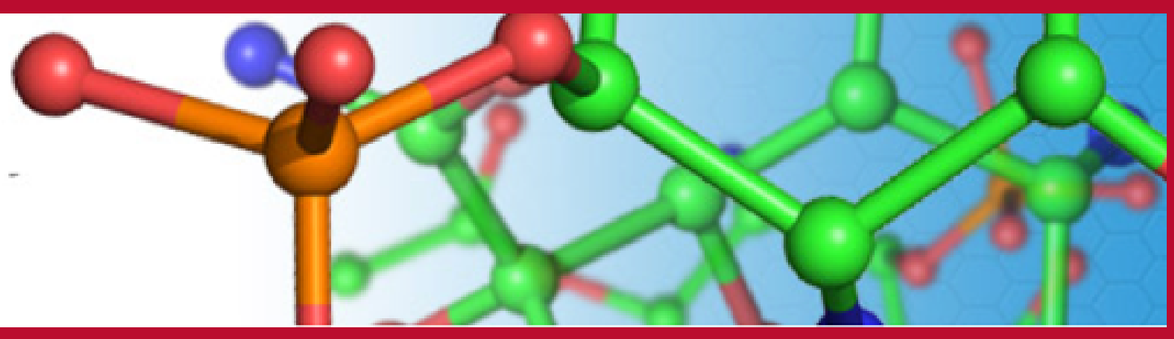
DEPARTMENT OF CHEMISTRY & CHEMICAL BIOLOGY



2021 ANNUAL NEWSLETTER

A MESSAGE FROM OUR DEPARTMENT CHAIR

Dear Alumni, Colleagues, and Friends,

I hope that this newsletter finds you and your loved ones healthy and safe.

I am extremely happy to report that we successfully completed the Fall 2021 semester completely face-to-face. All classes and meetings were held in the traditional face-to-face manner. It was wonderful to see all our students, faculty, and staff in person - many I hadn't seen in over a year. All of this was accomplished with very few COVID cases within the department, and as far as I am aware, there was not a single person that contracted COVID in our building or classrooms. This was quite an accomplishment, and undoubtedly due to each and everyone's actions.

2021 was an incredible year! The Chemistry and Chemical Biology department accomplished many amazing feats. For example, the department completed its Academic Program Review, where the team of outside reviewers stated "the graduate faculty are to be congratulated on their research productivity and accomplishments. Many of the faculty are internationally recognized for their scholarship." Additionally, we completed the 2nd (and final) phase of the renovations to Clark Hall. We all moved back into the building in August and September. In the newly renovated space, all faculty offices are co-located on the second floor, and I really enjoyed frequent face-to-face interactions with all faculty, staff, and students. I will share a few more of the many wonderful achievements within the department in the accompanying newsletter.

As always, thank you for your continuing support and stay well.

Sincerely,
Jeremy S. Edwards
Distinguished Professor and Chair

NEW FACULTY

Dr. Dongchang Chen joined UNM Chemistry and Chemical Biology in January 2021 as Assistant Professor

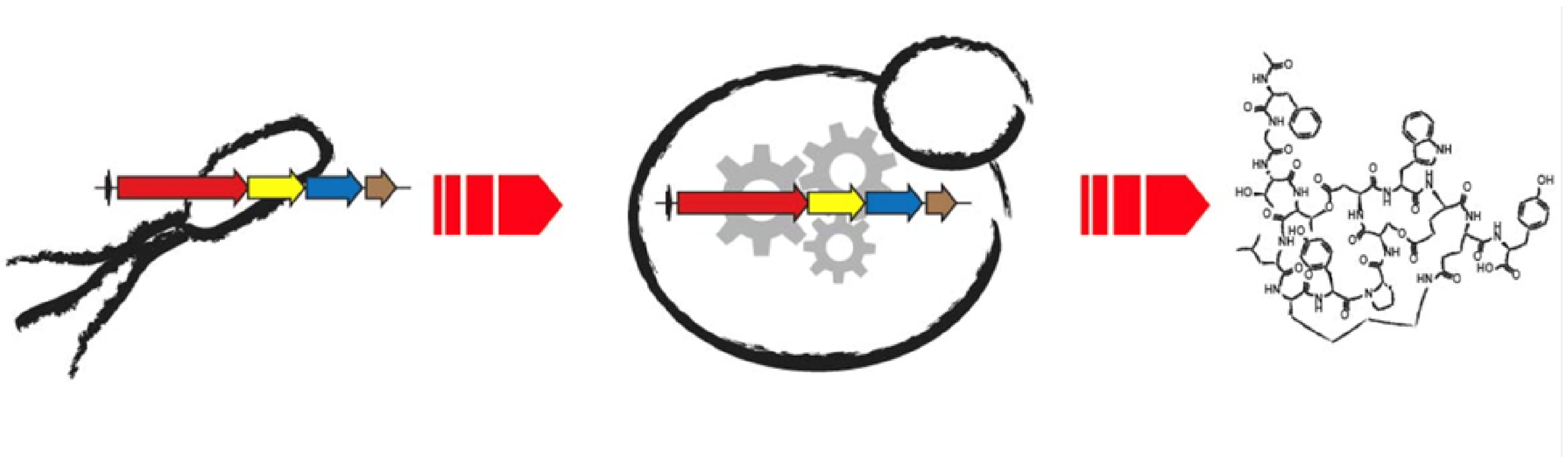
Dr. Chen joined UNM Chemistry and Chemical Biology in January 2021 as a tenure-track Assistant Professor. Dr. Chen's research seeks to resolve critical chemical processes for energy storage and conversion materials via advanced spectroscopic approaches. The obtained knowledge will serve as guiding principles for systematic materials design and address outstanding challenges in energy and environmental applications.

Dr. Chen worked as a postdoc researcher in the Energy Storage and Distributed Resources Division of Lawrence Berkeley National Laboratory since 2017. His postdoctoral work focused on the principles and design strategies for high-energy density Li-ion battery cathode materials. He obtained his Ph.D. degree in chemistry from Georgia Institute of Technology, where he studied reaction mechanisms and surface/interfacial phenomena for various energy storage applications via in situ/operando Raman spectroscopy. He received his B.Sc. Degree in chemical physics from University of Science and Technology of China in 2011.

FACULTY HIGHLIGHTS

Prof. Mark Walker recipient of $1.7 million grant

This grant is an NIH MIRA award and provides $1.7M of total funding over 5 years. The grant will support Prof. Walker's group to study the enzymatic pathways that make ribosomally synthesized and post-translationally modified peptides, which are a class of natural products. This new grant will provide a deeper understanding of how the enzymes that make this class of natural products function, which will allow Prof. Walker to generate large libraries of natural product-like compounds that can be screened to identify those with useful biological activities more efficiently.



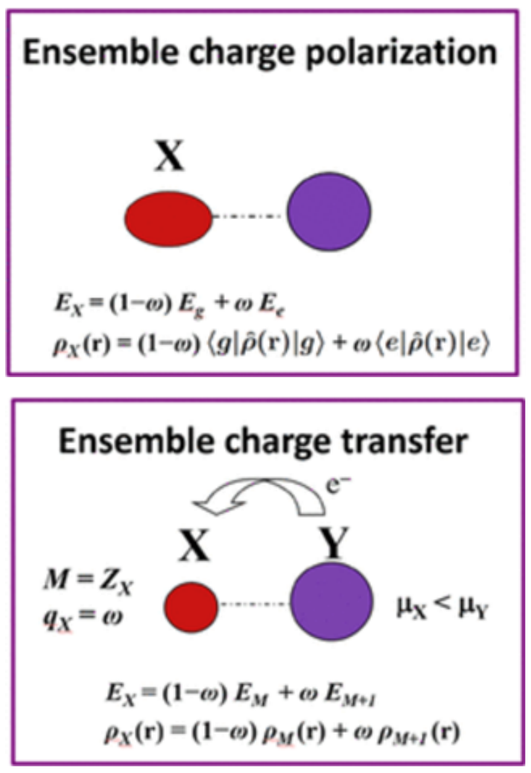
FACULTY HIGHLIGHTS

Prof. Susan Atlas published an invited paper in the Journal of Physical Chemistry A

The article was part of a Festschrift issue honoring Prof. Lawrence R. Pratt. The article is entitled "Embedding Quantum Statistical Excitations in a Classical Force Field." Prof. Atlas combines ideas from statistical mechanics and electronic structure theory to propose a physics-based, atomistic force field for molecular dynamics (MD) simulations of complex materials, including proteins. The force field couples electronic and atomistic length scales through an ensemble density functional theory formulation of the embedded-atom method originally developed for elemental materials. Charge transfer is expressed in terms of ensembles of ionic state basis densities of individual atoms, and charge polarization, in terms of atomic excited-state basis densities. This provides a highly compact yet general representation of the force field, encompassing both local and system-wide effects.

Prof. Susan Atlas is co-PI on a $3,000,000 NSF Grant

This grant will support a "Focused Research Hub in Theoretical Physics" at the Center for Quantum Information and Control (CQuIC), where Prof. Atlas also serves as a Steering Committee Member. The grant, led by Regents' Prof. Ivan Deutsch, Physics and Astronomy, will enable CQuIC to enhance the development of early-career scientists through the creation of an interdisciplinary postdoctoral fellowship cohort with broad expertise in physics, computer science, electrical engineering, and chemistry. The Hub also includes partners at Sandia National Laboratories, Los Alamos National Laboratory, and Honeywell Quantum Solutions to help build a diverse and inclusive next-generation QIS workforce. Prof. Atlas serves as a science Project Director and as Diversity Officer for the Hub.



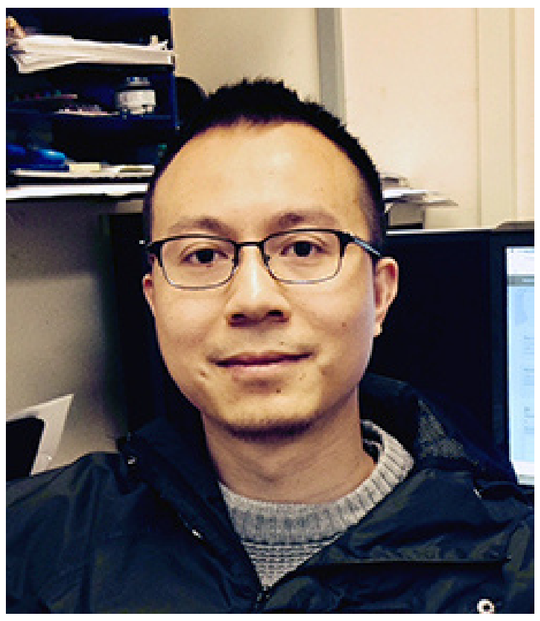
Chemistry Chairman's Discretionary Fund

If you would like to make a donation to the Department of Chemistry and Chemical Biology, please consider the *Chemistry Chairman's Discretionary Fund.* This discretionary fund is used to provide program support and to meet the immediate and unexpected needs of the department.

https://www.unmfund.org/fund/chemistry-chairmans-excellence-fund/

FACULTY HIGHLIGHTS

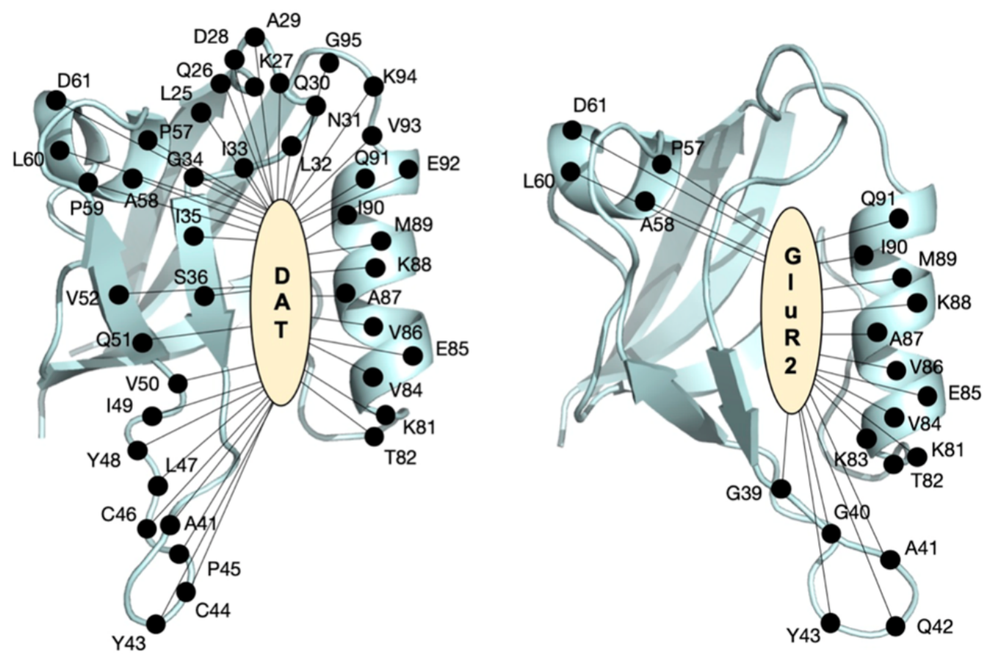
Prof. Yi He collectively published an article with the Oak Ridge National Laboratory (ORNL)



The article was published in ACS Applied Materials & Interfaces analyzes the design of single-ion conducting polymer electrolytes (SICPEs). His work highlighted that the polarity of side chains has a limited influence on ion dissociation for copolymer-type SICPEs. The Li+ -ion dissociation seems to be controlled by the charge delocalization on the polymerized anion. With good miscibility between plasticizing neutral units and ionic conductive units, the ambient ionic conductivity of synthesized SICPEs is still mainly controlled by the Tg of the copolymer. This work sheds light on the dominating role of PEO in SICPE systems and provides helpful guidance for designing polymer electrolytes with new functionalities and structures.

Prof. Yi He received a grant from the National Science Foundation

The NSF grant is focused on studying the Protein Interacting with C Kinase-1 (PICK1) which is a eukaryotic signaling molecule that is a key regulator of receptor trafficking. PICK1 has been shown to play a role in a large number of diseases, including breast cancer, schizophrenia, addiction, and addiction relapse. The objective of this grant is to computationally probe the key residues and physical interactions associated with the structural and mechanical properties of each subdomain that are directly related to the biological function of PICK1.



Prof. Brian Gold awarded funding from the National Institute of General Medical Sciences of the National Institutes of Health

The funding, under the NM-INBRE Developmental Research Project Program will provide for the project, “Rethinking Enzyme Catalysis for Improved Therapeutics.” NM-INBRE champions biomedical and community-based research excellence in the state of New Mexico through the development of innovative, supportive and sustainable research environments for faculty and students, community engaging health initiatives, while building a network of lead scientists and educators at the state, regional and national level.

FACULTY HIGHLIGHTS

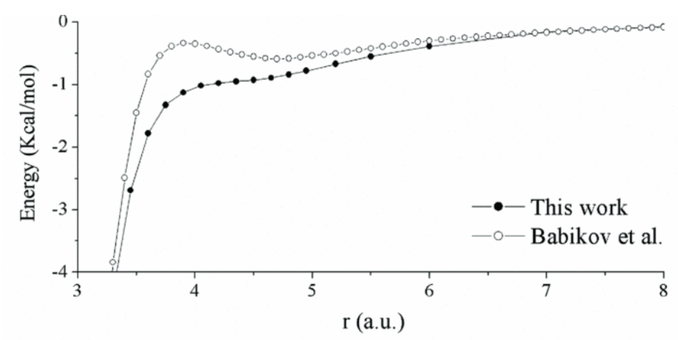
Disinguished Prof. Guo was Elected as a Fellow of American Association for the Advancement of Science (AAAS).

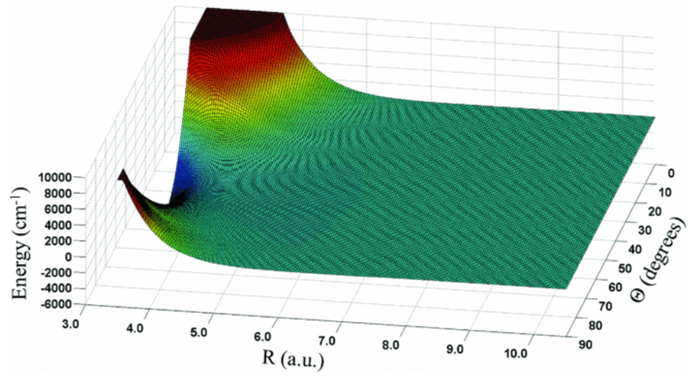
In a tradition stretching back to 1874, these individuals are elected annually by the AAAS Council. Fellows have included Thomas Edison, W.E.B DuBois, and Maria Mitchel. AAAS Fellows are a distinguished cadre of scientists, engineers and innovators who have been recognized for their achievements across disciplines.

This honor is reserved for only the top 0.1% of scientists world-wide. This honor for Professor Guo recognizes his distinguished career achievements in research and service to the chemistry community.

Distinguished Prof. Hua Guo lead a collaborative group of researchers from the UNM and Texas A&M University

The group sought to understand more about the photo-chemistry of Earth's ozone. The work was published in the Proceedings of the National Academy of Sciences of the United States of America (PNAS), and it offers a long-awaited explanation for the "odd" behavior of ozone molecules in our atmosphere. The discovery was made using quantum mechanical calculations.





Guo's paper addresses an intriguing observation about ozone behavior that has puzzled chemists for the past 30 years. Guo writes, "About 30 years ago, an experimental study revealed a strange behavior of the O_2 molecule as a result of the breaking-up of ozone. The O_2 photofragment was shown to have a strong preference to its rotational states with even quantum numbers, while the rotational states with odd quantum numbers are much less populated. Here, the rotational quantum number dictates how fast the O_2 molecule rotates and it contains important information about how the O_3 molecules break up in an excited electronic state."

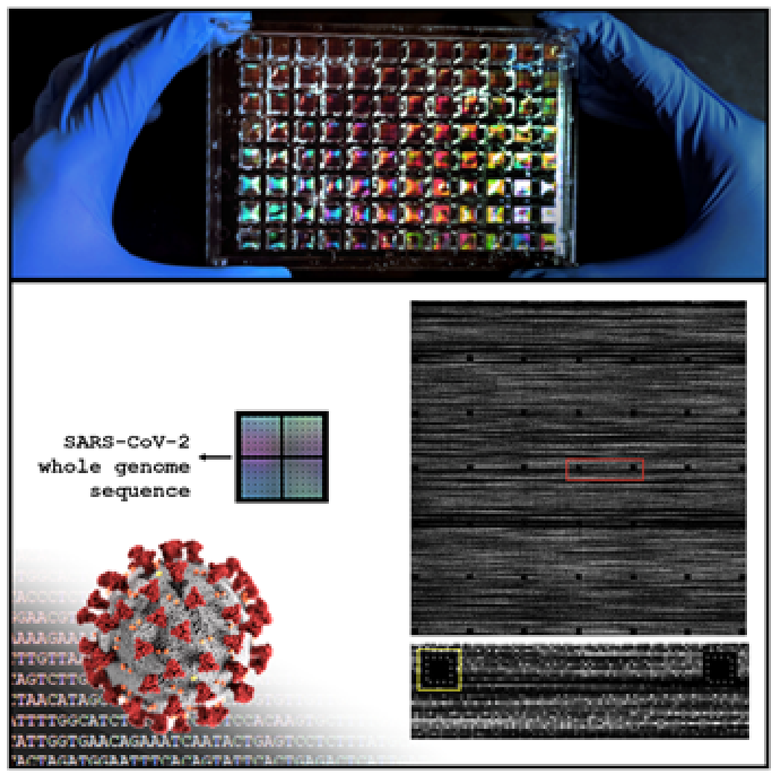
Prof. Jeffrey Rack named Co-Op Faculty Coordinator for the Interdisciplinary Science Cooperative

Launched in 2019 in the brand new state-of-the-art Physics and Astronomy Interdisciplinary Science (PAÍS) facility, the University of New Mexico (UNM) Interdisciplinary Science Cooperative (IS Co-op) is dedicated to fostering relationships across disciplines throughout campus and beyond in order to strengthen our research and educational outcomes. From various collaborative spaces designed to inspire teamwork, to events and project support designed to promote and engage new ideas, the IS Co-op is creating a foundation of success for the University and beyond.

FACULTY HIGHLIGHTS

Distinguished Prof. Jeremy Edwards article published in Langmuir

Prof. Edwards led a research group that developed a new high throughput and inexpensive full SARS-CoV-2 genome sequencing technology. The technology is able to rapidly sequence the full viral genome and identify new and existing variant strains. The technology has been used to sequence hundreds of viral genomes from COVID patients in New Mexico.



For more information visit:
https://pubs.acs.org/doi/abs/10.1021/acs.langmuir.0c02927

Distinguished Prof. Jeremy Edwards' group sequenced the whale shark genome

The Edwards group collaboratively sequenced and analyzed the genome of the endangered whale shark, the largest fish on Earth, and compared it to the genomes of 84 other species ranging from yeast to humans. We found strong scaling relationships between genomic and physiological features. For example, in the whale shark, large gene size and large neural gene size strongly correlate with lifespan and body mass, suggesting longer gene lengths are linked to longer lifespans. For more information visit: https://www.pnas.org/content/117/34/20662.short

UNM CCB hosted the the American Chemical Society Division of Organic Chemistry Graduate Research Symposium

The DOC Graduate Research Symposium, which provides an opportunity for 50-75 graduate students in organic chemistry to interact with leaders from academia, industry, various funding agencies, and publishers at a single venue will took place on November 18-21, 2021 on the UNM campus.

For more information visit:
www.organicdivision.org/grs/

STUDENT HIGHLIGHT

Amy Overstreet Stevens awarded into the National Science Foundation Graduate Research Fellowship Program

Her work addresses relevant health concerns in New Mexico by applying computational techniques to drug design and discovery. Her two primary research projects focus on (1) substance use disorders and (2) Type 2 Diabetes Mellitus (T2DM). Her work addresses substance use disorders by exploring the PICK1 protein. PICK1 is one of the key regulators in biological cycles related to substance use disorders. She has applied molecular dynamics simulations to explore the biological dimer of PICK1, the dynamic allosterism of the PICK1 PDZ domain, and the interactions between PICK1 and the lipid membrane. Her work is providing missing 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. Additionally, Amy is addressing the burden of T2DM through protein design of nanobodies. Previous work has isolated monoclonal antibodies that have efficacy in altering the function of GluT4, a key protein involved in T2DM. Nanobodies have been identified as functional forms of antibodies with advantages in design and permeability due to their smaller size. She is designing nanobodies to target GluT4 and alter its function to enable the uptake of glucose into the cell. Amy is first author of five manuscripts (one published, one submitted, and three in-progress) and a supporting author of three manuscripts (one published, one submitted, and one in-progress).

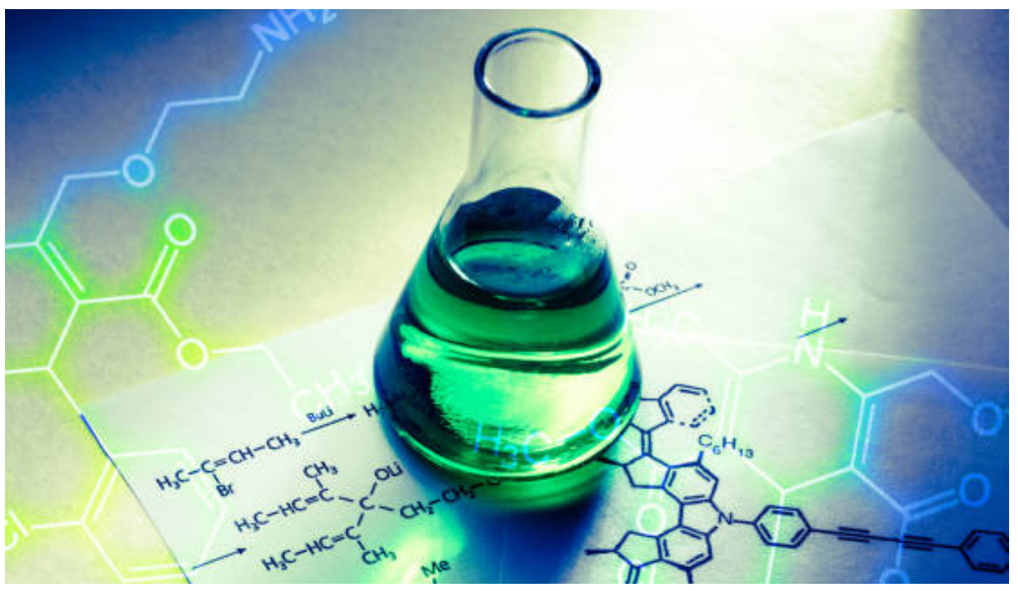
DEPARTMENT NEWS

Department of Chemisty and Chemical Biology begin hiring search for three Assistant Professors

The Department of Chemistry & Chemical Biology at the University of New Mexico invites applications for three openings at the Assistant Professor level to begin in August 2022. These are full-time, tenure track positions in experimental organic chemistry, broadly defined. Areas of particular interest include synthesis/catalysis, bioorganic/medicinal, chemistry, soft materials, and organic semiconductors.

To learn more, visit the job posting, **here.**

JOBS



DEPARTMENT NEWS

Elements of Success - COMING SOON!

For many years, those interested in supporting the success of Chemistry students were able to make a donation to "buy" a periodic element plaque as part of the Elements of Success campaign. The donor had honored individuals with an engraved plaque which was displayed on the wall for all to see.

Unfortunately, during the renovation, the original display was unable to be saved. However, as we settle into the newness of the Clark Hall facilities, we want to ensure that those who have supported us along the way are remembered with a plaque listing the names of all previous donors and honored individuals. That being said, it is important that we adapt and find a way to amalgamate new and old, and a beautifully designed display will be an exciting addition.

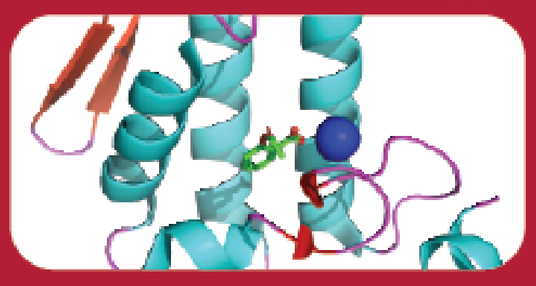
We know one thing for sure - the greater UNM community has made it clear that they want have new opportunities to leaving a lasting legacy, and they want to support the students at UNM. Coming soon, a newly re-vamped Elements of Success campaign will be launched with multiple giving levels for donors to participate! The details and design are still being determined, but the goal is clear – these funds will be used to benefit our students.

If you are interested in making a donation to the Elements of Success that will directly benefit the students in the Department of Chemistry and Chemical Biology, please visit https://www.unmfund.org/fund/elements-of-success-foundation/, and keep an eye out for more information on the campaign.

PhD and MS Graduate Programs in Chemistry and Chemical Biology

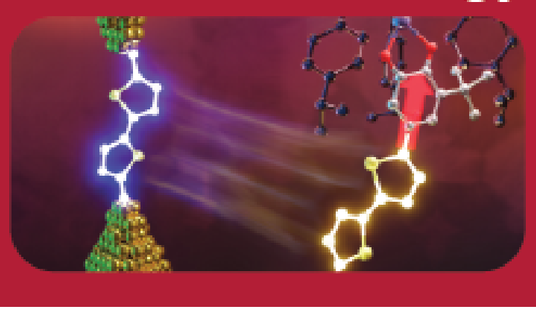
Research Opportunities

Chemical Biology



Computational Chemistry

Materials & Energy



Why Choose UNM?

- New Mexico's Flagship University
- State-of-the-Art Facilities
- Research funded by the NSF, NIH, DOE, DOD and more
- Competetive Financial Support
- Tackle Global Challenged with:
  - Los Alamos National Laboratory
  - Sandia National Laboratory
  - Air Force Research Laboratory

Visit chemistry.unm.edu for more information

Application Deadline
1/15/2022

DEPARTMENT NEWS

ROSE Scholar Program

The Research Opportunities for Science Educators (ROSE) Program kicked off its inaugural summer program for high school science teachers in June 2021. Eight ROSE Scholars from across the state (Roswell, Cuba, Farmington, Las Cruces, and Albuquerque) participated in a 4-week immersive research program on the UNM Albuquerque campus, hosted by principal investigators in the Department of Chemistry and Chemical Biology. The Program was co-organized by Prof. Steve Cabaniss, Prof. Jeff Rack, and Prof. Susan Atlas, with financial and administrative support from the Department of Chemistry and Chemical Biology (Prof. Jeremy Edwards, Chair); the Office of the Vice President for Research; the NM Public Education Department; and Program assessment by Prof. Abigail Stewart, University of Michigan. Objectives of the program included enabling teachers to refresh their knowledge and develop new skills, while gaining a better understanding of, appreciation for, and inspiration from current scientific research, and establishing authentic relationships between UNM faculty and science educators in local and regional communities, including inspiring high school students to apply to UNM for undergraduate studies.

Five CCB labs participated in the Program, providing diverse, state-of-the-art research opportunities to the Scholars: “Synthetic peptide libraries for accelerated drug discovery” (Prof. Brian Gold); “Revealing the activation mechanisms of a critical protein involved in substance use disorders” (Prof. Yi He); “New approaches to antibiotic discovery” (Prof. Mark Walker); “Development of photoactive materials” (Prof. Jeff Rack); and “Modeling the effect of amino acid mutations on the SARS-CoV-2 spike protein; Machine Learning modeling of the atom-in-molecule” (Prof. Susan Atlas). The Program received enthusiastic reviews from both Scholars and participating faculty, and an expansion to 25 Scholars and additional chemistry research laboratories is planned for Summer 2022.

DEPARTMENT NEWS

Clark Hall Open House Highlights Gratitude and Forward Thinking

After a year and a half of moving out of workspaces, working remotely, demolition, rebuild, and the return to campus, the Department of Chemistry and Chemical Biology was thrilled to celebrate the completion of the Clark Hall Renovations by hosting an Open House and Ribbon cutting. Guests from the University of New Mexico community were invited to join in the festivities, enjoy light refreshments, and take guided tours the totally renovated facility and laboratories on November 5, 2021.

The program, hosted in the beautiful new open space and lobby, included remarks from Chair Jeremy Edwards, Provost James Holloway, Interim College of Arts and Sciences Dean Arash Mafi, and Professor Stephen Cabaniss. As they spoke, themes of gratitude and forward thinking were veined throughout.

They celebrated the successes and achievements of our faculty, and expressed gratitude for not only the tremendous efforts of all of those who made the renovation successful, but also to the voters who chose to approve of these renovations, for those who believe in the power of science, to those who know that scientific advancement and interdisciplinary collaboration are a necessary path for future successes. Following the ceremony, Professor Edwards had the honor of cutting the ceremonial ribbon and officially kick off refreshments and tours.

We would like to thank the Project Team for their Herculean efforts, those who facilitated the tours, and everyone who attended the Open House for your continued support of the Department of Chemistry and Chemical Biology.