion performances across diverse nanophotonic platforms, contributing valuable insights to the ongoing fabrication endeavors. The ability to control the conversion of photons at different frequencies facilitates the creation of entangled photon pairs, essential for quantum key distribution and other quantum communication protocols. This feature contributes to the development of secure communication systems with applications in quantum cryptography. In conclusion, this collaborative effort not only contributes to the fundamental understanding of chiroptical phenomena but also paves the way for transformative nonlinear optical mechanisms in energy harvesting, quantum communication, and photonic integrated circuit device applications. **(meets metric)**

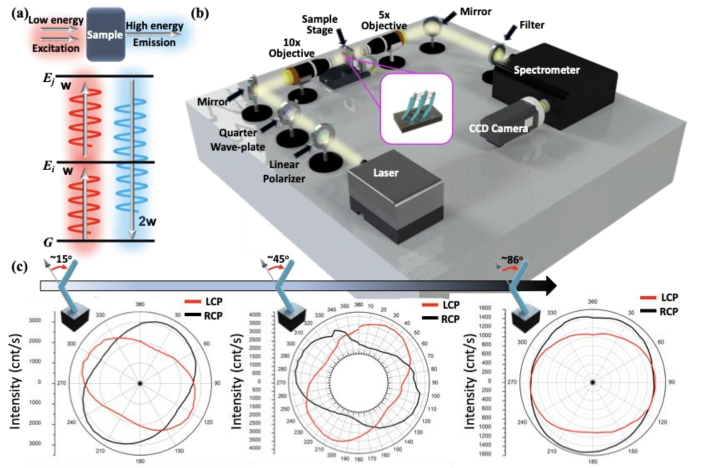

Figure 18. (a) General principle of upconversion process. (b) optical set-up for investigating the upconversion luminescence performance at second harmonic frequency. (c) Sample azimuthal rotation evolution of upconversion performance at second harmonic frequency for the metamaterial platform with different distortion angle of the second columnar segment of broken L-shape metamaterial (β: 15º, 45º, and 86º from left to right) under both right circularly polarized (RCP, red solid line) and left circularly polarized light(LCP, black solid line) sources. The laser power and excitation wavelength are taken as P_{laser}=100mW and λ_{ext}=1030nm, respectively. Measurements were performed based on the collaboration with Prof. Hoang from Univ. of Memphis.

Kilic was also invited to give the opening plenary talk titled as "*Spectroscopic ellipsometry based optical analysis of hybrid metamaterial platforms*" in the 12th Workshop on spectroscopic Ellipsometry (WSE), Prague-Czech Republic, in September 2023. Additionally, **Kilic, E. Schubert,** and **M. Schubert** jointly submitted four abstracts for presentations at APS 2024 March Meeting, and two of these abstracts have been accepted for presentation by two female graduate students. The linear chiroptical response of the metamaterial systems has been submitted to Nature Communications and is currently under review. The *in-situ* spectroscopic ellipsometry based growth monitoring of ZnO ALD is in the submission stage to the *Journal of Vacuum Science Technology-A* (IF = 2.9). Another paper is currently under revision in *Advanced Optical Materials* (IF = 9) on revealing the universal effective medium properties of slanted nanocolumnar structures from a wide variety of material choices.

As a part of this EQUATE FRG2 program, under the supervision of **M. Schubert, E. Schubert,** and **Kilic**, one female student was trained on performing theoretical simulations on linear and nonlinear optical responses of various metamaterial designs. Another female student was trained on atomic layer deposition system which is another key fabrication segment for the fabrication of complex metamaterial systems for the development of efficient single photon generation mechanisms, for example.

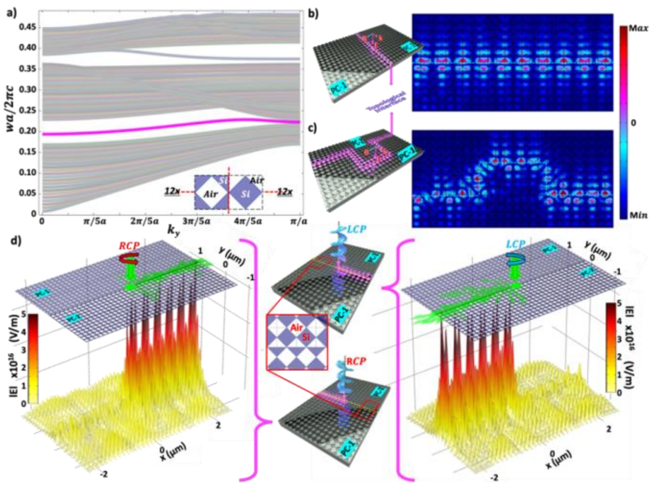

Figure 19. (a) Projected band structure for the photonic boundary between the semi-infinite PC-1 and PC-2. The magenta line shows edge state dispersion. The coupling of electric field amplitude at different interface scenarios: (b) straight case (c) pulse-shape case with sharp corners. In both cases, the superlattice structure is made out from 24 by 24 unit cells. As the half of this structure consists of PC-1, the other half is PC-2. (d) the directional propagation of circularly polarized light at the interface: the theoretical demonstration of chiral topological edge state. While right-handed circularly polarized light (RCP) propagates to +x-direction, the left circularly polarized (LCP) propagates through the opposite direction.

Kilic will present one oral and one poster presentation regarding the research outputs (in collaboration with **E. Schubert** and **M. Schubert**) of optical and magnetic properties hybrid columnar metamaterial platforms in the upcoming APS March Meeting to be held in Minneapolis, MN in March 4-8, 2024. In the same conference, two female students will present their works (*in-situ* spectroscopic ellipsometry based real time growth monitoring of ZnO ultra-thin films and Spin-locked topological edge state from all-dielectric metasurface design), as well.

For **Objective 2.b Robust Entangled Photon Generation from Nanoscale Structures**, FRG2 conducted **2.2.1. Spin-locked topological edge state from all-dielectric metasurface design.** Two-dimensional photonic topological insulators (2D-PTIs) have garnered attention for their potential applications in quantum information technologies and advanced photonic integrated circuits. **Kilic** collaborated with **E. Schubert**, and **M. Schubert** in the design and optimization of new photonic interface from a simplified photonic crystal with an all-dielectric checkerboard structure. The interface is engineered by introducing a 2D lattice mismatch with a half-lattice constant shift along both x- and y-directions. The resulting super-lattice structure induces the emergence of an ultra-narrow band leak mode in the linear optical response, characterized by an extraordinarily large Q-factor ($f_{rsnc}/\Delta f_{FWHM}$ where f_{rsnc} and Δf_{FWHM} are the spectral location and full width half maxima (FWHM) of the resonance peak, respectively) value of ~ 4 x 10^6, indicating minimal energy losses within the system. This feature enables longer photon lifetimes and holds promise for achieving a superior signal-to-noise ratio. Despite the identical energy dispersion diagrams on both sides of the interface, differences in Zak Phases are observed, providing clear evidence of a topological edge state. The theoretical efforts showed that at the resonant frequency, the light couples to the interface (see **Fig. 19b and 19c**) and moreover, depending on the handedness of incident beam, the propagation has a directional property, as well (see **Fig. 19d**).

Further investigation into the nonreciprocity performance, incorporating the non-linear Kerr effect, reveals a notable blue shift in the topological leak mode within the transmission/reflection spectra with increasing beam intensity. Additionally, we demonstrate the feasibility of enhancing both spectral controllability and nonreciprocity properties of the topological edge mode through the introduction of a defect, such as an air hole and/or a pillar, at the interface (see **Fig. 20**). We envision that the findings presented in this research contribute valuable insights into the manipulation of photonic topological insulators, providing new avenues for the development of next-generation photonic devices and quantum technologies.

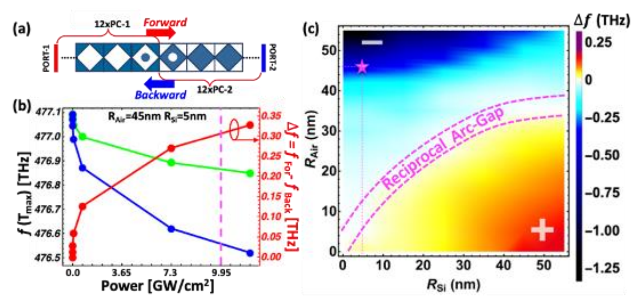

Figure 20. Engineering the Nonreciprocity of Topological Edge Mode: "Ternary Switch". (a) Schematic diagram of theoretical framework which will be used in the non-reciprocity induced by Kerr effect nonlinearity in the topological edge state checkerboard metasurface design. (b) power dependent evolution of topological leak mode extrema points in forward (green) and backward (blue) light illumination and the nonreciprocity is defined as the difference between them: $\Delta f = f_{for} - f_{back}$. Spin of nonreciprocity as a function of defect size and type. The inclusion of an air hole defect induces the leak mode in the transmission spectrum for forward illumination "lagging" behind the backward illumination case. This is reversed with the introduction of a Si pillar defect at the interface, causing the leak mode in the transmission spectrum for forward illumination "leading" the backward illumination case, instead.

Bao group built an experimental set-up to produce and measure Spontaneous parametric down-conversion (SPDC) two-photon entangled pairs (**Fig. 21**). **Bao** integrated all equipment required for the experiment including tunable femtosecond laser, single photon detectors, microwave, and optical equipment and built up the setup, **Fig. 21**. **Bao** built SPDC setup that is capable in generating entailed photon pairs. **Kilic** developed a theoretical model framework that can provide insight information on the topological edge state and second order nonlinear processes which can be utilized to investigate topologically protected entangled photon-pairs. **Bao** trained a graduate (PhD) student in setting optical components of the SPDC setup to generate entangled photon pairs. Kilic trained a female graduate student to study high order nonlinear optical processed and topological insulators. **Bao** published a paper on deterministic and replaceable transfer of silver flakes for microcavities in *Frontiers of Physics*. Currently, **Kilic** is preparing another manuscript titled "Spin-locked topological edge state from all-dielectric metasurface design" for submission to a special issue on Topological and Chiral Matter in *Applied Physics Letters* (IF = 4). **(on schedule/meets metric)**

Figure 21. Setup in Bao's lab with newly installed coherent fs laser and SPDC .

For **Objective 2.c Efficient Single Photon Generation from Nanoscale Structures**: recently, single photon emitters (SPEs) have been observed in two-dimensional (2D) materials like hexagonal boron nitride (hBN, **Fig. 22a**). The 2D hosts facilitate enhanced SPE quantum properties compared to bulk systems due to their narrower (< 10 nm) emission linewidths, improved mechanical properties that allow the realization of mechanical oscillators with high quality factor, and ease of integration to optical components for integrated quantum photonics. Despite the extensive recent progress in understanding and utilizing the quantum properties of SPEs in 2D systems such as hBN, future developments are severely limited by low photon emission rates and quantum yield. **(on schedule/meets metric)**

Laraoui collaborated with **Kilic** and obtained promising results on enhancing the quantum properties of SPE, summarized in **Fig. 22e** and **Fig. 22f**. We first produced SPEs in layered 35 nm thick hBN flakes (size is 50 mm), annealed at high temperature

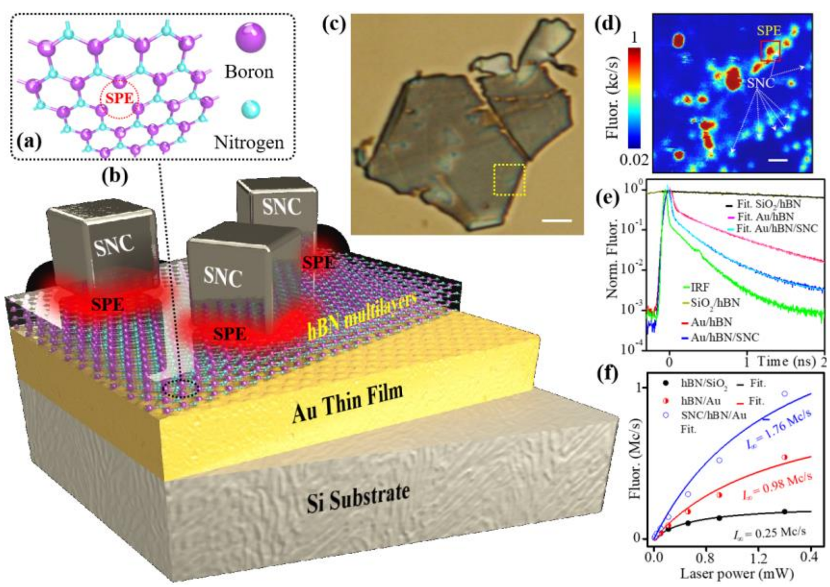

Figure 22. (a) A sketch of the hBN lattice with SPE. **(b)** Schematic of hybrid nanophotonic cavity composed of hBN sandwiched between Au film and SNCs to enhance the quantum properties of SPEs. **(c)** optical image of hBN flake (scale bar is 10 mm). **(d)** Fluorescence image of 35 nm thick hBN flake indicated in **(c)** by a dashed square (scale bar is 1 mm). **(e)** Measured (scattered) and calculated (solid line) lifetime for SPE in hBN flake transferred to SiO_2, Au/Si substrate without (solid red line) and with (solid blue line) SNCs. **(f)** Measured (scattered) and calculated (solid lines) fluorescence intensity as function of the laser power for SPE in hBN flake transferred to SiO_2 (filled circles), Au/Si substrate without (half-filled circles) and with (open circles) SNCs.

(1100 °C) under O2 annealing. We found > 90% of the emitters in **Fig. 22d** are SPEs with narrow (<10 nm) emission spectra and have g(2) <0.5, indicative of single photon emission. We have demonstrated plasmonic enhancement of SPE properties by spin-coating of 98 nm silver nanocubes (SNCs) on top of the hBN flake in **Fig. 22d**: a decrease of quantum emitter lifetime by 200 times (from few ns to 20 ps), an increase of SPE fluorescence by 7 times (up to 2 Mc/s). This is the first result done on SPEs in hBN and we expect > 2000 order of magnitude enhancement of SPE fluorescence when fabricating deterministically metallic nanocavities on top of hBN as in **Fig. 22**.

Kilic developed a COMSOL model to fit the experiments carried out by Laraoui on enhancing the quantum properties of single photon emitters by using plasmon metallic nanocavities.

Laraoui trained a postdoc and an undergraduate student from UNL on performing experiments in quantum optics. The postdoc has successfully completed the two-year contract, published a high impact (9) paper Advanced Optical Materials, and joined Honeywell research labs in Minneapolis, MN, as an Advanced R&D Engineer.

Laraoui and **Kilic** published a high impact paper in *Advanced Optical Materials* which was selected for the back cover of the issue published in August of 2023. A paper on the results summarized in **Fig. 22** is under review at the high impact (11) journal *Laser and Photonics Reviews*.

For the **Seed project: Quantum Size Effect on Radiative and Electronic Transport,** in Year 3 the **Ghashami** group collaborated with **Laraoui**'s lab to investigate the fundamental mechanisms underlying photon and electron transport within micro/nanoconfinements using quantum sensors based on nitrogen vacancy in diamond. Special attention was given to nanostructured surfaces and 2D materials (e.g., hBN and WSe_2). To accomplish the research objective, it was proposed to use NV microscopy with a good spatial (< 20 nm) and thermal (few mK) resolutions to investigate the heat transport mechanism at the single-nanometer distances, and utilize a precise nanopositioning platform equipped with thermal control stages for sub-micrometer separations, as shown in **Fig. 23**. As the first task, fabrication and characterization of candidate materials/surfaces was required to provide a quantitative understanding of the role of material/surface characteristics in photon/electron emission. Inspired by the optimal design parameters of our theoretical modeling, our samples and nanophotonic structures were fabricated in collaboration with FRG2 SIs **Kilic** and **E. Schubert**, using glancing angle deposition

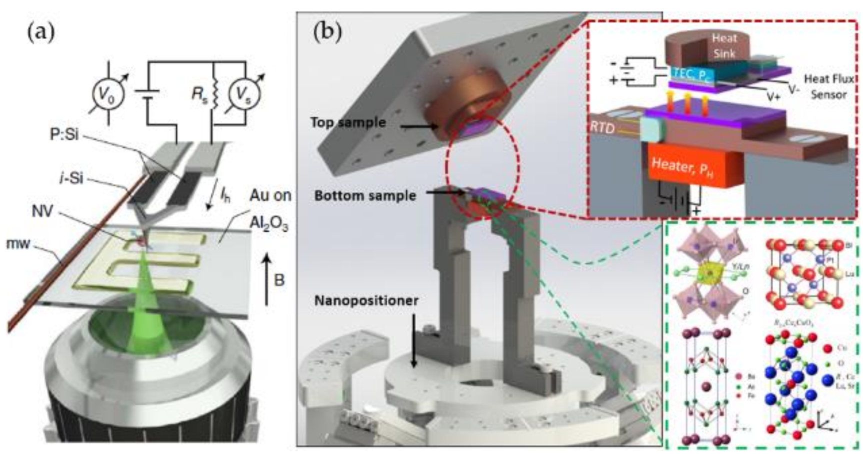

Figure 23. (a) Schematic of a thermal AFM cantilever with a diamond-nanocrystal-hosted NV attached to the tip. **(b)** Schematic of our high-vacuum nanopositioning platform used for precision measurement of energy fluxes between quantum materials.

(GLAD) techniques. The optical and radiative characteristics of these unique samples were carefully extracted using spectroscopic ellipsometry (in collaboration with FRG2's **M. Schubert**, to probe the surfaces' dielectric function and film structure. For temperature and electric field mapping, we used AFM to generate high-resolution nanoscale images and study the fabricated samples' local sites/forces. We employed an NV microscope, a state-of-the-art combined-platform hosting tuning-fork-based AFM, and an optical confocal microscope, see **Fig. 23a**, in collaboration with **Laraoui** lab, to perform imaging of various quantum properties with a spatial resolution (<20 nm) at variable temperatures (4-400) K. To experimentally demonstrate the quantum-size dependence of photon and charge transport, we proposed to perform precision energy flux measurements between two engineered surfaces separated by a nanoscale vacuum gap. **Mohammad Ghashami**'s group developed a precision nanogap controller setup inside a high-vacuum chamber to be able to host a pair of the fabricated samples. The high-precision nano-positioning platform, as shown in **Fig. 23b**, is configured with three closed-loop controlled piezo-actuating motors to control the width of nanoconfinement, and also a sensitive heat fluxmeter for direct reading of energy flux across gap. Using this apparatus, **Ghashami**'s group will conduct direct energy measurements between any two planar macroscopic surfaces. An integrated Fabry-Perot interferometer will also be integrated to measure and monitor the gap distance in real time.

Ghashami trained a Hispanic Ph.D. student on design and development of a nano-thermometry setup. The student also learned the design and fabrication of metamaterials using GLAD technique in collaboration with **Kilic** and **E. Schubert**. **Ghashami** held weekly group meetings where two undergraduate students were involved with the nanoscale heat flux measurements and performing basic AFM scans in collaboration with **Laraoui**. The Ph.D. student from **Ghashami**'s lab delivered three two oral presentations at ASME IMECE 2023 (held in New Orleans, LA) and the MRS Fall Meeting and Exhibition 2023 in Boston.

In Year 3, FRG2 SIs made significant impact in many research and education aspects, including:

- **Mathias Schubert** and **Eva Schubert** organized a full two-term online lecture series in Fall 2023 and Spring 2024 (16 lectures total), the Nebraska Ellipsometry Lecture series. This lecture is given by speakers from Europe, Asia, and North America, and attracts 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 toward 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 (ECCS 2329940) with Dr. Shubhendu Bhardwaj from ECE at UNL investigating Semiconductor-based Terahertz Traveling Wave Amplifiers for Monolithic Integration. As main organizer of the 2025 International Conference on Spectroscopic Ellipsometry, **M. Schubert** in November 2023 initiated the North American Ellipsometry Association group on LinkedIn which serves as a platform for professionals in the field of ellipsometry in North America to connect, share knowledge, discuss trends, and explore collaborative opportunities. The group has 121 members.

- **E. Schubert** received two NSF grants. The first, "Broadband and Tunable Enhanced Chiral Light-Matter Interactions at the Visible with New Ultrathin Helical Metamaterials," focuses on exploring enhanced chiral interactions between light and matter using innovative ultrathin helical metamaterials in the visible spectrum. The second grant, titled "NSF-DFG: Advances in Ion-Surface Interaction-Driven Manufacturing of One-Dimensional Metal Oxide Heterostructures," centers around the fabrication and characterization of metal oxide heterostructures driven by ion-beam assist deposition technique. In April 2024, **E. Schubert** was promoted to professor at UNL.
- **Abdelghani Laraoui** received an NSF grant for $800,000 in collaboration with Kapildeb Ambal and Jian Wang from Wichita State University, KS (also an EPSCoR state) within ExpandQISE program's Track-1 funding, for understanding and controlling decoherence in hybrid spin qubit-magnon systems for advancing education and building workforce in emerging quantum technologies. **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). For Spring 2024 (January-May), 15 students (4 female) registered for the class with 11 graduate students and 4 undergraduate students from Physics, Chemistry, Electrical & computer engineering, and Materials & Mechanical engineering departments.
- **Ufuk Kilic** remodeled and refurbished the ALD and GLAD lab facilities in the new labs at UNL and refurbished 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 female and African-American graduate students.
- **Sy-Hwang Liou** remodeled the magnetic force microscopy (MFM) setup to measure topological spin textures and trained EQAUTE funded students from FRG1 and FGR2 on the setup. **Liou** in collaboration with **Laraoui** supervised a female PhD on aspects of quantum sensing. The female student published two high impact papers at ACS Nano (IF = 17.1) and Nano Letters (IF = 10.8).
- In EQUATE Year 3, seed awardee **Mohammad Ghashami** received NSF's CAREER Award. He also organized a 1-day tour of his lab and facilities for middle school students from throughout Nebraska for the Big Red Summer Camp. The 16 students (6 girls and 10 boys) participated in hands-on experiences designed to engage them with basic physics of heat transfer and to encourage their further pursuit of STEM topics.

In terms of challenges, Wei **Bao** left UNL during EQUATE Year 3 and was replaced by SI Alexander **Sinitskii** (see FRG3). Bao's FRG2 research activities are replaced by SIs **Kilic** and **Laraoui**.

FRG3 – Quantum Information Processing (2023-2024)

As outlined in the strategic plan, Year 3 for EQUATE's FRG3 was marked by a significant growth in scope, with the addition of **Alexander Sinitskii** who replaces **Wei Bao** as an SI after Bao's departure from UNL in August 2023, as well as the return of **Tom Wong** after his leave. Sinitskii is a professor of chemistry at UNL and was a seed-grant awardee who joins FRG-3 to strengthen the experimental materials capabilities underlying both the exciton-polariton BEC research previously conducted by Bao as well as the crosswire quantum dot objective.

In particular, the theoretical work on crosswire quantum dots by **Mei** and **Sabirianov** has led to a promising effort by **Christian Binek** (FRG1) to synthesize and measure transport properties of the crosswire quantum dots made from graphene. The experimental effort will be enhanced by the introduction of Sinitskii who will work to fabricate these devices in other 2D materials such as di- and tri-chalcogenides.

Secondly, inter-FRG discussions have yielded an initial plan to not only continue work with exciton-polariton BECS as originally proposed by Bao, but to expand it into new directions with a collaboration between seed awardee **Yanan (Laura) Wang** and **Sinitskii**.

We are also excited to have **Tom Wong** (Creighton University) back from his leave at the National Quantum Coordination Office in Washington D.C. as of January 2024. We expect the work on quantum computing algorithms to accelerate with his return.

Key personnel are FRG3 leader **Wrubel** (Creighton University), Bao (UNL – participation ended in August 2023), **Armstrong** (UNK), **Wong** (Creighton University), **Mei** and **Sabirianov** (UNO), **Wysocki** (UNK), and **Sinitskii** (UNL – joined August 2023).

Thrust 1. Quantum Emulation

Objective 1.a: Surpassing the Standard Quantum Limit in a ^{41}K BEC (on schedule)

FRG3 successfully reconfigured the experiment from cooling and trapping potassium-39 to the 16x less abundant potassium-41 needed to achieve Bose-Einstein condensation. We successfully installed our optical dipole trap and are loading atoms from the magneto-optical trap into the dipole trap. **Fig. 24** shows an absorption image of the crossed dipole trap beams and a fit to measure the number of atoms in the crossing. We are currently loading about 1.5 x 10^4 atoms and are working to increase this number so that evaporative cooling can be used to achieve Bose-Einstein condensation.

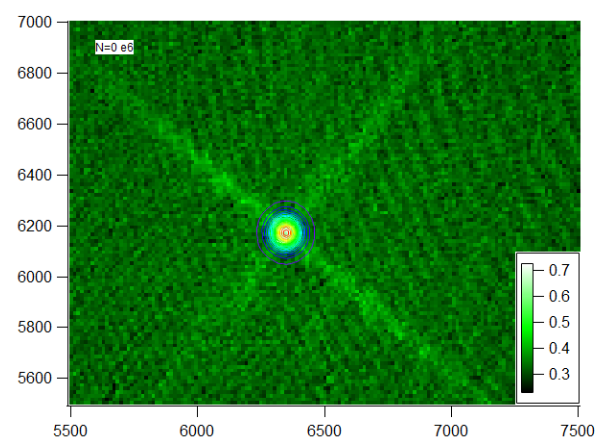

Figure 24. False-color absorption image of the crossed optical dipole trap laser beams. The circles show a fit to the central region of trapped atoms which measures the total number of atoms.

A main goal of this experiment has been the detection of the radio-frequency Feshbach resonance. Now that we are able to reliably capture atoms in the optical trap, we will be able to do our first searches for the radio-frequency Feshbach resonance before the end of Year 3.

After a six-month lead time, we have also received our primary imaging camera which will dramatically improve the signal-to-noise ratio of our images. The camera has been installed and tested, and we are currently developing the software interface needed to make use of the camera in our experiment.

The most significant result was loading ultracold potassium-41 atoms into the optical dipole trap. This paves the way for our first attempts at detecting the RF-Feshbach resonance before the end of Year 3.

We continue to push hard to achieve Bose-Einstein condensation and complete our Year 3 objectives. FRG3 also trained 4 undergraduates and 1 graduate student in techniques of laser-cooling and trapping, and mentored 1 postdoctoral fellow.

Postdoctoral fellow **Corbyn Mellinger** presented our results on the cold temperatures of our octupole magneto-optical trap at the APS Division of Atomic, Molecular, and Optical Physics Conference in June 2023. We are preparing to submit a manuscript to *Physical Review A* on Quantum Walk Algorithms in collaboration with SI Tom Wong. We published one master's thesis (currently under embargo).

We have been somewhat delayed by a drop in the number of master's students applying to the Creighton physics program, which leaves us with no graduate students in the lab this year. Progress towards BEC has been steady but slower than expected. To achieve BEC we need more atoms in the optical dipole trap. One way we will address the need for more atoms in the optical dipole trap is to implement a grey-molasses cooling technique which has been shown to decrease temperatures by about 10× in potassium and increase dipole trap loading rates dramatically.

For **Objective 1.b: Emulation of Novel Spin Systems (on schedule)**, the goals of this objective depend in large part upon the completion of the activities described in Objective 1a, which continue to be our main focus. Progress on the optical lattice will be delayed until Year 4.

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

On **Objective 1.d: Theory of Polarons in Dipolar and Spinor Gases (on schedule)**, we examined how the orientation and degree of asymmetry of an asymmetric repulsive Gaussian impurity affected the self-energy and density of a dipolar Bose-Einstein condensate gas. This follows the strategic plan of extending codes for more properties of the polarons. We plan to start looking at some properties of Lee-Huang-Yang (LHY) liquids, which is the next term in the mean field expansion of a Bose fluid, specifically on signatures of superfluidity within such a liquid like a quantum droplet. Finally, we plan to start working on making modifications to our code to implement optical lattices, which is a part of FRG3's Year 4 objectives.

We found that the shape of the Gaussian impurity with the lowest self-energy was spherical, perhaps somewhat surprising as the dipolar gas has a preferred direction. It seems the spherical shape still creates the minimum disturbance to the gas. For the density, we found significant deviations near the impurity as expected but at a far enough distance, the density resembled that of the pure gas, illustrating the healing length of the condensate. Near the impurity, the dipolar gas reacted differently depending on the geometry of the impurity, particularly with increasing deformation perpendicular to the dipole polarization axis. Usually the density, which forms a single central peak in the absence of an impurity, bifurcates into two satellite peaks with their location dependent on the orientation and deformation of the impurity.

FRG3 **postdoc Neelam Shukla** (UNK) attended and presented at three scientific conferences, one of which was in her previous field. She is training in new computational techniques such as Monte Carlo, machine learning, and parallelization of codes. She will also take two short classes at the upcoming March Meeting in quantum computing. Also, UNK's Armstrong is mentoring an undergraduate student who is working mostly with Shukla on nuclear fusion/plasma calculations. They have made great progress, and plan on submitting a manuscript for publication this spring, which is fantastic for our undergraduate researcher.

EQUATE FRG3 work has been disseminated in several presentations. **Shukla** gave a talk at the June 2023 DAMOP meeting in Spokane, WA and will speak at the upcoming APS March Meeting in Minneapolis, MN. She also presented a poster at the Gaseous Electronics Conference in Ann Arbor, MI, in October. **Armstrong** gave a talk at the Institute of Science and Technology-Austria to the research group of a collaborator there. Finally, Armstrong was invited to participate in The Symposium on the Occasion of Aksel Jensen's 80th birthday (he was second post-doctoral supervisor) at Aarhus University, Denmark. We continue to work on publishing our research, and expect to be able to submit this spring.

In terms of **Changes/Problems**, this year FRG3's UNK team began to focus not so much on the impurity/polaron, but either its effect on the medium that it is implanted into or the medium itself (the LHY liquids): a slight deviation from the Strategic Plan.

With **Thrust 2. Quantum Computation,** for **Objective 2.a: Quantum Walk Algorithms (meets metric)**, we improved the runtime of nonlinear quantum search algorithms by tuning the relative weight of cubic and quintic terms in the nonlinearity. One publication nearly ready for submission to *Physical Review A* on "Quantum Search with a General Cubic-Quintic Nonlinearity." In terms of **Changes/Problems,** Wong originally planned on returning to Creighton University—from the National Quantum Coordination Office at the White House Office of Science and Technology Policy (OSTP)—in Summer 2023. Instead, he returned in January 2024, delaying the start of his concerted efforts on EQUATE.

For **Objective 2.b: Crosswire Quantum Dots for Quantum Computing (on schedule)**, we focused on the materials of promise for 2D arrays of quantum dots (QDs). Using density-functional theory (DFT) we calculated the electronic states of cross-wire QDs in graphene, as well as h-BCN. This allows us to construct the effective Hamiltonian of such realistic systems that involve all accounted interactions including the quadratic spin-spin interaction.

We continued to explore magnetic and transport properties of potential 2D materials. We analyzed anomalous Hall effect (AHE) in Cr_2Te_3. We find strong canting effects of the magnetic moments on the AHE, and explained the temperature dependance of the AHE conductivity, including the change in the sign. We are currently analyzing decay rates of a chain of atoms (i.e., two-level systems) on a Fibonacci lattice and similar systems.

We characterized the magnetic and transport properties of Cr_2Te_3, and found strong unconventional temperature dependence of the AHE and a change in the sign of the AHE as temperature increases. We explained the effect by evaluating exchange coupling frustration on the lattice resulting in canting of the spin of self-intercalating Cr that varies in temperature.

We analyzed magnetic interactions in doped Fe_3Te_4. We find that doping with 3d-metals does not promise an increase in Curie temperature and, therefore, does not make room temperature applications more feasible. We also observed proximity effect in h-BCN/WSe_2 heterostructures using DFT calculations, and Identified potential adsorption sites of impurity atoms on h-BCN.

We developed a high-throughput approach to analyze the change in electronic states of 2D materials and 1D QDs.

In terms of **training and development**, FRG3's University of Nebraska at Omaha (UNO) team trained a postdoctoral fellow, **Jaeil Bai**, who has performed analysis of quantum 2D materials such as Cr_2Te_3, Gr/metal nanostructures, as well as h-BCN chiral nanodots. Bai presented results of his studies at the American Physical Society, March 2023. Dr. **Alsaad** has received training in applications of DFT to study quantum materials. He performs calculations of heterostructures of h-BCN with TM magnetic atoms and monolayers. He performs calculations of magnetic interactions using VASP, wannier90 and TB2J. In addition, he performed studies of 2D and 3D quantum materials such as Fe_3Se_4. He presented results of these studies at the APS March meeting as well.

This UNO team supervises Dr. **Yinglu Jia**, a newly hired research associate, on two projects--

- Mechanism studies of laser assistant crystalline growth of GaN, and
- High-throughput calculation of altermagnetic materials

--plus an undergraduate student, **Edgar Ramirez-Soto**, a physics major at UNO who has learned basics of DFT calculations and performing the studies of chiral quantum materials. He is supervised in part by Dr. Alsaad.

In terms of dissemination, FRG3's UNO team submitted 5 manuscripts for publication (4 already published), and another manuscript is in preparation. The group's postdoctoral fellows and visiting scientists have given presentations.

For **Objective 2.c: Computational design of new spin-qubit materials (on schedule)**, we identified promising adatom/surface combinations for spin-qubit applications:

1. Lanthanide adatoms (Tb, Dy, Ho) on graphene:
   (i) Strong spin-orbit coupling of lanthanide adatom can provide large anisotropy barrier for spin stability.
   (ii) Scarcity of nuclear spin in graphene (abundant ^{12}C nuclei have no nuclear spin) may lead to a large coherence time.
   (iii) Excellent electronic properties of graphene allow for reversible ionization of adatoms by gating. In his previous research, the PI has demonstrated that magnetic anisotropy and hyperfine coupling of lanthanide atoms depend dramatically on the ionic state. It is, therefore, expected that magnetic properties of the adatoms can be efficiently controlled by gate voltage.

2. Transition metal adatoms (Fe) on two-dimensional In_2Se_3:
   (i) Since In_2Se_3 is ferroelectric and there should be a significant bonding between adatom and the surface, the magnetic properties of the adatom may be controlled by switching electric polarization of In_2Se_3.

For both systems, preferred adsorption sites have been determined and the relaxed atomic structures have been obtained. For all considered lanthanide adatoms, the graphene hollow site has the lowest energy. However, the energy for both the on-top and the bridge sites is less than 0.1 eV higher, and therefore these sites may be experimentally realized as well. For the Fe@In_2Se_3 system we identified two competing adsorption sites with energy difference of about 0.1 eV. Interestingly, the energetic ordering of these sites can be reversed by electric polarization switching.

Electronic structure has been computed for both types of adatom/surface combinations. For lanthanide adatoms on graphene, the non-spin-polarized density functional theory (DFT) calculations (keeping the 4f states in the core) demonstrate a small charge transfer from lanthanide 6s states to carbon π states and, consequently, the graphene Dirac point is shifted below the Fermi energy. For description of magnetic properties, the lanthanide 4f states must be explicitly included. Since DFT cannot properly describe the multiplet structure of the partially-filled 4f levels, the electronic structure is computed using the multiconfigurational quantum chemistry method for a cluster model. The resulting low-energy spectrum originates from the strong coupling between the lanthanide ground 4f multiplet split by the graphene crystal field and the lanthanide 6s/5d LS states. The latter are determined by the lanthanide oxidation state and, therefore, the low-energy spectrum changes dramatically with the oxidation state even though the 4f occupation stays the same. For the Fe@In_2Se_3 system the electronic structure can be accurately described using DFT+U method. We found that the band structure strongly depends on the adsorption site and the electric polarization direction. In fact, the Fe 3d occupation and Fe magnetic moment are significantly different for different adsorption sites and different polarization directions.

Calculations of magnetic interaction parameters are partially completed. For lanthanide adatoms on graphene, the magnetic anisotropy barrier has been calculated for small cluster sizes. For the +3 ionic state, the barrier can be described using the Stevens crystal field parameters (computed). The anisotropy barrier strongly depends on the ionic state. Calculations for larger clusters and computation of hyperfine coupling parameters will be done in the future. For the Fe@In_2Se_3 system, the magnetic anisotropy energy has been calculated. The anisotropy shows significant dependence on the adsorption site and the electric polarization direction. The results are currently being analyzed.

Significant aspects include demonstration of strong sensitivity of magnetic anisotropy barrier to the ionic state of the lanthanide adatom on graphene, and demonstration of control of the magnetic properties of Fe adatom on In_2Se_3 by the electric polarization switching.

In addition, electronic-nuclear spectrum for the ground state of the $Eu(BA)_4$ molecule has been calculated and a good agreement with the literature experimental data has been demonstrated. Calculated transition probabilities between the levels indicate that an efficient light-nuclear-spin interface can be realized in this system.

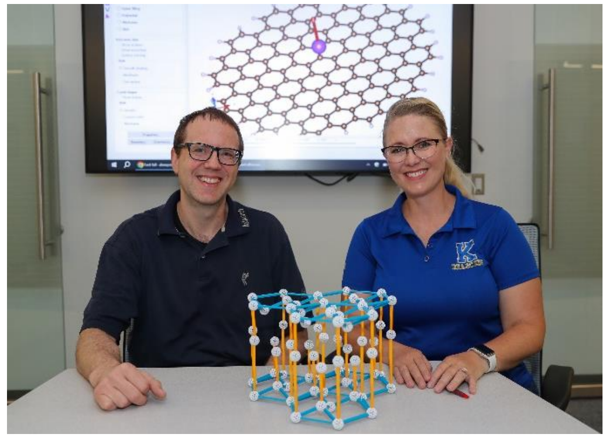

Figure 25. Alex Wysocki (UNK Physics) meets with Kearney High School teacher Alison Klein during her RET work in Summer 2023. UNK photo

In this area, FRG3's **Wysocki** trained a postdoctoral researcher in multireference quantum chemistry calculations. Wysocki also trained a RET researcher (Kearney High School science teacher **Alison Klein**, via EQUATE outreach placement), on density functional theory electronic structure calculations and multiconfigurational quantum chemistry calculations (**Fig. 25**). Additionally, Wysocki trained an undergraduate student in density functional theory electronic structure calculations, and started to train a freshman undergraduate student in solid state physics and electronic structure calculations.

Wysocki gave a contributed talk at the 2023 APS March Meeting (March 5-10, Las Vegas, NV) titled "Nuclear spin spectra for ground and excited multiplets of Eu-based molecule." Wysocki also gave a presentation at the Magic+ Conference (July 24-28, Bedlewo, Poland) titled "Magnetic properties of transition metal and rare-earth adatoms: An ab initio study".

FRG3 researcher **Monirul Shaikh** presented a poster at the 35th Workshop on Recent Developments in Electronic Structure Methods (June 13-16, 2023; Merced, CA) titled "First principles studies of magnetic adatoms on ferroelectric surfaces."

Regarding Y3 **Impacts** by FRG3's Wysocki group, several outreach activities were conducted:

What	**When**	**Where**	**Who**
Part of the team organizing and running the APEs summer camp introducing students to various concepts from physics, astronomy, and engineering	*May 23-25, 2023*	*UNK*	*20 high school students*
Led the Electric Circuits Activity for the ESU 10 Elementary Science Olympiad	*Dec 6-7, 2023.*	*ESU 10, Kearney*	*12 sessions; each engaged approx. 30 elementary school students*
Visited the Science Olympiad team at Kearney High School to talk about quantum computing	*Dec 14, 2023*	*Kearney High School*	*13 high school students*

For **Objective 2.d: Experimental Realization of Crosswire Quantum Dots in Transition Metal Di(Tri)chalcogenides (meets metric)**, we worked on the synthesis and characterization of 2D materials of interest for quantum applications. These materials included transition metal dichalcogenides (MoS_2, HfS_3, SnS_2) and carbides (i.e., MXenes, such as Ti_3C_2) that could serve as platforms for quantum experiments and devices within all three FRGs.

We developed a new method for the synthesis of MXenes modified with various transition metals (*ACS Nano* **2023,** *17*, 18747); demonstrated MXene-based nanoresonators (*Nanoscale* **2023,** *15*, 1248) and gas sensors (*ACS Applied Nano Materials* **2023,** *6*, 9226).

We studied electronic and optoelectronic properties of HfS_3, a quasi-1D transition metal trichalcogenide material; demonstrated polarization-sensitive phototransistors (*Journal of Materials Chemistry C* **2023,** *11*, 9425).

We demonstrated photodetectors based on 2D SnS_2 modified with methylammonium lead iodide perovskite (*ACS Applied Electronic Materials* **2023,** *5*, 705). **Wysocki**'s group trained three graduate students (Jehad Abourahma, Michael Loes, and Rashmeet Khurana) in synthesis and characterization of 2D materials.

Wysocki's team presented an invited EQUATE seminar (summer 2023) titled "Graphene Nanoribbons for Quantum Technologies." This group has published 9 papers that acknowledge EQUATE support: four of these as lead PI, and five as a contributing author. In addition, the publication Lipatov, A., et al. *Journal of Materials Chemistry C* **2023,** *11*, 9425-9437 was featured on the front cover of the journal, and the publication Bagheri, S., et al. *ACS Nano* **2023,** *17*, 18747-18757 was highlighted in *Science*. In terms of **Changes/Problems**, one change for FRG3's Wysocki group is adding more collaborative research with other FRG3 members.

SOLICITATION-SPECIFIC PROJECT ELEMENTS:

Education, Outreach and Workforce Development (2023-24)

In EQUATE's strategic plan, the goal of the EQUATE Workforce Development effort is to prepare the next generation of highly qualified and motivated students, educators, and researchers through comprehensive programs, activities, and mentoring.

For **Objective 4.1: Equip Nebraska students (grades 6-12) with resources for success in STEM workforce**, Year 3 showed an increased interest in ***Young Nebraska Scientists (YNS) Summer Camps*** with 7 faculty-led camps, most reaching participation capacity. Two new camps were offered directly through YNS including *Discovering Food Science: Exploring Dairy the Milky Way*, a residential high school camp, and *Pizza, The Rise of the Dough*, a camp for both middle and high school students. Year 2 was the first year for "Camp on the Go": taking our mobile camp to Columbus, NE--a hub for many rural Nebraskans. For Year 3, an educator from Columbus, NE who helped with our previous camp brought her students to the NCMN. The students in grades 2 - 7 were exposed to quantum topics through hands-on activities. YNS summer camps were attended by 143 students (61.5% female and 34.2% URG). Ninety-two campers were exposed to EQUATE-specific topics. **Metrics: Yr 1 development, Yrs 2-5, 85 participants (30 at EQUATE-specific summer camps) annually.**

In summer 2023 YNS, in conjunction with Nebraska Center for Materials and Nanoscience (NCMN) and the JA Woollam Foundation, hosted 20 **YNS High School Researchers** (**Fig. 26**) in laboratories at the University of Nebraska-Lincoln (UNL). The students were hosted by EQUATE researchers including **Lai, Laraoui, Streubel, Guo, Xu, E.Schubert, Hong, and Adenwalla**. Additionally, 2 students participated in the program as part of the Wong Laboratory on the University of Nebraska at Omaha (UNO) campus. Twenty students presented posters at the UNL Summer Research Fair. Overall, 50% of HSRs were female and 41% were from underrepresented groups in STEM. **Metrics: Yrs 1-5, 8 students annually.**

Figure 26. Twenty YNS High School Researcher (HSR) students were hired in Summer 2023 via the EQUATE project. This number exceeded the budgeted amount for eight HSRs; additional funds were contributed by local industry partner, J.A. Woollam Company, which also led the students on a factory tour where ellipsometers are made for worldwide use in research.

During EQUATE's Year 3, 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 particle wave duality. Additionally, a module was developed using the RAIN program for a citizen science-based mobile lab. 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. In the 2023-2024 school year, mobile labs have reached approximately 792 students so far with 28% URG and 49.6% female. The schools include Omaha Westside, Minden, Lincoln, Kearney, Hemingford, Spalding, and Wheeler High Schools. **Metric: 1,000 students/yr with 3 EQUATE-specific kits offered during Yrs 2-5.**

EQUATE's ***Faculty Mentoring through EQUATE Seed Grants*** program solicits proposals requesting one year of funding through a university-wide call for proposals. Seed proposals should be focused on a particular research topic in quantum science and technologies, and typically involve one or two PIs at the tenure-track assistant professor level. 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). Five proposals were submitted for consideration, and one was selected for funding in December 2023. The proposal chosen was from **Shireen Adenwalla** of UNL Physics and Astronomy, who proposed "Strain Driven Skyrmions in Thin Film Heterostructures." She will work with Alexey **Kovalev**, EQUATE FRG1 SI, on this research. **Metric: Yr 1: 2 awards, Yrs 2 -5: 1 award annually.**

Broadening Participation

Nebraska's tribal colleges and tribal councils have been working with University of Nebraska-Lincoln (UNL) Chemistry Professor **Mark Griep** to prepare three grant proposals to increase research opportunities for faculty and students. The first proposal is to the United States Department of Agriculture, National Institute of Food and Agriculture (USDA NIFA) for hemp production. Nebraska Indian Community College agreed to create a test field and to be the first to test out any new educational materials created from the project. The second is a $1 billion Dept. of Energy proposal submitted by a Nebraska government official, where the Santee Sioux and Winnebago Tribal Councils agreed to participate in an infrastructure development grant program sought to initiate the hydrogen economy. Unfortunately, the Nebraska project was not selected for funding. The final proposal was described in an NSF EPSCoR Track II grant application that was submitted on January 22, 2024. It seeks to empower under-resourced communities with the tools to prepare for future flooding events. It is a collaboration led by Nathan Huynh at UNL with colleagues in Iowa, Louisiana, and South Carolina. In Nebraska, the Santee Sioux Tribal Council agreed to help us understand what happened in the Santee community during the 2019 flood. They are still awaiting a decision on the first and third grant applications.

Faculty from LPTC and NICC are working with Griep to plan 3 family outreach events in March 2024 at the tribal communities. Native scientists will speak about their work. EQUATE's **Binek** will work with tribal elders to discuss how each tribe's origin story relates to quantum. Additionally, there will be hands-on STEM activities for families. It is expected that approximately 50 people will attend each event.

From EQUATE's Strategic Plan, Objective 4.4, the project's Broadening Participation efforts also include: **College prep groups (NCPA, Upward Bound, Girls Inc, etc). Metric: 100 URM/yr: low-income, first-generation students**

Nebraska EPSCoR and NCMN continue to work with Girls Inc. Eureka! program managers in both Omaha and Lincoln, Nebraska. Approximately, 44 (100% female, 43% URM) young women participated in quantum and engineering activities spanning several days during EQUATE Year 3.

New this year, Nebraska EPSCoR is supporting the Nebraska **College Preparatory Academy (NCPA)** "Black Girls Lead in Business." This intensive program brings 75 young women to the University of Nebraska at Omaha (UNO) campus for two days to learn about business, entrepreneurship, research, and technologies such as virtual reality. The summit helps to demystify college, build the girls' confidence in math, and allows the girls to interact with faculty / students at UNO along with area business leaders as they create a business plan for a new technology they invent.

Figure 27. A middle school student tries playing Dr. Binek's guitar, which causes flames to dance in a wave pattern, during a summer visit to EQUATE labs.

Wignall, **Sangster**, and NCMN's **Huttenmaier** participated in a repeating afterschool program held at 5 Title 1 middle schools in Lincoln, Nebraska. EQUATE staff spend time with students, teaching them about quantum topics and doing hands-on activities. Organized by the Office of TRIO at UNL, this program strives to support low-income, first generation, and/or disabled students so they may reach their full potential. Through this program, outreach staff impacts 80 students (56% female and 47% URM) several times per year. Additionally, the students visit UNL during the summer for hands-on activities and tours (**Fig. 27**).

The UNL College of Engineering's **Discover Engineering Days (DED)** introduce middle school students (grades 6-8) and their teachers to various fields 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 utilize engineering habits such as collaboration, problem solving, creativity, and critical thinking skills. The DED offers 7 workshops over the course of the year, averaging approximately 100-150 students at each meeting. EQUATE Outreach is involved with this program throughout the year, teaching the students about Triboelectric Energy and how it relates to Quantum. Students involved in this program come from both rural and urban schools, with strong representation of URM and female attendees.

Regarding **Objective 4.4: Increase the number of underrepresented minorities in STEM fields,** in the summer of 2024, Nebraska EPSCoR provided scholarships for 79 low-income students (44% female, 18% URM) 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" in their learning.

The **2024 Women in Science Conference** is designed to expose high school students to a wide variety of science-related fields and encourage them to pursue majors and careers in science, technology, engineering, and mathematics, through the work of women currently working in the sciences. The conference takes place in April at UNL. **Metric: 90 students and 10 teachers**

All Girls All Math (AGAM) Camp met in-person (for the first time since 2019) for a week of math-based adventures on the UNL campus. It was attended by 19 students (100% female, 40% URM) from all over the United States. Students learned about cryptography and coding, attend virtual tours of both national and local museums, and participate in small group activities such as virtual escape rooms which challenged participants to use mathematical reasoning, problem solving skill, and communication ability.

Nebraska EPSCoR provides support for five student researchers from the state tribal colleges to attend the **Nebraska Academy of Sciences (NAS)**. The meeting is held yearly in April and is expected to take place as usual. **Metric: 5 students at NAS**

Communication and Dissemination

Objective 4.5 Increase public awareness of EQUATE

In Year 3, EQUATE presented a one-day conference in March 2024 in the tradition of the Nebraska Research and Innovation Conference (NRIC), with 80+ attendees and 30+ posters. FRG2 leader **Abdelghani Laraoui** convened speakers from Princeton University, Georgia Tech, University of Chicago, and more—in the theme of *Diamond Quantum Sensing: Challenges and Opportunities*. NRIC events in Years 4 and 5 will be led by FRG3 and by EQUATE's Outreach team. (meets metric)

In Year 3, EQUATE logged **104** journal **papers and presentations**; the metric (four per EQUATE investigator) was exceeded with **56** published journal papers and **48** conference presentations, as of February 2024.

Nebraska EPSCoR's **Annual PR Report** (**Fig. 28**) for 2023 featured EQUATE FRG2 research on its cover. More than 1,000 copies of this publication were printed or viewed at epscor.nebraska.edu, with distribution to a mailing list of 800 recipients. (meets metric)

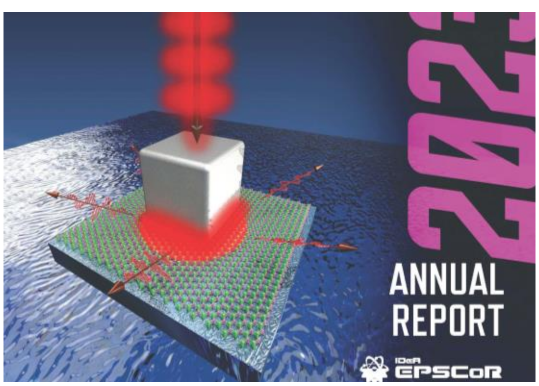

Figure 28. The cover of Nebraska EPSCoR's 2023 annual report publication depicts EQUATE FRG2 research, with multiple pages of project coverage included.

The EQUATE **website** (equate.unl.edu) continued to serve, with 2,275 users making 4,969 pageviews from Feb. 1, 2023 - Jan. 31, 2024. Compared with 2,216 users making 6,223 pageviews from Feb. 1, 2022 - Jan. 31, 2023, the EQUATE website did not meet the metric of 10% growth year over year in Year 3. It could be helpful to engage more viewers by resuming the addition of webinar recordings from the sessions by EQUATE speakers, as in 2022 and 2021, and by updating the Outreach section's content. Summer program students can be engaged in a “scavenger hunt” to find facts in the EQUATE website for prize rewards. (did not meet metric)

EQUATE’s **social media** presence, tagged by #NebEQUATE, had an active Year 3 with 76 mentions, above the Year 2 baseline of 55 mentions – which included sharing REU stories, journal publications, outreach events, and other EQUATE achievements. (meets metric)

EQUATE Management Team (MT) Meetings took place monthly in Year 3 (meets metric); with the EQUATE faculty hiring unsuccessful in Year 2, the MT asked the UNL Physics Department Chair to report at each meeting on the progress of the hiring in Year 3. It was excellent news in January 2024 to learn of the acceptance of an EQUATE faculty position offered to **Zuochang Zhang**, from University of California, Berkeley. EQUATE continued its monthly seminar series, and several of the new faculty candidates gave relevant talks which were attended by project participants and interested colleagues.

Emerging Areas and Seed Funding

EQUATE’s seed funding program has added relevant talent and topics to the project. As Year 3 concludes, the following list of researchers and their work (**Table 1**) has enhanced EQUATE’s outcomes.

Table 1.

Seed grant recipient	**Project Year**	**Title of funded seed project**
Yanan Laura Wang	1	Dynamic Control of 2D Single-Photon Quantum Emitters via Strain Engineering
Siamak Nejati and Alex 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 and Abdelghani Laraoui	2	Quantum Size Effect on Radiative and Electronic Transport
Shireen Adenwalla	3	Strain Driven Skyrmions in Thin Film Heterostructures

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 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 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 has also become a resource for the state of Nebraska on quantum topics, and 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. Al Geist has been accompanied by high-ranking military representatives such as Dr. James L. Stewart, Spectrum Warfare Systems Department Chief Scientist who also serves as the NATO Chairman for the Suppression of Enemy Air defense. In January 2023, EQUATE educated Brigadier General AnnMarie K. Anthony from the Joint Electromagnetic Spectrum Operations Center and Mr. Pedro Ramirez, Technical Director of the Nuclear Command, Control, and Communications (NC3) Enterprise Center about work done by EQUATE researchers on quantum materials and quantum technologies. EQUATE scientific director **Binek** was accompanied by FRG2 leader Dr. Abdelghani **Laraoui** who supported the conversation on FRG2-related work on quantum communication, specifically the creation and transmission of identical and entangled photons. EQUATE is proud to serve our nation as a recognized knowledge resource for STRATCOM.

FRG2's Laraoui also leads an NSF ExpandQISE Track-1 award for approximately $800,000, which includes Wichita State University physicist Kapildep Ambal and chemist Jian Wang. Their project seeks more robust materials such as ultrathin magnetic films and two-dimensional magnetic materials—with an application toward controlling spin qubits in diamond at longer distances that can work at higher temperatures. For this work Laraoui facilitates access to the Nebraska Center for Materials and Nanoscience (NCMN), a key factor in the success of the EQUATE effort, including NCMN's cryogenic scanning probe microscope.

EQUATE also notes a collaboration in Year 3 involving both research and broader impacts between FRG3's **Alex Wysocki**, University of Kearney physics faculty, and Kearney High School science teacher Alison Klein. Klein's RET (Research Experience for Teachers) in summer 2023 was EQUATE-funded; Wysocki has continued to mentor KHS students throughout the school year.

Sustainability

EQUATE continues to make significant strides towards ensuring its sustainability. Aligned with the strategic plan, the research and collaborations undertaken by EQUATE lay the groundwork for proposals that extend beyond the organization's lifespan. A standout achievement in 2023 was the securing of an NSF CAREER Award of EQUATEs seed grant awardee Dr. **Mohammad Ghashami** for his work on the physics of near-field thermal radiation in systems with multiple components. He received the early career award in April 2023. Dr. Ghashami's EQUATE seed award on quantum size effects on radiative and electronic transport, which he received in year 2 of EQUATE, was instrumental in setting the foundation for his earning of the NSF CAREER award.

In 2023 several EQUATE participants submitted another $2M NSF major research instrumentation (MRI) proposal to NSF. This effort was spearheaded by EQUATE's scientific director **Binek** with substantial contributions from FRG2 and FRG1 leaders and senior investigators. The major instrumentation proposal aims at a new 100keV electron beam lithography system which, among many other things, would help many EQUATE researchers to fabricate quantum technological nanostructures for example those described in the report in the context of quantum crosswire qubits and spintronic devices.

The previously reported submission of an NSF pre-proposal titled "QuSeC-TAQS: Probing quantum entanglement in correlated spin systems via qubit spectrometry and spin correlation measurements" was invited to be submitted as a full proposal. Unfortunately, the proposal was ultimately not funded. However, the encouraging reviews stimulated a subset of FRG2 and FRG1 investigators to write and soon submit a modified version of a similar proposal (in response to NSF's Dear Colleague Letter titled "Funding Opportunities for Engineering Research in Quantum Information Science and Engineering") under leadership of FRG2 leader **Laraoui**. Dr. Laraoui has a record of accomplishment in submitting successful proposals which serve EQUATE's sustainability. Another example is his 2023 awarded $800k NSF grant from the Program entitled Expand Capacity in Quantum Information Science and Engineering" where he collaborates with investigators from another EPSCoR jurisdiction (Kansas) at Wichita State University.

The most significant achievement in sustainability is a catalyst award as part of UNL's Grand Challenges. Overall UNL is offering $40 million over five years in seven areas which have been identified as UNL's Grand Challenges themes. As previously reported, EQUATE played a pivotal role in advocating for Quantum Science and Engineering as one of the Grand Challenges themes. Scientific director **Binek**, a key figure in formulating the theme, also joined the steering committee approved by the chancellor's executive leadership team. Collaborating with Dr. Susan Hermiller (UNL Mathematics), a team of 21 UNL faculty (including EQUATE SIs and leaders), Binek resubmitted a catalyst proposal titled "Quantum Approaches Addressing Global Threats," which got funded for five years with $4.7M. This extremely interdisciplinary and diverse quantum research activity fortifies EQUATE's sustainability and broadens the participation in quantum research significantly beyond the traditional STEM community through inclusion of the Arts and Humanities.

Management, Evaluation and Assessment

EQUATE Management Team (MT) Meetings took place monthly in Year 3 (meets metric, EQUATE Strategic Plan Objective 4.5); EQUATE MT meetings are well-attended by each FRG leader as well as Nebraska EPSCoR staff. (If unavailable, FRG leaders designate a substitute representative from their team.) These sessions meet in Lincoln and include Zoom presence for FRG3's Dr. Wrubel, who teaches in Omaha, as well as for the project's external evaluator (KSU OEIE). EQUATE MT meetings enhance project communication and collegiality, and allow for monitoring and updates on project activities including outreach sessions, EQUATE's monthly seminar series, and the project's annual conference.

The Office of Educational Innovation and Evaluation (OEIE) at Kansas State University serves as the external **evaluator** for Nebraska's Established Program to Stimulate Competitive Research (EPSCoR) Emergent Quantum Materials and Technologies (EQUATE) program, funded by the National Science Foundation (NSF). OEIE aids the project in assessing its progress, implementation, and impacts through data collection with project leaders, team members, and external partners/stakeholders, and through analysis of project publications. According to OEIE's Evaluation Plan for EQUATE, the project's annual evaluation report compiles responses from participant surveys, assets assessment, external partner focus groups, and interviews of new hires and seed awardees. For details, please see the full Year 3 evaluation report uploaded with the reporting submission documents via NSF EDOCS.

Assessment of EQUATE also occurs with the project's External Review Panel (ERP), which consists of five faculty members from higher education institutions throughout the nation who specialize in quantum materials topics. The 2024 ERP was comprised of Axel Hoffmann, University of Illinois at Urbana-Champaign (Panel Chair); Michael E. Flatté, University of Iowa; Ilya Krivorotov, University of California, Irvine; and Allan Macdonald, University of Texas at Austin. The panel's EQUATE visit was set for mid-March 2024; the ERP report and project response will be included in EQUATE's upcoming Year 4 report.

SPENDING AND UNOBLIGATED FUNDS

At the time of this reporting (for June 1, 2023 – April 30, 2024), 76% of EQUATE Year 3 funds have been liquidated. However, we anticipate that approximately $371,000 will soon be liquidated, based on the monthly spending rate, because EQUATE's higher education partners (Creighton, University of Nebraska at Omaha, University of Nebraska at Kearney, Little Priest Tribal College, and Nebraska Indian Community College) have not yet fully billed the project for expenses incurred after 1/31/2024.

In addition, we expect 5 Nebraska small colleges to bill us for $149,000 to finance the purchase of STEM teaching and research equipment before the TRE Award expires on 5/1/2024.

After these commitments are met, EQUATE spending will be above 90% for the current reporting year, which complies with the EQUATE cooperative agreement's Programmatic Terms and Conditions.

SPECIAL CONDITIONS

EQUATE's Programmatic Terms and Conditions specified that two new faculty members would be hired by the project in Year 2. The hire at the University of Nebraska at Kearney (UNK) was completed in Year 2, which brought Assistant Professor **Alex Wysocki** to the EQUATE project and FRG3. The EQUATE-funded hiring of an assistant professor at the University of Nebraska-Lincoln (UNL) was delayed in Year 2, after the chosen candidate's late-stage decline of the hiring offer. EQUATE PI **Matt Andrews** apprised the project's NSF program leadership at that time, and the hiring process restarted ahead of Year 3. The hiring of University of California, Berkeley's **Dr. Zuochang Zhang** was successful in January 2024, and Dr. Zhang will begin work at UNL in August 2024.

TABULAR/GRAPHIC REPRESENTATION OF PROGRESS TO DATE

The following table, from the most recent (Year 3) 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 on schedule; Red = task/s behind schedule; underline indicates metric and bold text indicates milestone.) Also, this Year 3 representation includes "Tracked Changes" edits (text in red ink) due to necessary adjustments acknowledged by EQUATE FRG leaders; EQUATE's complete Strategic Plan including Year 3 Tracked Changes edits was uploaded at NSF EDOCS and, upon approval by the cognizant Program Officer, that update becomes accepted as the official Strategic Plan version for EQUATE until further notice.

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** Metrics: Extract the Néel temperature, magnitude of boundary magnetization, or direction of the Néel vector	Probe spin structure and canting of boundary magnetization Explore 90-degree AFM DWs	Investigate switching dynamics **Achieve electrical rotation of Néel vector** Metrics: Demonstrate via magnetic, magneto-optical, or NV center microscopy measurements	Pump-probe dynamic investigation of Néel vector rotation	Binek, Laraoui
Characterize magnetic state of chromia heterostructures	Characterize the electronic structure of Pd on chromia	**Identify ferromagnetism in Pd induced by interfacial chromia** Metrics: Extract the Curie temperature or the magnitude of	Investigate exchange coupling of Pd on chromia	**Fabricate 2D TMTC, such as TiS_3 and HfS_3, on chromia** Metrics: Demonstrate via electrical and chemical techniques	**Identify induced polarization in TiS_3 and HfS_3 on chromia** Metrics: Extract the magnetization via magnetic or spectroscopy	Dowben, Binek

		magnetization			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 oxide films** Metrics: Identify the associated Raman peaks	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 heterostructures based on antiferroelectrics and ferromagnets, i.e., $Ni/BiInO_3$. Metrics: Quantify magnetic field-controlled current-voltage curves and anticipated capacitive behavior.	Synthesis/ investigate new PST materials. Theoretical modeling of new PST materials. Raman studies of spin/carrier relaxation	Guo, Hong, Streubel, Tsymbal
Fabrication and characterization of PST tunnel junction		**Fabrication of tunnel junction** Metrics: Demonstrate the device	**Characterize tunneling resistance** Metrics: Demonstrate the I-V	**Imaging tunnel current** Metrics: Demonstrate via conductive probe AFM	**Characterize tunneling anomalous Hall/spin Hall effects** Metrics:	Binek, Hong, Laraoui, Tsymbal

devices		layout and fabrication flow via optical image and AFM Develop first-principles approaches to calculate anomalous and spin Hall effects	characteristic of tunneling behavior Theoretical modeling of tunneling results	imaging or NV center microscopy Theoretical modeling of tunneling anomalous Hall/spin Hall effects	Demonstrate via magnetotransport measurements Study thickness dependence of tunneling effects	
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 samples Develop micro-magnetic theory approaches for modeling THE	**Resolve magnetic state via anomalous Hall effect and THE** Metrics: Demonstrate via magnetotransport measurements Fabricate yttrium iron garnet films via metal-organic decomposition epitaxy	Characterize the magnetic properties of strain-free $NiCo_2O_4$ films via magnetometry. Metrics: Determine the magnetic Curie temperature and susceptibility.	**Imaging of magnetic structures** Metrics: Demonstrate via MFM/ MOKE/XPM/NV center microscopy Theoretical studies of Berry phase due to quantum-spin fluctuations	Theoretical modeling of field-gradient manipulation and quenching of quantum states	Hong, Kovalev, Streubel, Xu
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 entanglement 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 experimental 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 on spin lifetime	Investigate spin transport in graphene on B-chromia, focusing on 90-degree rotation Utilize x-ray magnetic linear	Investigate quantum interference effects in graphene on B-chromia Metrics:	Binek, Dowben, Kovalev, Streubel

		Demonstrate via magnetotransport measurements **Establish the characterization capability for ferromagnetic resonances in magnetic thin films.** Metrics: Determine the ferromagnetic resonances and magnetic homogeneity of YIG films.	in graphene **Theoretical modeling of spin transport** Metrics: Extract spin relaxation time	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	Dowben, Hong, Tsymbal
Probe dynamic Coulomb screening in 2D vdW interfaced with halide perovskites and ferroelectric	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**	**Spatially resolve domain structures in ferroelectrics or defects in halide perovskite** Metrics: Demonstrate via optical spectra	Probe the modulation of carrier and valley populations via Coulomb screening/ polarization effects of the	Guo

oxides			**screening** Metrics: Identify the magnitude of coupling strength Modulating of TMDC edge transitions	mapping Assess local variations of carrier dynamics modulated by substrate Coulomb screening or ferroelectric polarization	substrate	
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 molecular spin state	**Fabricate SCO molecular 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	**Study effect of dielectrics on the spin state of SCO** **Thin film deposition and device fabrication of Co2+/3+ SCO molecules** Metrics: Demonstrate via AFM, electric, or spectroscopy characterizations	**Fabricate SCO/ ferroelectric heterostructures** Metrics: Demonstrate via AFM, electric, or spectroscopy characterizations **Build transistors/ phototransistors based on Co2+/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**	**Study SCO properties in heterostructures in response to heat and light stimuli** **Extract exchange coupling in SCO molecular bilayer systems** Metrics: Identify the magnitude of exchange coupling strength	**Identify effect of ferroelectric 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**	**Dowben, Lai, Xu , Streubel**

Build a Zener - Mach solid state interferometer as a logic gate		**Establish the group theory of a Zener - Mach solid state inferomete as a logic gate** Metrics: Propose the operation scheme			**Build a Zener - Mach solid state interferometer from spin crossover molecules** Metrics: Demonstrate the logic operation	Dowben
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 electrochemistry characterizations	~~Design and fabricate Fe(HB(pz)$_3$)$_2$/MOF composites~~ ~~Property characterization~~ 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 characteristics** Metrics: Demonstrate via SQUID, VSM, SEM, TEM, transport or AC conductivity measurements	**Fabrication and characterization of voltage-controlled devices with Fe, Fe/Ni, Fe/Pd SCO complexes** Metrics: Demonstrate via SQUID, VSM, transport measurements	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	~~Probe framework phonon modes in MOFs with various metal cations and organic linkers~~ 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 invitations	**Interview candidates** Metrics: Arrange interview visits **Make offer** Metrics: Provide a startup	Ensure new hire connects with FRG leader and project science director for effective mentoring	Welcome new hire to campus and introduce them to EQUATE team	TBD	Binek, Laraoui, Hong, Tsymbal, Streubel, Xu

		package ~~Welcome new hire to campus and introduce them to 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				Modify the setup to accommodate SiC spin characterization and sensing.	Laraoui

	setup					
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 temperature and magnetic field in YIG, CoFeB METRICS: understood effects of thickness of CoFeB and YIG on magnon modes (frequency, linewidth, damping).	Determine spin-magnon coupling coefficients and type of magnon proposes relevant in YIG METRICS: determined the NV-spin magnon coupling coefficients in YIG	**Study spin-magnon interactions in other FM insulators such TmIG** METRICS: Optimized the hybrid diamond-FM waveguide for single NV spin qubits-magnon coupling.	**Explore magnons as quantum buses and understand effect of magnetic noise on spin coherence lifetime T2 of single NVs** METRICS: determined the feasibility of using magnons as quantum busses to couple distant spin qubits.	Laraoui
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 development	**Build and optimize NV setup for low-field (LF) - magnetic resonance (MR) imaging.** METRICS: by	Integrate hyperpolarization protocols based on solid state effect and double spin resonance to NV- LF-MR		Enhance the NV magnetic sensitivity using hybrid NV-FMN nanoparticles		Liou, Laraoui

	end of year NV-LF-MR setup is ready for measurements.	setup				
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 equipment: single photon detectors for single NV NMR, MW and optical equipment, NMR magnetsMETRICS: By end of Year 1 the equipment is integrated to					Laraoui, Liou

	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 improvement	**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
Spectroscopy of color centers in UWBG semiconductors	Test THz-EPR on diamond NV centers to check the sensitivity.	**Demonstrate THz-EPR-E on defect spin systems in Gallium Oxide bulk crystals.** Metrics: demonstrated THZ-EPR-E single of defect spin systems in Ga_2O_3 bulk crystals	**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 single crystals	**Demonstrate characterization of photoionization and carrier excitation dynamics of potential quantum emitters in SiC, Ga_2O_3 and AlN** Metrics: demonstrated photoionization and carrier excitation dynamics of quantum emitters in Ga_2O_3, SiC, and AlN.	**Demonstrate time evolution of characterization of photoionization of quantum emitters in SiC, Ga_2O_3 and AlN** Metrics: demonstrated time evolution of photoionization of quantum emitters in Ga_2O_3, SiC, and AlN.	M. Schubert

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 enhancement** <u>Metrics: optimized ultrathin nanostructures for enhanced nonlinear optical properties.</u>		Design chiral quantum optical devices based on the fabricated structures.		Kilic
Fabrication and Epitaxial growth of optical nanostructures	Fabricate new anisotropic and chiral nonlinear structures using iGLAD bottom-up growing technique. **Nanofabrication system optimized.** <u>Metrics: Fabricated anisotropic chiral nonlinear structures.</u>	Develop new ALD epitaxial growth techniques to design nonlinear optical structures		**Obtain circular polarized high harmonic generated waves from the fabricated helical structures** <u>Metrics: demonstrated circular polarized harmonic generation form the fabricated chiral structures</u>	Use TiN, and lattice resonances in the nanophotonic structures to achieve stronger and tunable nonlinear responses.	E. Schubert, M. Schubert
Measurement setup development	Implement g(2)(t) mapping, photon statistics and life-time measurements to study of chiral nanostructure	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.** <u>Metrics: built and optimized</u>		M. Schubert, ~~Bao~~, Laraoui

	s.			the nonlinear optical measurement setup.		
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 nonlinear process of SPDC. **Model the SPDC process.** Metrics: modeled the SPDC process in different ultrathin nanocomposite structures	Optimize and determine ultrathin nanostructure that can achieve maximum SPDC leading to a strong entangled photon pair generation.			Measure various quantum optical effects, such as photon statistics and interference.	Kilic~~, Bao~~
Fabricate entangled photon sources.			Fabricate nonlinear metasurfaces and integrate them with conventional BBO nonlinear crystals to enhance the SPDC efficiency.	**Fabrication of SPDC metasurfaces** Metrics: Fabricated SPDC metasurfaces		E. Schubert, M. Schubert
Develop experimental setup for quantum photon statistics measurements.	Develop experimental 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.	~~**Measure the SPDC efficiency and entangled photon generation.**~~ ~~Metrics: detected SPDC processes and demonstrated entangled photon pair generation~~	~~**Measure various quantum optical effects, such as photon statistics and interference.**~~ ~~Metrics: understood the quantum optical effects via SPCD.~~	~~Bao~~ Bao left UNL; his tasks in years 4 and 5 will be 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 the SPDC setup.					Bao / Laraoui
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 configuration for single-photon quantum sources	Kilic
Fabrication of single-photon sources.			Fabricate single-photon optical sources, e.g. hBN, SiC, AIN integrated with novel composite structures	**Optimization the fabrication of efficient single-photon quantum optical sources from nanoscale structures.** Metrics: fabricated photonic nanoscale structures with enhanced single-photon		E. Schubert

				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.	**Characterize single photon emission by measuring the photon correlation function mapping.** Metrics: characterized single photon emission by using photon correlation mapping	~~Bao,~~ 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 characterization.					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

Development 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-Interfer-ometery 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-Fr	Wrubel
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 experiments, previously only possible with cold atom or GaAs	Build the full sample preparations and photoluminescence capability in exciton polaritons	**Demonstrate old landmark 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				Bao
Explore unique experiments at room temperature with perovskites, such as spin-orbital physics, best only			Demonstrate spin-orbital physics in perovskite microcavity at room temperature perovskites	~~Explore and demonstrate room-temperature exciton-polariton BEC capability involving spin-orbital coupling~~	~~**Demonstration of unique quantum fluid experiments at room temperature such as supersolid**~~ ~~Metric: Measurem~~	Bao departed UNL in August of 2023

possible or impossible with cold atom					~~ent of a quantum phase transition in room-temperature exciton-polariton BEC~~	
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	Create codes to calculate observables for dipolar polarons in connection to optical lattices produced by PI Wrubel; Write code for impurities as potential probes of the density, temperature, or spin of	**Complete computer codes for structural polaron properties and polaron-polaron interactions in different interaction regimes** Metric: Computer code solving for structural polaron	Armstrong

				their environment	properties and polaron-polaron interactions **Adapt optical lattice codes for 2D to calculate energies and 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				**Determine the distribution of 1D nonlinear**	**Predict computational efficiency of**	Wong

quantum walks in realistic systems				**quantum walks** <u>Metric: Predicted distribution of 1D nonlinear quantum walks</u>	<u>**nonlinear search algorithms on networks that are highly connected***</u> <u>**Predict computational efficiency of nonlinear search algorithms on periodic lattices in 1D, 2D, and 3D***</u> <u>***both milestone & metric**</u>	
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 of N interacting qubits in 1D (or possibly 2D) finite lattices.	Develop a code (Matlab) computing quantum states in cross-road QD, interaction between qubits and their dynamics (code for numeric simulation of time evolution of QD arrays)	Construct effective Hamiltonian of the quadratic spin-spin interaction with long-range force and strong correlation	**Calculate the decay rates of a single QD and finite-size array of QDs coupled to the resonant waveguide mode** <u>Metric: Predicted decay rates of single QD and finite-size array of Qds coupled to the resonant waveguide mode.</u>			Mei and Sabirianov
DFT analysis of 2D				Calculate energy states of 2D	**Based on the DFT modeling,**	Mei and Sabirianov

materials to characterize the properties of proposed crosswire QD applications including graphene-based systems, TMDs, and thin film ferromagnetic systems.				array of cross-road quantum dots with materials of promise (target for fabrication with our collaborators)	**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	
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,	Year 1	Year 2	**Year 3**	Year 4	Year 5	Responsible

Milestones in bold)						
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 process (UNK)	Applicant screening; offer/s made and accepted	New incumbent begins work; meets EQUATE team	Ensure new hire connects with FRG leader and project science director for effective mentoring.	TBD	TBD	Department of 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/year with minimum of 5 experiences/yr**	**Made available to 200 teachers/year with minimum of 5 experiences/yr**	**Made available to 200 teachers/year 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 EQUATE mentors for early-career faculty**	**New hires (EQUATE-funded) arrive at UNK, UNL**			**Cumulative: 5 early-career faculty mentored**	Binek, Wrubel
Objective 4.4: Increase the number of underrepresented minorities in the STEM field.						
Activities	Specific accomplishments, milestones, and/or outputs					
	Year 1	Year 2	Year 3	Year 4	Year 5	Responsible
Sponsor Tribal College student researchers	**5 students present at annual Neb Acad Sciences**	**5 students present at annual Neb Acad Sciences**	**5 students present at annual Neb Acad Sciences**	**5 students present at annual Neb Acad Sciences**	**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 # views per year**	+ 10% year-over-year	+ 10% year-over-year	+ 10% year-over-year	+ 10% year-over-year	NCMN's Behrendt, w/input via 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 +	Mail to 800 recipients + online	Mail to 800 recipients +	Mail to 800 recipients +	Mail to 800 recipients +	Allen

	online views	views	online views	online views	online views	
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