Research Opportunities for Science Educators (ROSE)

Pilot Project Report

Part A. Activities

July, 2021

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Executive Summary

The Research Opportunities for Science Educators (ROSE) pilot program was a collaboration between the University of New Mexico (UNM) and the New Mexico Public Education Department (PED). The idea was originally conceived by researchers in the Department of Chemistry and Chemical Biology at UNM and the final version of the pilot program was developed through discussions among these researchers and PED officials over a period of several weeks in Spring 2021. The goal of the program is to help improve the quality of science education in New Mexico by enabling educators to refresh their knowledge and develop new skills, while gaining appreciation for and inspiration from current scientific research. Another long-term goal is to substantively change perception of the research enterprise, as high school science teachers experience the excitement and satisfaction of cutting-edge research first-hand and convey this to their students.

Applications were solicited from New Mexico high school chemistry/science teachers across the state, and finalists were invited to join principal investigator (PI)-led research laboratories at UNM for one month as resident researcher-Scholars. Demand for the program far outstripped available positions in hosting labs, with 39 official applications and 3 additional inquiries for 5 positions. Additional funding from the UNM research office allowed a total of 8 Scholars to be funded, 2 from Albuquerque and 6 from smaller communities throughout NM. All selected Scholars teach at schools with high percentages of under-represented minorities in the student bodies. The Scholars' projects in five research groups included molecular modeling, chemical synthesis and chemical biology.

Assessment of the program is ongoing, through personal interviews with the ROSE Scholars and PI lab directors. An independent third party is conducting the personal interviews and anonymizing the results. Initial results indicate that the pilot program was an extraordinary success. Participants were enthusiastic about their experiences and willing to recommend the program to colleagues. A second round of follow-up interviews will be held in the fall to gain insight into how the 2021 cohort of Scholars have incorporated their experiences within their classroom lessons, and a final assessment report will be issued in late 2021.

Based on the success of the 2021 summer pilot, we are excited about the possibility of improving and expanding the ROSE Program it in the future, and we look forward to future collaborations with NM PED and hope to include other partners as well.

Motivation

New Mexico typically ranks in the bottom decile of US states in quantitative educational outcomes like high school graduation rates and standardized test scores[1]. In spite of the presence of three national laboratories (two DoE, one DoD) and a relatively high percentage of STEM Ph.D. recipients in the state, New Mexico ranks in the bottom quartile of all states for eighth grade science proficiency[2]. The NM Public Education Department (PED) considered only 1/3 of high school juniors (11th grade) to be proficient in science in 2019[3]. This problem is particularly severe for underrepresented minority (URM) students and students from rural areas, as detailed in the Yazzie-Martinez lawsuit decision[4].

Chemistry is a notable weak spot in high school science instruction for New Mexico. Openings for "chemistry teacher" positions consistently attract far fewer applicants than those for "biology teacher" or "science teacher" [5]. This may be related to the New Mexico teacher licensure system, which does not require a chemistry background for secondary science teachers. New Mexico HS students had a consistently lower passing percentage for the AP Chemistry exam than for the AP Biology and Physics exams over the period 2015-2019[6].

The University of New Mexico (UNM) is a high-research activity (R1) university with over 800 sponsored research projects in FY 2019[7]. STEM research is conducted in new or recently renovated state-of-the art laboratories, including several interdisciplinary facilities like the Center for High Technology Materials (CHTM), Center for Alcohol and Substance Abuse (CASA), Center for Advanced Research Computing (CARC), Center for Quantum Information and Control (CQuIC), and new PAÍS (Physics and Interdisciplinary Science) building. Over 200 faculty and 1000 graduate students are engaged in STEM research ranging from fundamental quantum mechanics and particle physics to applications-oriented engineering and field ecology projects working on Mars rovers and the evolution of the human species.

UNM and the Department of Chemistry and Chemical Biology (CCB) have a vested interest in supporting and improving science education generally and chemistry education specifically in NM public schools. Reaching out to individual students has real benefits, but does not scale to the large numbers of NM high school students we would like to reach. By working with high school science teachers, we can leverage the research resources of an R1 university to benefit many more students, albeit indirectly. As noted in the initial program summary (Appendix A): "ROSE will improve the quality of science education by allowing educators to refresh their knowledge and develop new skills while gaining appreciation for and inspiration from current scientific research."

1. https://nces.ed.gov/programs/coe/indicator/coi
   https://www.nationsreportcard.gov/profiles/stateprofile/overview/NM
2. https://ncses.nsf.gov/indicators/states/indicator/eighth-grade-science-proficiency
3. https://webnew.ped.state.nm.us/bureaus/accountability/achievement-data/
4. http://nmpovertylaw.org/wp-content/uploads/2018/09/Graphic-Yazzie-Martinez-Decision.pdf
   https://webnew.ped.state.nm.us/bureaus/yazzie-martinez-updates/
5. Personal experience from SE Cabaniss school board service.

6. New Mexico Math and Science Advisory Council Public Elementary and Secondary Mathematics and Science Achievement for School Year 2019-2020, available at https://webnew.ped.state.nm.us/bureaus/math-science/msac-math-and-science-advisory-council/
7. https://viewbook.unm.edu/research-brochure/8-9/

Planning and Preparation Timeline

The ROSE pilot project emerged from discussions among three CCB faculty. Prof. Jeff Rack noted during an NSF review panel that CCB community outreach to high schools and underrepresented minorities has been piecemeal relative to many other departments and lacks documentation of long-term effectiveness. In discussions with Prof. Steve Cabaniss and Prof. Susan Atlas in March 2021, the idea emerged to invite teachers from high schools and primarily undergraduate institutions (PUIs) to participate in ongoing research at UNM as a way of establishing connections to schools across the state and enhancing the chemistry expertise of their faculty.

The organizers (Rack, Cabaniss, Atlas) created a short proposal for this idea under the program name Research Opportunities for Science Educators (ROSE), included here as Appendix A. The original intent was to obtain support to implement some version of the program in Summer 2022, after pandemic restrictions were relaxed and the Clark Hall (UNM Chemistry building) renovations were completed.

On April 12, 2021, the organizers and CCB department chair Jeremy Edwards met with NM PED deputy secretary Gwen Warniment and Jacqueline Costales to discuss the ROSE proposal outlined in Appendix A. Dr. Warniment proposed a small pilot project for summer 2021 to be supported financially and logistically by PED.

On April 30, the organizers met with Yanira Vazquez and Shafiq Chaudhary, to determine the number of people who could participate, and discuss organizational and operational details of the Program. All other correspondence prior to, during, and after the Summer 2021 Program was through email.

Organizer Biographical Sketches

Steve Cabaniss has taught analytical and environmental chemistry for over 30 years at Kent State University (1989-2002) and UNM (2002-present). His research examines the behavior of metals in natural waters and soils, including uranium contamination on the Colorado Plateau. He served as department chair for CCB (2012-2018) and on the governing board for the Albuquerque Institute of Mathematics and Science (AIMS) from 2006 to 2014 including 4 years as board president.

Jeffrey Rack began his professorial career at Ohio University in 2001 and moved to UNM in 2016, where he continues to teach general chemistry, inorganic chemistry and photochemistry. His research interests center around photochemistry and photophysics of materials and transition metal complexes. He presently serves as Secretary for the Division of Inorganic Chemistry (DIC) of the American Chemical Society (ACS), DIC Councilor for ACS, and is Vice-President for the Inter-American Photochemical Society.

Susan Atlas has been a faculty member at UNM since 1994, following a postdoctoral fellowship at Los Alamos National Laboratory. She teaches courses in introductory physical chemistry, statistical mechanics, parallel computing, electronic structure, and computational genomics. Her research is focused on the theoretical chemical physics of biophysical, biochemical, and materials systems. She has served as Director of the UNM Center for Advanced Research Computing and as Program Director in the Division of Chemistry at NSF.

Scholar Recruitment and Selection

The pilot program was announced May 5, 2021 in the PED's NM STEM Connect Newsletter, which is sent to science teachers across the state. Between May 5 and May 15 (the closing date), we received 39 total applications and three independent email requests about applying. The applicants were independently evaluated and ranked (by Cabaniss, Rack, and Atlas) based on the following criteria: whether or not the applicant will teach high school chemistry next academic year, will teach high school science next academic year, total number of years teaching experience, and self-identified area of research interest. This selection yielded a group of 15 prospective ROSE Scholars. Final selection from this group was based on matching individual high school science teacher interests with PI interests, applicant availability, personnel capacity in host (PI) laboratories, and geographic location of the applicant and their school. Preference was given to those educators who teach in rural areas or who teach large numbers of underrepresented minority students and/or had specific interests or background relevant to a particular research project. Declination letters were sent to all applicants who were not selected.

June Activities/Timeline

Program activities began with the arrival of scholars and orientation the morning of June 1. Scholars met with faculty organizers and PIs, completed paperwork required to give them access to UNM facilities (keys, card access, etc.), and participated in a chemical safety program. ROSE scholars began their respective research programs on June 2. Each Friday (June 4, June 11, June 18, and June 25), ROSE Scholars, host PI's, and other special guests were provided lunch, where we met to informally discuss aspects of the experience. On June 25, ROSE Scholars participated in the ROSE Symposium, where each Scholar presented a brief lecture on their experience. The ROSE pilot program was completed on June 25.

Research Descriptions

Prospective ROSE Scholars were provided a menu of research projects to select areas of interest. This selection was used to pair the science educators with a PI host. Those areas were:

Chemical Synthesis	Molecular Modeling	Nanochemistry
Biochemistry	Chemical Education	Solar Energy
Materials Chemistry	Photochemistry	Polymers
Proteins & peptides	Catalysis	Genomics
Drug discovery	Electrochemistry	

A more detailed description of each research project as provided by the host PIs can be found in Appendix G.

Assessment Procedures and Outcomes

Evaluation of the pilot program is in progress, and an assessment report will be prepared for distribution late in the Fall 2021 semester. The report will include information collected from the Scholars on their expectations for the program during the orientation session (form in Appendix E) and more extensive interviews of scholars and PIs conducted shortly after the pilot project ended (completed for Scholars, in progress for PIs), and during the Fall 2021 semester (planned for Scholars in late September/early October).

Interviews are being conducted and summarized by Dr. Abigail Stewart, who is the Sandra Schwartz Tangri Distinguished University Professor of Psychology and Women's and Gender Studies at the University of Michigan (UMich) (lsa.umich.edu/psych/people/faculty/abbystew.html). Prof. Stewart directed the UMich ADVANCE program for women and minority STEM faculty from 2001 to 2016, and more recently co-authored (with Virginia Valian) "An Inclusive Academy: Achieving Diversity and Excellence" (2018, MIT Press). She consults for the UNM ADVANCE program (https://advance.unm.edu/about-us/).

The primary purpose of these interviews is to help improve the program in subsequent summers, from advertising and selection of Scholars through on-campus activities and responses to how the experience "carries through" to the classroom in the fall. PIs are being asked to comment on program workload and disruption, as well as interactions with Scholars. The initial interviews with Scholars focused on program logistics and activities and their responses, while the later interviews will emphasize changes (if any) in the classroom.

The pilot program exceeded our expectations on several levels, including the enthusiastic responses of the teachers (ROSE Scholars). A few excerpts from Prof. Stewart's report on the first round of scholar interviews follow in italics; quotes from individual teachers are also in quotation marks.

The program was, as is evidenced below, enormously and universally successful, in the eyes of the ROSE Scholars. Participants came with high hopes, and those hopes were met and exceeded. They greatly valued, in particular, the opportunity to do hands-on research with mentors they perceived as both patient and supportive, and brilliant. They felt this experience provided them with many resources to bring to their teaching.

All 8 of the 2021 participants would like to participate again.

All of the participants expect to maintain ties with people in the program.

Would you recommend this program to others? All of the participants said, yes, though two qualified their responses by saying: "I think it has to be a teacher that is willing to come in and know that, you know, they need to ask questions."

The participants outlined the program's powerful impact on them in every case. For that reason I have left in their verbatim quotations about it. Some focused on the impact of learning and experiencing new things; others on the way in which past and current knowledge integrated and created a more meaningful whole. In every case, though, participants reported that the impact was positive and substantial.

"Everything seems to connect at the quantum level: biology, physics and chemistry…"

"I'm just jazzed to tell them about the research, you know like, to be able to get involved in something that you don't get to experience as a teacher… and it was just such a great experience to see how the applied lab techniques, the instrumentation they used, what kind of things we should probably think about covering more, that ties into this… I think that's what I'm really want to bring back to my peers is: just what did we work on [in the ROSE Program], and how does this tie to what we're working on [in high school]."

Since the pilot emphasized individual research projects, each Scholar answered differently about how they might incorporate skills from ROSE into their pedagogy:

"…in biology, we talk about enzymes, the binding of enzymes, and the protein. And so this is a very good example because we can, I can even teach my students to actually do the simulation using a free program just using our laptops"

"I learned how to let the student visualize the data. For example, I modeled interactively with our Python plot package… And that could be very good to teach biology students and chemistry students, or the physics and say: You see this is our atoms and molecules, this is how they enter to connect to the cell membrane, so it could be a very authentic project for the teaching."

Several of the Scholars noted the diversity within the research groups and wanted to take that observation back to their students:

"…now when I develop a lesson plan I can rely on my experience about how these things are studied. And I also learned new concepts that I can embed throughout my lessons. What does the research look like? Bringing that perspective to them, maybe let them do projects, and really recruit them not just to UNM—it's not boring, it's not oriented just to males, the group I participated in was very diverse!"

"…in the lab, the people that I work with: there is diversity, and I want to emphasize that the research is not [only] for men. Researchers are doing experiments doing work in the lab are not only men. This is this work is also for women, different background. Right. So I want to highlight that. And I really wanted to invite my, my students to pursue college, and want them to experience research. My goal is to motivate them. My goal is to inspire them to pursue their dreams to do to pursue STEM career."

We also asked whether the experience had changed their impression of UNM. Note that five of the eight scholars live outside the Albuquerque metropolitan area, while two teach in APS and one teaches in Cuba but lives in Rio Rancho.

Five of the participants outlined particular ways in which their view of UNM had changed.

One commented that it is a very nice campus; and another that they learned about it from the administrators who came to lunch. One pointed out that "Now I think I'm very confident that I have a connection to UNM." Another pointed out that "I never thought that they have these interdisciplinary department here. I didn't realize that they have an interdisciplinary department wherein, you know, they actually apply all these different principles to zero in on the common ground. I'm very surprised and lucky to know that, because I can share it more to my kids with the students." Finally, one said that, to their surprise, they "saw some really cool things at UNM that made her know it's friendly, has rethought use of space outdoors, to study, to sit, not just one concrete slab." They now think it's an "Excellent place to go."

Based on the overwhelming response to the initial advertisement and the enthusiastic positive responses of the ROSE scholars in the initial interviews, the organizers want to offer an expanded version of this program in Summer 2022.

Acknowledgements

The ROSE pilot project was supported by the New Mexico Public Education Department and the University of New Mexico, Office of the Vice President for Research, and the Department of Chemistry and Chemical Biology (CCB). NM PED provided stipends, travel allowances, and housing for five of the Scholars. The UNM Office of the Vice President for Research provided stipends for three ROSE Scholars. CCB provided administrative support for the program as well as funding for the weekly lunch meetings.

Special thanks to Gwen Warniment, Jacqueline Costales, Shafiq Chaudry and Yanira Vasquez (NM PED), Mary Jo Daniel and Ellen Fisher (UNM OVPR), Dan Garcia, Tim Schroeder and Arash Mafi (UNM Administration) and to Teri Anderson, Sharon Boyd, Bobby Ortiz and Felicia Rider (UNM CCB), who all provided crucial support to the program in many different ways. We are especially indebted to the graduate students and postdoctoral researchers helped make the inaugural ROSE program an extraordinary success. They are Glorianne Dorce, Mark Aldren Feliciano, Tongtong Li, Shenghan Song, Amy O. Stevens, Rajani Thapa Magar, Emigdio Turner, and Pavel Yamanushkin.

Appendix A. Preliminary Program Description

Research Opportunities for Science Educators (ROSE)

Program description

ROSE will bring New Mexico science educators (SEs) from high schools and primarily undergraduate institutions (PUIs) to the UNM Albuquerque campus for 8 weeks in summer to work on a research project with a faculty investigator. These faculty will be experienced principal investigators with ongoing funded research projects. The SEs will have access to UNM library and lab facilities and will receive training in research and safety techniques, which will improve their understanding of the science they teach and expand knowledge of state-of-the-art methods for transmission to colleagues and students at their home institutions. Educators will have the opportunity to present and publish their results, and to learn about projects in other research groups at UNM. Educators will receive a stipend, and on-campus housing will be provided for those who desire it.

Science educators at NM high schools and PUIs are eligible to participate if they a) have taught science classes for at least five years or b) have a bachelor's degree or higher in a laboratory science and have taught for at least two years. Educators will apply by February 1 and will learn of their acceptance by March 15 for the following summer; educators are expected to return to teaching in the following Fall. Selections will be made by a committee of participating faculty, and preference will be given to educators who teach in rural areas, teach large numbers of underrepresented minority students, and/or have specific interests or background relevant to a particular research project.

Informal events will allow the SEs to network with each other, share their research experiences, and meet faculty and learn about research in other laboratories and departments. The summer will conclude with a more formal poster session in which the SEs present their results to UNM faculty and students.

Benefits

To New Mexico high schools and PUIs: ROSE will improve the quality of science education by allowing educators to refresh their knowledge and develop new skills while gaining appreciation for and inspiration from current scientific research.

To UNM: ROSE will help recruit well-prepared STEM students by familiarizing their teachers with our faculty, laboratories and research opportunities. In addition, the program will establish authentic relationships between UNM faculty and science educators in the local and regional communities which may lead to additional collaborations and enhanced grant opportunities addressing broader societal impacts. In principle, a science educator may be able to return to the same PI's lab over a period of multiple summers.

To national funding agencies: ROSE will increase the number of college applicants and improve the preparation of high school STEM students while aiding and publicizing funded research projects.

Appendix B. Announcement from NM STEM Connect May 5, 2021

Research Opportunities for Science Educators (ROSE) at the University of New Mexico

Open to New Mexico High School Educators

Are you interested in performing cutting-edge research in modern facilities? Would you like to learn the latest in the development of chemical theories? Would you like to know more about research opportunities at the University of New Mexico? The UNM Department of Chemistry and Chemical Biology (CCB) is partnering with NM PED to offer a pilot program designed to bring science teachers to CCB for four weeks in June (June 1 to June 25) to work with our scientists. Participants will receive a stipend of $1,200 per week, and housing support/mileage reimbursement is available for those traveling more than 60 miles one way. All participants will receive a UNM parking pass.

Applying is easy! We ask that you identify potential areas of interest, which are listed on the application information form. To learn more about the individual opportunities, please see the accompanying list of abstracts. Some of these projects require in-person participation, while others are entirely virtual. They are all exciting! This opportunity will allow you to participate in an active, federally funded research project that seeks to answer important scientific questions in areas including: Chemical Synthesis, Nanochemistry and Nanoscience, Molecular Modeling and Computation, Photochemistry, Solar Energy, Electrochemistry, Biochemistry, and many others.

We hope that you will give this opportunity serious consideration, in spite of the compressed timeline. **We look forward to receiving your application by May 14**. You should expect a reply (offer of support, specific faculty project) by May 18 and will need to accept or decline this by May 21 to allow time for contract processing before the program begins June 1. Please email Professor Rack (jrack@unm.edu) if you have further questions or concerns.

Appendix D. Table of ROSE Scholars and their Institutions

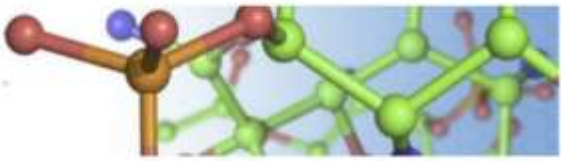
Scholar	**School**	**UNM PI**
Mariejune Abergos	Early College High School Roswell	Jeff Rack
Geizi Dejka	San Juan College High School	Yi He
Daniel Delgado	Cuba High School	Susan Atlas
Inez Jacobs	Mark Armijo Academy (APS)	Mark Walker
Shigang Liu	Las Cruces High School	Susan Atlas
Demvia Maslian	New Mexico Military Institute	Yi He
Margarita Romero	Arrowhead Early College HS	Jeff Rack
Brian Schreiber	Atrisco Heritage Academy (APS)	Brian Gold

Appendix E. Orientation "Expectations" Form

On the first day of the program, as the ROSE Scholars arrived for orientation, a brief questionnaire was distributed for the Scholars to complete, with questions about their expectations for the ROSE Program. A copy of the questionnaire is included on the next two pages.

NEW MEXICO Public Education Department

DEPARTMENT OF CHEMISTRY & CHEMICAL BIOLOGY



Impressions on Entering the ROSE Program

Welcome to the Summer 2021 ROSE Program. As the inaugural cohort of ROSE Scholars, your thoughts about research, and what you hope to get out of the program, will be very helpful for us to hear, as we begin these four weeks together. Please take a few moments to complete this survey, bearing in mind that "there are no right answers"!

Name: _____

Email: _____

1. **What is your impression of what happens in a research group and how research is 'done'?**

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2. **How do you hope to benefit from this program personally?** _____

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3. **How do you think participation in this program will benefit your school and students when you return to teaching this fall?** _____

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Appendix F. Orientation hand-out on research

An Introduction to Scientific Research for ROSE Scholars

For those who have never engaged in a research project, the "nuts and bolts" of the process may seem mysterious. Are there "regular hours"? Who provides orientation and direction? What are the schedule and effort expectations? What is produced at the end? It depends. This trite answer may not seem very satisfying, but research by its nature is difficult to predict and describe in advance.

Scientific research attempts to increase the sum of human knowledge by asking questions where the answers are unknown. Answering these question may require locating, understanding and integrating existing knowledge (library or internet 'research'), making new measurements or performing new calculations with existing tools, constructing new apparatus or algorithms, synthesizing new molecules or materials, writing computer code and/or devising new theories and ways of understanding. A typical research group will engage in several of these activities while pursuing the answers to their questions. And once you know the answer to one question, it frequently suggests others…

At a research university, the director of each research group is the principal investigator or 'PI', responsible for the overall direction of research (what questions shall we ask?), obtaining the funding to pursue the research and assigning tasks to individual researchers, who may be students (graduate or undergraduate), research staff, or Ph.D. level scholars like post-doctoral associates who are part of the research group.

The ROSE PIs for this summer are professors in the Department of Chemistry and Chemical Biology (CCB), all directing long term research efforts which you will be joining. Based on your interests and project needs, the PI will assign you a task or tasks and arrange for someone (perhaps the PI, perhaps an experienced researcher in the group) to "show you the ropes" and help guide your progress. Depending on the project, you could end up synthesizing a candidate drug, calculating the molecular structures of a protein complex, writing code to implement a new theoretical method or measuring the excited state lifetime of a new molecule.

What are the hours (or time requirements)? A ROSE stipend is full-time, 40 hours per week support, but the schedule and hours spent in lab can vary considerably. A molecular simulation can be run at any time of day, but a molecular synthesis may require scheduling a block of time- 2 hours? 6 hours?- when other people will be in the lab. Using department facilities or shared instruments may require arranging time slots with other users. You and your PI should discuss expectations early in June, including required meetings (research group, training), general lab schedule and practices, and lab/instrument/computer access.

How do I get research supplies? Your PI will need to approve any spending requests, directly or indirectly. You should ask about the purchasing procedure in your research group, and whether the PI is anticipating your spending any research funds.

What is produced? Research results are legally the property of the responsible institution (UNM) with the proviso that the contributions of funding agencies and participants are appropriately acknowledged. As a research project proceeds, the results are typically distributed in the form of reports to funding agencies, conference presentations and publications in the scientific literature. Most of these have multiple authors, since most projects have multiple participants. Your results may be incorporated in these (with your contribution acknowledged), but this is unlikely to happen this June! Instead, you will leave a record of your activities and results with your PI. The format of these records can vary widely (data files? handwritten or online lab notebook? compounds synthesized?) and you should discuss this with your PI to be sure you are recording the appropriate information (and in the appropriate format). We will also ask you to share your results with the other ROSE scholars and PIs on June 25 (presentation format to be determined).

Appendix G. Research Project PI summaries

ROSE Research projects for June 2021 (pilot project)

PI: Prof. Susan R. Atlas
http://chemistry.unm.edu/people/faculty/profile/susan-atlas.html

Understanding 'atoms in molecules'

Bonding is at the heart of chemistry. In our lab, we are studying how the nature of an atom changes when it forms a chemical bond with another atom as part of a larger molecule or complex. This question, originally posed over 100 years ago by G. N. Lewis in his article introducing dot structures ("The Atom and the Molecule," J. Am. Chem. Soc., 38, 762–85 (1916)), is proving central to modern understanding of the structure and dynamics of molecules and materials. Our work uses computational modeling of the electron density spatial distribution as the foundation for analysis. Current research in our lab involves simple diatomics (LiF, a paradigm of ionic bonding) and CO (a paradigm of covalent bonding) and amino acids, the building blocks of complex biomolecules. Using these simple structures as testbeds, this project is exploring new theories of the atom-in-molecule using neural networks and machine learning. The project is mathematical and computational in nature; prior experience with computer programming (any language) will be helpful. All work for this project can be performed remotely over the internet; research meetings will conducted via Zoom.

Modeling the effect of amino acid mutations on the structure and dynamics of the SARS-CoV-2 spike protein receptor binding domain (RBD)

As of May 2021, the COVID-19 global pandemic has resulted in > 150M cases and 3.2M deaths worldwide (Viruses **13**, 1126 (2021)). COVID-19 infection is caused by the penetration of single-stranded viral RNA into a host cell. This occurs via fusion of the viral capsid envelope with the host cell membrane. A primary mechanism for this fusion is the binding of the SARS-CoV-2 "spike protein" receptor binding domain to a host cell ACE2 receptor. mRNA vaccines train the immune system to recognize the spike protein, to produce a robust antibody response to the virus. However, new SARS-CoV-2 variants such as B.1.1.7 (Alpha) and B.1.617.2 (Delta) have emerged, with multiple mutations in the viral genes encoding the spike protein. These mutations result in amino acid substitutions and deletions, potentially affecting spike protein structure and function, ACE2 binding affinity, and vaccine effectiveness. In this computational project, we are investigating the impact of spike protein receptor binding domain (RBD) amino acid substitutions on RBD structure and dynamics, with the remaining atoms of the solvated spike protein held fixed. Simulations utilize the NAMD molecular dynamics simulation code and VMD visualization package (https://www.ks.uiuc.edu/), and the supercomputing resources of the UNM Center for Advanced Research Computing.

PI: Prof. Brian Gold
www.GoldChemistry.com

Synthetic Peptide Libraries for Accelerated Drug Discovery

Chemotherapies and molecular diagnostics highlight the importance of a molecular arsenal to battle essentially all types of cancer. Despite the success of current chemotherapeutics, the associated side effects and development of drug resistance necessitate the development of new drug compounds. Hurdles to the development of new therapeutics stem from the rapid generation and screening of chemically diverse drug molecules. Our research focuses on synthetic strategies to rapidly generate compounds for the development of new cancer drugs and diagnostics.
This work is supported by the National Institute of Health via UNM's Center for Metals in Biology and Medicine and benefits from collaborations with UNM's Center for Molecular Discovery. Research fellows will be exposed to principles of bioorganic structure and reactivity, enzymology, and structure-based design, and can gain experience in chemical synthesis, computational chemistry, biochemistry and chemical biology, and drug discovery.

Rethinking Enzyme Catalysis for Improved Therapeutics
HIV/AIDS remains among the worst global pandemics in modern history, while hypertension and Alzheimer's disease are public health crises that either directly or indirectly (heart attack and stroke) attribute to three of the top six leading causes of death. These distinct ailments share related therapeutic targets. Our goal is to exploit the similarities of these enzyme targets to rapidly develop next-generation inhibitors with profound clinical potential.
This work is supported by the National Institute of Health via the New Mexico IDeA Networks of Biomedical Research Excellence (NM-INBRE) and benefits from collaborations with UNM's Center for Molecular Discovery. Research fellows will be exposed to principles of bioorganic structure and reactivity, enzymology, and structure-based design, and can gain experience in chemical synthesis, computational chemistry, biochemistry and chemical biology, and drug discovery.

PI: Prof. Yi He
http://helab.unm.edu

Revealing the activation mechanisms of a critical protein involved in substance use disorders
Substance use is a wide-reaching concern in the United States today and heavily contributes to the burden of disease in our nation. Here at home, New Mexico has the highest alcohol-related death rate in the nation and ranks 17th in drug-related deaths. Furthermore, the use of drugs and alcohol lead to systemic social problems in New Mexico. Substance use is related to systemic social problems, including health, criminal justice, education, and social welfare. In recent years, a promising solution to this wide-reaching problem has emerged through a unique human protein – Protein Interacting with C Kinase-1 (PICK1). PICK1 is a scaffolding protein that is one of the key regulators in biological cycles related to substance use disorders. Our study utilizes computer simulations to provide information that is key to assist drug developers in designing a small molecule inhibitor to target PICK1 and ultimately support individuals suffering from the effects of substance use disorders.

PI: Prof. Jeffrey Rack
http://rackresearchgroup.wordpress.com

Development of Photoactive Materials
Research in the Rack Group is focused on the development and study of photoactive compounds and materials for applications in quantum information science and optical limiting devices. We make a series of laser measurements ranging from femtoseconds (10^{-15} s; a billionth of a millionth of a second) to hundreds of microseconds (10^{-6} s; a millionth of a second) to understand how these materials respond to light. In one project (funded by the Army Research Laboratory), we prepare materials that exhibit optical limiting properties, which are used to protect light detectors, such as cameras. This project involves the synthesis of photoactive compounds, their incorporation within polymeric materials, and/or laser investigations into how these materials react with light. In another project (funded by the National Science Foundation), we synthesize compounds and materials that change color when exposed to light. These materials can be used for information storage and other applications. We are interested in the details of how this reaction occurs, and how we can use this change to affect other properties, such as magnetism. There are many opportunities in these projects, and we are always looking for new people to help meet our research goals.

PI: Prof. Mark Walker
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New Approaches to Antibiotic Discovery
Chemicals produced by living systems, or natural products, have had a tremendous impact on human health. For example, nearly one third of all small molecule drugs approved by a regulatory agency over the past nearly four decades have been natural products or derivatives of natural products, including over 70% of antibiotics and 40% of anticancer drugs. While very useful molecules have been identified among the hundreds of thousands of natural products that have been characterized to date, genome sequencing efforts over the past decade and a half have revealed that we have only characterized the products of a small fraction of the biosynthetic pathways that exist in nature. The products of these pathways have the potential to greatly impact the diagnosis and treatment of disease, and it is critical that we develop new approaches to accelerate the identification and characterization of new natural products and natural product-like compounds.

This project will focus on using molecular biology and biochemical techniques to characterize enzymes that are involved in the production of new types of natural products.

Appendix H. Safety training slides

The safety training slides from Teri Anderson and Sharon Boyd are attached as a pdf (the original PowerPoint slides are much larger due to presence of videos).