2026 Science

DMR-2423992 PREM

Hole concentrations in doped gray tin on InSb and CdTe measured with infrared ellipsometry

Jaden Love (MS: Summer 2025)

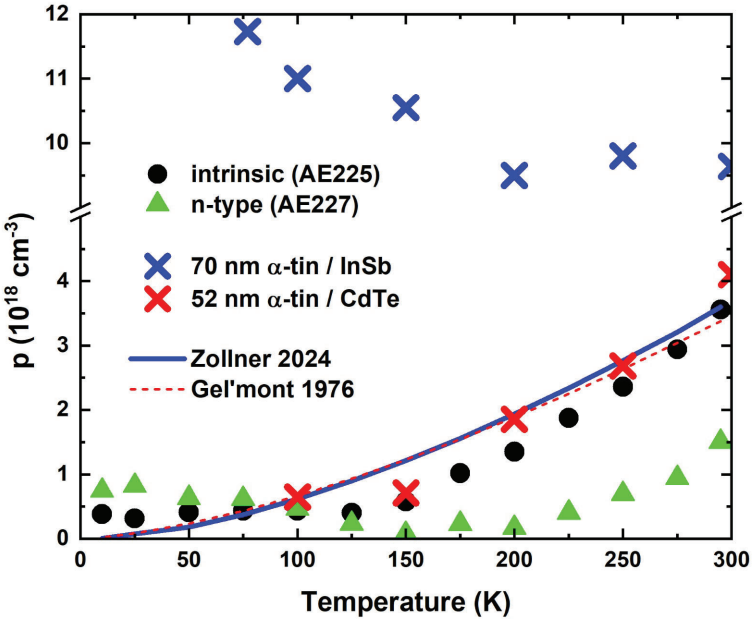
S. Zollner, B. Kiefer, I. Vasiliev, M. Zhou, L. Miao, New Mexico State University

Status: Jaden measured the temperature dependent dielectric function for two 30 nm gray tin (α-Sn) layers grown using molecular beam epitaxy (MBE) on InSb (100) bulk substrates. The interface preparation directly influences the properties of the gray tin layer. It is of high importance to characterize these differences in pure α-Sn to compare as a reference sample alongside $Sn_{1-x}Ge_x$ alloys with varying tin concentrations.

Outcome: We have quantified the carrier density for the 30 nm films prepared on different interfaces by applying an optical sum rule to determine the density as a function of temperature. Our results are compared with literature values and agree well especially for the intrinsic grey tin layers. This study demonstrates a non-destructive method for determining the carrier density that provides good agreement with theory.

This publication was recently completed and can be found in the Journal of Applied Physics:

Jaden R. Love, Carlos A. Armenta, Atlantis K. Moses, Haley B. Woolf, Jan Hrabovský, Stefan Zollner, Aaron N. Engel, Christopher J. Palmstrøm: *Hole concentrations in doped gray α-Sn on InSb and CdTe measured with infrared ellipsometry*, J. Appl. Phys. **139**, 185704 (2026).
https://doi.org/10.1063/5.0315746



Future Plans:

Analyze the absorption by free charge carriers at very long wavelengths (Drude response).

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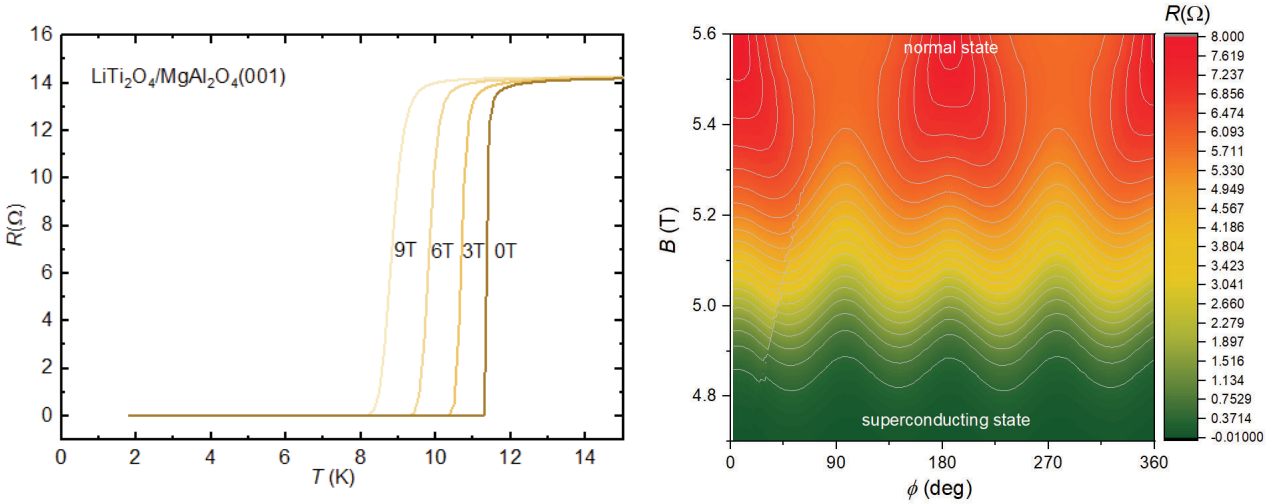
Engineering Superconductivity in Correlated Oxide Thin films

S. Zollner, B. Kiefer, I. Vasiliev, M. Zhou, L. Miao, New Mexico State University

Elijah Robinson and Aidan Brealey-Rood
(Physics Undergraduate Students)

- RuO_2 has recently attracted significant interest due to the possible coexistence of superconductivity and altermagnetism.
- We have successfully grown RuO_2 and $LiTi_2O_4$ thin films using pulsed laser deposition at NMSU. Superconductivity in $LiTi_2O_4$ was characterized at NMSU and is shown in the figure, while the superconducting transition of RuO_2 is below the current temperature limit of our measurement system.
- These samples were sent to Harter at UCSB for optical measurements to understand differences in their superconductivity.
- Future work will push these systems toward the two-dimensional limit.



(Left) Resistivity versus temperature of a $LiTi_2O_4/MgAl_2O_4(001)$ thin film for different magnetic fields. (Right) Resistivity map as a function of magnetic field strength and angle near the superconducting transition of a $LiTi_2O_4/MgAl_2O_4(001)$ thin film, exhibiting 2-fold behavior.

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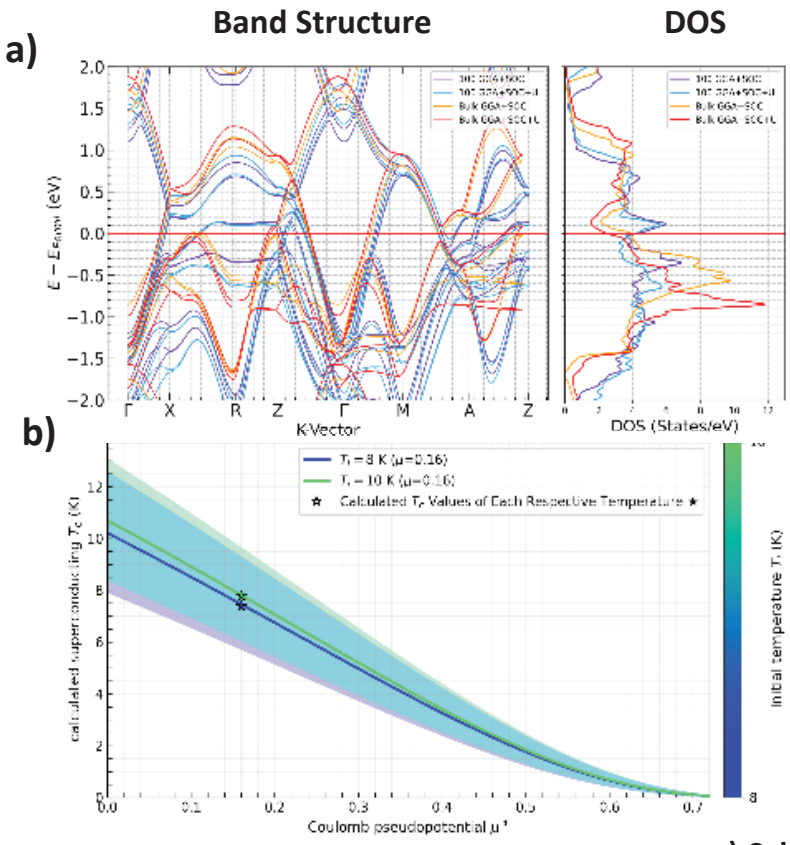
Ab Initio Studies of the Electronic Structure and Superconducting Properties of RuO_2 Thin Films

S. Zollner, B. Kiefer, I. Vasiliev, M. Zhou, L. Miao, New Mexico State University

Gabriel Manzanares (MS, 2025)



- Recent discovery of strain-induced superconductivity in rutile RuO_2 thin films has attracted considerable attention. Superconducting behavior of RuO_2 films has been linked to the changes in the electronic structure of strained RuO_2 crystal lattice resulting in significant increase of the density of states at the Fermi level.
- Ab initio density functional computational methods were applied to study the influence of epitaxial strain on the electronic and superconducting properties of RuO_2 thin films grown on TiO_2 substrates.
- The results of this study suggest that applied epitaxial strain may lead to the stabilization of superconducting phases in RuO_2 thin films.
- Gabriel Manzanares has successfully defended his Master of Science dissertation and graduated with an M.S. degree in Physics in December 2025.

a) Calculated band structures and DOS of strained (100) RuO_2 thin films grown on TiO_2 substrate.
b) Estimated superconducting transition temperature T_C of strained (100) RuO_2 thin films.

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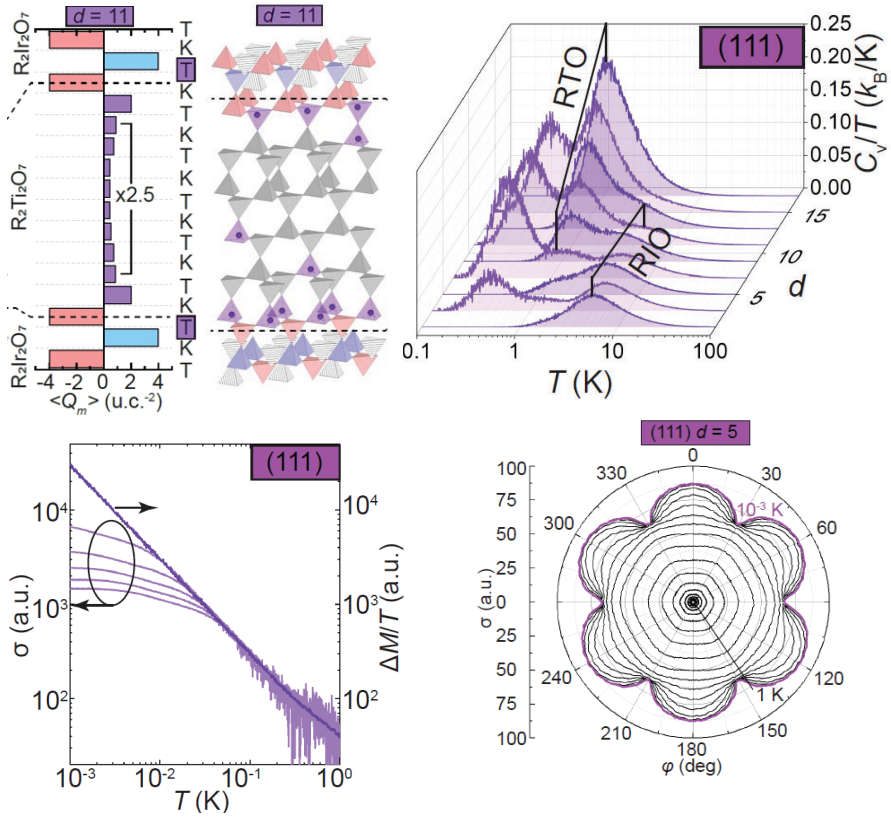
Manipulation of magnetic monopole quasiparticles in oxides

S. Zollner, B. Kiefer, I. Vasiliev, M. Zhou, L. Miao, New Mexico State University

Andres Chappa
(Physics Undergraduate Student, BS Spring 2026)

- Two-dimensional magnetic monopole gas (2DMG) is an emergent low-dimensional state with nonzero net magnetic charge density, providing a platform to study fundamental behavior and application of magnetic monopole quasiparticles.
- Andres Chappa used Monte Carlo simulations to engineer 2DMG properties in oxide heterostructures, tuning monopole density, entropy, transport, and symmetry through heterostructure thickness and crystalline orientation (see the figure on the right). He is preparing a first-author manuscript entitled “Heterostructure Engineering of a Two-Dimensional Magnetic Monopole Gas with Tunable Transport and Symmetry.”
- Andres Chappa also contributed as second author to related works: “Enhanced-Entropy Phases in Geometrically Frustrated Pyrochlore Magnets,” Phys. Rev. B 112, 214427 (2025), and “Monopole Traps for Position-Based Information Coding,” currently under review in Phys. Rev. B.



2026 Science

DMR-2423992 PREM

Large Language Models for Materials Discovery

Daniel Reyes (MS: Spring 2027)
Gavin Campos (BS; Spring 2026)

S. Zollner, B. Kiefer, I. Vasiliev, M. Zhou, L. Miao, New Mexico State University

We are developing an LLM-guided materials discovery workflow (LLM-agnostic), inspired by LLMatDesign:

Iterative loop:
(1) Propose parent-material edits *(add / substitute / remove / exchange)*
(2) Offline evaluation *(ML/DFT relax + property regression + stability screen)*
(3) LLM reflection *(update constraints / prompts)*
(4) Iterate.

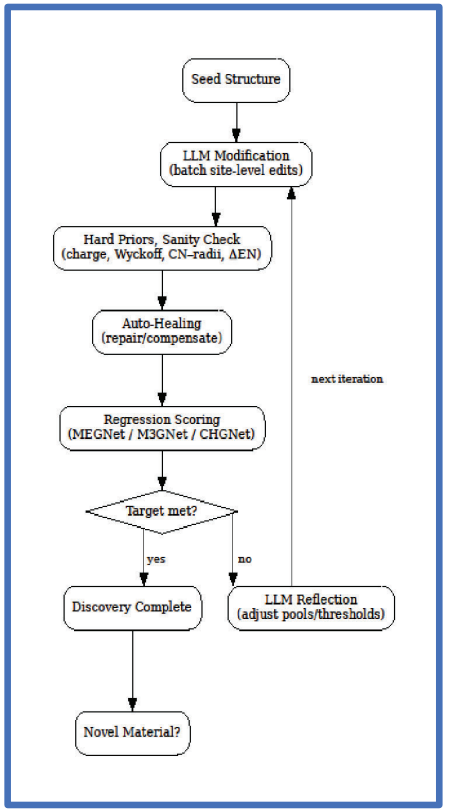
Current status: Candidates often match property targets but fail thermodynamic stability. Example:

$AlHfSiBNFO_4$

$E_g(target/LLM)$ = 4.0 eV; $E_g(DFT; BK)$ = 3.5 eV
$E_{hull} > 0$ ➔ unstable

Next improvements: Strengthen offline guidance via ML relaxation + surrogate stability screening and add a compensation step to automatically repair failed edits.

Outcome: A robust, high-throughput discovery pipeline that plugs into existing LLMs and improves hit-rate while reducing expensive DFT cycles.



2026 Science

DMR-2423992 PREM

Design and Synthesis of Topological and Spintronic Materials

S. Zollner, B. Kiefer, I. Vasiliev, M. Zhou, L. Miao, C. Frank, New Mexico State U.

- We are a young solid-state chemistry laboratory at NMSU. Our primary goal is to train undergraduates and graduate students in the essential techniques of solid-state and condensed-matter synthesis and measurement. As the lab capabilities expand, we are working on on designing and synthesizing bulk materials with topologically nontrivial band structures, motivated by both basic science and potential applications in emerging technologies.

- Laboratory Setup and Training

- Installed high-temperature furnaces and trained undergraduate students in their operation.
- Designed and installed a steel manifold for flame sealing; the system is leak-free as of 12/2025!
- Set up a new steel manifold for a flame sealing station. System is leak free as of 12/2025!
- Secured approval for light RAM work (D.U. received 11/2025); students completed required RAM training modules.

- These capability expansions enable new research:

- Growth of large single crystals and thin films to measure anisotropic properties of transition-metal oxides previously studied only as powders, as well as selected intermetallic compounds
- Transfer of these synthesis and characterization skills to a second project focused on controlled defect formation and doping to tune the properties of heavy-fermion systems, particularly unconventional superconductors.

Pictured Undergraduates:
Arthur Simental, Jordan Barela, Jade Clark

2026 Broader Impacts

DMR-2423992 PREM

Outreach and Recruitment Highlights (2025 – 2026)

S. Zollner, B. Kiefer, I. Vasiliev, M. Zhou, L. Miao, New Mexico State University

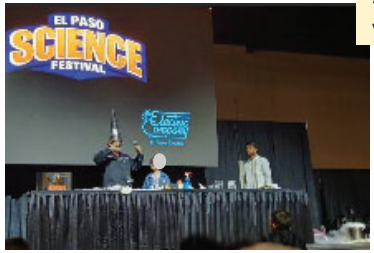
From August 2025 to September 2026, our department participated in 36 outreach events. These events were aimed at local K-12 & community college students.

- **Community Events & Student Competitions:** These are large-scale events where we have hundreds to thousands of interactions with K-12 students and their family members. The largest of these events are the El Paso Science Festival (12,000+ attendees!), NM TSA, Big Bang Bash, One Huge Fiesta, the Dona Ana 250th anniversary, and Learn-A-Palooza.

- **Departmental Events:** Each year we host our "Physics Fun Day" and Physics Summer Camp. This year Physics Fun Day was a roaring success welcoming over 300 students to join us for hands on activities and demonstrations. This year we will host 10 participants at the week-long Physics Summer Camp, and the program will teach the fundamentals of classical and modern physics and introduce special topics. Additionally, we will host 30 students from the TRiO program who will have two days of activities focused on E&M, optics, and optical measurement techniques.

- **Visiting Schools:** Throughout the semester our department is visited by groups of students from local schools as well as from the DACC. We host an open lab period where visiting students are rotated through demonstrations covering a variety of topics. For older students, these visits include tours of our research facilities. Occasionally we are invited to visit their campus where we will set up a classroom or auditorium space to share information about our programs and show demonstrations.

- **S.T.E.A.M. Nights:** These events are hosted by local elementary and middle schools. Each one has several hundred participants who visit our table for interactive demonstrations. These events successfully generate curiosity and are engaging even for very young kids.



"El Mago" presents at the El Paso Science Festival while volunteers are tabling and hosting demonstrations.

Physics Fun day was featured in the Las Cruces Bulletin!
https://www.lascrucesbulletin.com/stories/physics-comes-to-life-at-nmsu-event,164146

Physics comes to life at NMSU event

Hands-on demonstrations brought Las Cruces students face-to-face with science

2026 Broader Impacts

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University of California Santa Barbara REU Highlights (2025 – 2026)

A. Bleszynski Jayich, W. Ibsen; University of California Santa Barbara

UC Santa Barbara hosts NMSU Undergraduates for an 8-week mentored research experience at NSF Quantum Foundry Facilities. In 2025, three interns joined with Quantum Foundry Interns for an immersive introduction to QIS research. Two interns will join in Summer 2026.

Key Components of the REU Program

- ✓ Mentored research project in QF Facilities
- ✓ Weekly science communication training & professional skills workshops
- ✓ Structured research on-boarding activities with lab mentors
- ✓ Quantum Foundry research and laboratory talks and tours
- ✓ Networking events with university faculty and local industry members
- ✓ Research Symposium including talk and poster session

Jesse Reyes, NMSU REU participant presenting poster on *Polar Distortions on $PtBi_2$*

Program Group Photo including coordinator Wendy Ibsen with Ethan Cichon, Danissa Ortega, Jesse Reyes, and Lead Mentor, Andrea Capa Salinas.

Jesse Reyes, Ethan Cichon, Danissa Ortega are welcomed by UCSB graduate students Ruben Saatjian and Jack Tregidga of the Harter Lab.

NMSU Interns working on their research projects. Top left, Jesse and Jack using the dilution refrigerator. Top right, Danissa at the microscope. Bottom, Ethan checking the sample placement.