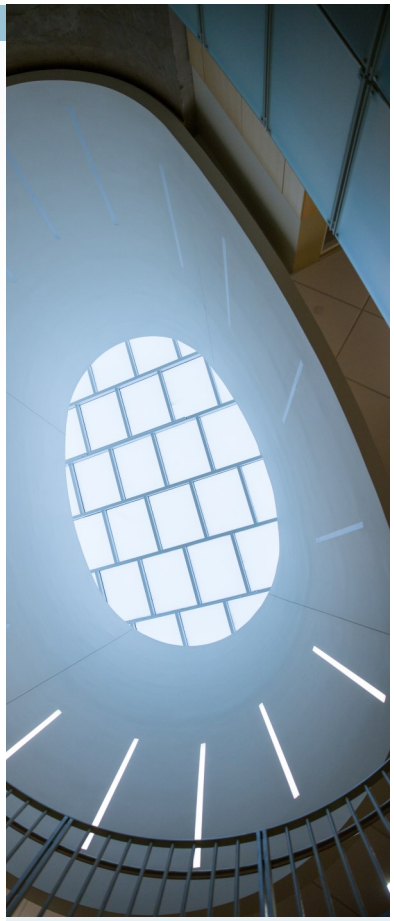
Spring 2023

Department of Chemistry NEWSLETTER



Faculty Focus: Huiyuan Zhu

Huiyuan Zhu, Ph.D. started with UVA Chemistry in August of 2022 as an Assistant Professor coming from Virginia Tech where she was an Assistant Professor in Chemical Engineering since 2018. In June of 2023, she was promoted to Associate Professor without term. Her arrival on grounds has been followed by several big announcements. In February-2023, it was announced that she had been named a 2023 Sloan Research Fellow. Her award became the third year in a row where the Alfred P. Sloan Foundation chose a fellow from UVA Chemistry. On August 25, 2022, as part of an announcement by Department of Energy Secretary Jennifer Granholm, UVA Chemistry was awarded a clean energy technology grant of which Prof. Zhu is a major collaborator (See "DOE Grant" pg.10).

Huiyuan Zhu, Ph.D.

Her research aims to develop new synthetic strategies for well-defined nanocrystals and 2-dimensional (2D) materials with atomically precise surfaces and interfaces that can lead to a fundamental understanding of how atomic structure affects catalyst performance and to use this new knowledge to design optimized catalysts for critical energy conversion and chemical transformation processes. Her research specifically focuses on electrochemi-

Continued on page 2

Donald F. Hunt Retirement

Donald F. Hunt, Ph.D.

On January 2, 2023, Donald F. Hunt retired from the University of Virginia after 55 years of service. In September of 1968, Donald F. Hunt began what would become an impressive career that spanned five decades at the University of Virginia. During this time, Prof. Hunt, a University Professor since 1993, published 425 articles in peer-reviewed journals accumulating nearly 63,000 citations. Since 2003, articles coming out of the Hunt Lab accumulated over 1,500 citations per year. Prof. Hunt mentored over 130 graduate students and postdocs and was honored by his mentees with the creation of the endowed Donald F. Hunt Graduate and Postdoctoral Fellowship in Chemistry. Prior to coming to UVA, he spent a year at the Massachusetts Institute of Technology as a National Institute of Health Postdoctoral Trainee in Mass Spectrometry under the guidance of Professor Klaus Biemann. Professor Hunt obtained both his B.S. and Ph. D. (1967) degrees from the University of Massachusetts. Research for the doctoral dissertation was carried out under the direction of Professors Marvin Rausch and Peter Lillya in the area of organotransition metal chemistry. Professor Hunt was chosen as a recipient of both an NIH Fogarty Senior International Fellowship and a John Simon Guggenheim Fellowship in 1981-82. In 1990, he received the Charles H. Stone Award sponsored by the American Chemical Society. In 1992 he was named Virginia's Outstanding Scientist and also received the Pehr Edman Award for outstanding achievements in the application of mass spectrometry to the contemporary microsequence analysis of proteins. The Distinguished Contribution Award from the American Society for Mass Spectrometry was presented to Dr. Hunt in 1994 for his development of electron-capture, negative-ion mass spectrometry. In 1996 he was the first recipient of the Christian B. Anfinsen Award from the Pro-

Continued on page 3

Inside this issue

Newsletter Staff

Jill Venton, Department Chair and Publisher

Seth Matula, Department Business Administrator , Editor and Contributor

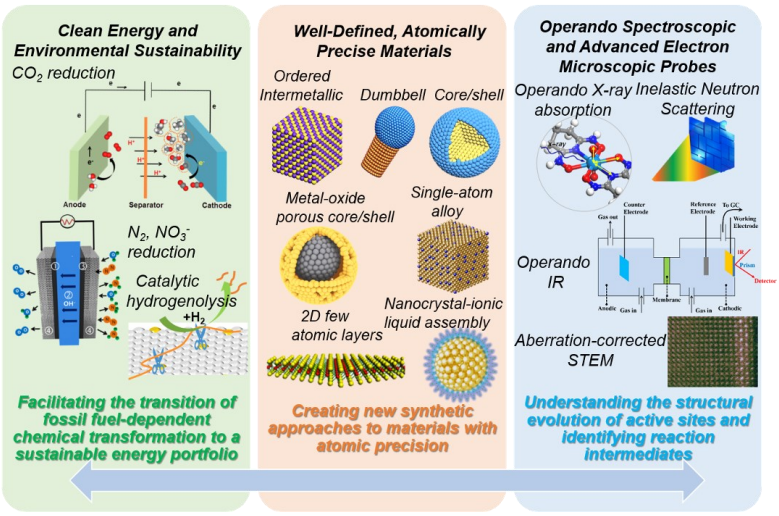
Delaney Hammond, Undergraduate Student and Contributor

Faculty Focus: Huiyuan Zhu *Continued*

cal CO2 conversion, sustainable nitrogen cycling, and heterogeneous thermocatalytic reactions (e.g., acetylene semi-hydrogenation). Three questions fundamental to catalysis are to be addressed: (1) What are the catalytic active sites and how do they evolve under reaction conditions? (2) How to steer the reaction pathway toward desirable products via modulating active sites and their environments? (3) How to circumvent or ultimately, go beyond adsorption-energy scaling relations?

Prior to 2018, she was on the research staff in the Nanomaterials Chemistry Group at the Oak Ridge National Laboratory in Oak Ridge, TN on a Liane B. Russell Fellowship. In 2020, she was awarded a Doctoral New Investigator Award from the ACS Petroleum Research Foundation, an Emerging Investigator from the Journal of Materials Chemistry, the ORAU Ralph E. Powe Junior Faculty Enhancement Award, and a Jeffress Trust Award. In 2022 she was awarded a CAREER award from the National Science Foundation. Prof. Zhu says, "Sustainable production of chemicals and fuels underpins the future. The rational design of catalysts is a key enabler."

Professor Zhu earned her B.Sc. in Chemistry from the University of Science and Technology China in 2009 and her Ph.D. in Chemistry from Brown University in 2014.



Chair's Letter by Jill Venton

It's been quite a year in the halls of Chemistry at University of Virginia. With the university and society back to business after the pandemic, our classes and labs are running at full capacity, and it is exciting to see so much in person teaching and research. We also have hosted events to showcase our department. In August, Jennifer Granholm, US Secretary of Energy visited the department to announce new energy centers in sustainability and renewable energy. We were pleased that UVA was awarded a new center with lead investigator Prof. Sen Zhang, and co-investigators Profs. Brent Gunnoe, Charles Machan, and Huiyuan Zhu. Secretary Granholm, DOE Director of Science Dr. Asmeret Asefaw Berhe, and UVA President Jim Ryan toured several laboratories, and graduate students and faculty gave short presentations on their research.

In October, we welcomed 80 alumni back to the chemistry department after a $100 million dollar renovation project. Alumni toured labs, attended poster sessions, and networked with students in the afternoon of the event. Alumnus John Butler, a specialist in DNA analysis from NIST, gave a plenary Graham lecture. Then students, faculty, and alumni enjoyed dinner in our new student common areas. The newly renovated chemistry building contains new active learning classroom, updated chemistry teaching labs, new staircases for connectivity, and utility upgrades. The new classrooms facilitate a move to active learning, and chemistry is a leader in two new grants from the Howard

Continued on page 4

Department Faculty Leadership

B. Jill Venton
Department Chair

Charlie Grisham
Associate Chair

T. Brent Gunnoe
Graduate Prgms. Dir.

Laura Serbulea
Undergrad Prgms. Dir.

Rebecca Pompano
DEI Director

Donald F. Hunt Retirement *Continued*

tein Society for development of new technology in the field of protein chemistry. He received the Chemical Instrumentation Award sponsored by the American Chemical Society in 1997. This award recognizes Professor Hunt for development of instrumentation capable of sequencing peptides and proteins at the attomole level. In 2000, Professor Hunt was the recipient of both the Frank F. Field and Joe L. Franklin award presented by the American Chemical Society for outstanding achievement in the field of mass spectrometry and the Thomson Medal from the International Mass Spectrometry Society. He received Distinguished Accomplishment Awards from the Human Proteome Organization (HUPO) in 2006 and the Association of Biomolecular Resource Facilities in 2007. In 2010, Professor Hunt received the University of Virginia's Distinguished Scientist Award. He received the 2017 American Chemical Society (ACS) Award in Analytical Chemistry, for his 'pioneering efforts to develop mass spectrometry methods and instrumentation that facilitated characterization of peptides and proteins and provided the foundation for the field of proteomics'. In 2014, he was elected as a member of the American Academy of Arts and Sciences. Professor Hunt is a co-inventor on more than 30 patents.

New Faculty Hire: Michelle Personick

Michelle Personick, Ph.D.

UVA Chemistry has hired Michelle Personick as an Associate Professor of Chemistry who will begin in the Fall of 2023. Prof. Personick comes to UVA from Wesleyan University in Middletown, CT. In 2009, she received her undergraduate degree from Middlebury College and a Ph.D. in Chemistry from Northwestern University in 2013. From 2013 to 2015, she was a postdoctoral researcher at Harvard University and a member of the Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC) Energy Frontier Research Center, where she studied selective oxidative transformations of alcohols on nanoporous gold alloy catalysts. Personick joined the chemistry faculty at Wesleyan in July 2015. In 2016, she was awarded the Victor K. LaMer Award from the American Chemical Society (ACS) Division of Colloid and Surface Chemistry in recognition of her research.
The Personick Group is advancing the state of the art in the synthesis of precise nanomaterials and is using these precision materials to define catalytic structure-function relationships at an elevated level of mechanistic detail. Prof. Personick says, "I'm excited to contribute to the highly collaborative research environment at UVA. Addressing important challenges in sustainable energy and catalysis requires combining approaches and ideas from a variety of research fields—both within and outside of chemistry. I was drawn by UVA's commitment to supporting the growth of fundamental, interdisciplinary research efforts in this area, as well as by the collegiality of the Chemistry Department and the dedication of the faculty to mentoring and student development."

Chair's Letter *Continued*

Hughes Medical Institute (HHMI) to promote achievement by all students and rethink how we teach large classes.
As you will read in this newsletter, UVA Chemistry is growing and we welcomed a new faculty member, Huiyuan Zhu to the faculty this fall. We also said goodbye to Professor Don Hunt, who retired from the university after over 50 years of service. The department is currently searching for 3 new faculty members and so we hope to continue building the faculty in years to come.
Our students are also achieving. You will read a feature on graduating 4th year Biochemistry major Celeste Costa. Our undergraduate students continue to earn external awards and achieve well on exams, including the ASBMB (American Society for Biochemistry and Molecular Biology) exam, where we had over 84% of students pass, well above the national average of 42%. Our graduate students have also earned prestigious fellowships, including DOE, NSF, and Jefferson Scholars Foundation scholarships.
Overall, it is a great time to be a chemist at the University of Virginia. We hope you enjoy these highlights about our faculty, students, and staff. Please keep in touch and consider giving a gift to the department to continue our mission to perform novel chemical research while training the next generation of chemical scientists.

Graduate Student Awards

Marc Bennett – Double Hoo Award
Frederik Brondsted – Jefferson Scholars Foundation Dissertation Year Fellowship
Josh Carder – 2023 UVA Chemistry Graduate Teaching Award
Drew Christiansen – NASA FINESST Fellowship
Emma Cook – Jefferson Scholars Foundation Dissertation Year Fellowship
Emma Cook – 2023 UVA Chemistry Adam Ritchie Outstanding Graduate Student Award
Emma Cook – ACS Division of Inorganic Chemistry Young Investigator Award
Megan Ericson – Double Hoo Award
Perrin Godbold – ACS CATL ChemCatBio Travel Award
Abigail Graham – 1st Place 2023 UVA Grad Thesis Slam
Ryan Hamblin – NGFP Fellowship
Olivia Murtagh—3rd Year Poster Award
Hannah Musgrove – 2023 UVA Chemistry Sidney Hecht Fellowship
Renna Nouwairi – 2023 Chemistry UVA Donald F. Hunt Graduate Fellowship
Renna Nouwairi – Best Oral Presentation, International Society of Forensic Genetics
Karl Ocius – 3rd Year Poster Award
Djuro Raskovic – 2023 UVA All-University Graduate Teaching Award
Djuro Raskovic – 2023 UVA Chemistry Graduate Teaching Award
Amelia Reid – Best Poster Award, International Conference on Carbon Dioxide Utilization
Brielle Shope – Virginia Space Grant Consortium Fellowship
Kamil Stelmach—NASA FINESST Fellowship
Kamil Stelmach – LaGrange Award
Bi Youan Tra – 3rd Year Poster Award
Rachelle Turiello – 3rd Place 2023 UVA Grad Thesis Slam
Rachelle Turiello – Audience Choice Award 2023 UVA Grad Thesis Slam
Rachelle Turiello – ARCS Endowment Award in Chemistry
Haley Scolati – NRAO Graduate Research Assistantship

Department of Chemistry
University of Virginia

Chemistry Strives Towards Inclusivity with the Driving Change Initiative

With a newly awarded grant from HHMI, the Chemistry Department hopes to reimagine how STEM classes are taught

This year, the UVA Chemistry Department has made important strides towards a more inclusive academic space. Last semester, the Howard Hughes Medical Institute (HHMI) awarded the University with a $2.5 million grant as part of its Driving Change Initiative.

Linda Columbus, Ph.D.

The initiative, which provided awards for six universities last fall, seeks to promote inclusion in the science, technology, engineering, and math (STEM) fields. Universities across the nation submitted proposals for the grant, detailing their plans for implementing programs that promote success among historically excluded groups.

Chemistry Professor Linda Columbus is the faculty director for Driving Change in the College if Arts & Sciences and was involved in formulating the departmental development of UVA's proposal to HHMI.

"Our goal is to drive genuine and lasting culture change so that undergraduate students from all backgrounds, particularly those who belong to historically excluded groups, will excel in STEM," Columbus said.

Thirty-eight finalists are chosen by HHMI to form the "Driving Change Learning Community,"

Continued on page 5

Undergraduates Receive ACS Scholars Program Awards

Alysha Johnson (l) and Jordan Baker (r)

Chemistry students Alysha Johnson and Jordan Baker have received awards from the ACS Scholars Program. The American Chemical Society, or ACS, provides renewable scholarships to students belonging to historically underrepresented groups. They provide awards to over 300 students annually, and have awarded over 3,500 students to date. By receiving ACS Scholars Program Awards, Johnson and Baker not only receive financial support, but are also welcomed into a large community of other accomplished chemistry students from underrepresented backgrounds.

Alysha Johnson is a first year undergraduate student from Suffolk, Virginia. Her research interest is in pharmacokinetics and pharmacodynamics, and she hopes to later pursue a career in pharmaceutical development or economic toxicology. Johnson said that she is excited to be a part of the ACS Scholars Program because it will allow her to connect with other Black chemistry students. "It is very hard to come by Black chemists, specifically women, especially in academic environments," Johnson said. "Most schools and institutions do not have a single Black woman researcher— so being connected to them through ACS gives me people I can share experiences with, both academically and personally."

Jordan Baker is a fourth year student who is interested in the intersection between chemistry, archaeology, and materials science. Baker said that being recognized by the ACS and connecting with other scholars in the program was encouraging. "When I first learned about the ACS scholars program, I had just joined my first research lab and was entering a new phase of my academic career," Baker said. "My acceptance into the ACS scholars program showed me that my hardwork in chemistry is paying off and there are people rooting for underrepresented groups in science." In the future, Baker hopes to become an analytical chemist to interpret recovered artifacts on archaeological sites.

Both Johnson and Baker have undoubtedly bright futures ahead of them. The ACS Scholars Program will help them advance in their pursuits no matter what path they choose. Congratulations to Alysha and Jordan on this fantastic achievement.

Driving Change Initiative *continued*

which meets every few months to discuss how to combat inequality in STEM programs. Driving Change hopes to "create a community whose members will support one another as we work to create inclusive environments, support student success, and recognize the institutional practices that are barriers to inclusion."

The universities in the learning community then submitted proposals for the grant, in which they express a commitment to implementing inclusive programs. Finally, HHMI chose six finalists that "made strong arguments for their readiness to embark on this change journey with experiments that held the best promise of helping the whole community."

"The HHMI proposal, with support from the Dean's and Provost's offices, provides financial compensation for time committed to develop, assess, sustain, and implement ideas departments propose to address the challenges they identify," Professor Columbus explained.

In order to foster inclusivity, the University's initiative focuses on two elements: student support and reimagined undergraduate programming. Over a two-year period, University staff and faculty, conducted a self-study to identify areas of improvement in the STEM Departments, then used the results to craft the proposal.

"We have outlined a journey for departments to study their programming and course work to identify and prioritize goals to improve student success in STEM," Columbus said. "We have experts in data collection and analysis, curricular design, effective teaching practices, and organizational efficacy to help departments reimagine their courses, major, and student journey through their program."

In addition to the grant from HHMI, contributions provided by the University, the College of Arts and Sciences, and the School of Engineering bring the total funding of the initiative to $7.7 million.

What made UVA's Driving Change proposal stand out was its focus on making change within departments, rather than through external units.

"Instead, the resources from these support units are brought to the departments and adapt to what the faculty need in terms of expertise, development, and process," Columbus said. "In addition, our proposal has the departments weighing in and shaping the process and journey the departments embark on."

To make the world a more equitable place, academic institutions must implement solutions to enact change at the college level. The Driving Change Initiative will allow UVA Chemistry to lay the foundation for a more inclusive world in the STEM fields and beyond.

Faculty Focus: Laura Serbulea

Professor Laura Serbulea serves UVA Chemistry as the Director of Undergraduate Programs and teaches organic chemistry courses, which include the accelerated organic chemistry lectures and laboratories. She earned her undergraduate degree at the University of Bucharest, Romania, and received her Ph.D. in Chemistry from University of California, Los Angeles. She joined the faculty at the University of Virginia in 2012.

In 2020, she was selected to serve for three years (2021-2023) as a College Mentor for the ACS sponsored Study Camp hosting the top 20 students from the U.S. National Chemistry Olympiad, in preparation for the International Chemistry Olympiad (IChO). At the 2022 Study Camp, which was hosted in-person by the University of Maryland College Park, she has conducted problem solving sessions on advanced topics in organic chemistry and have worked with the students in the laboratory and contributed to writing, administration and grading of theoretical and laboratory exams for the selection of the four students (and two alternates) to represent team USA at IChO. As a representative of USA at IChO, she has served on the International Jury and participated in the arbitration of theoretical exam scores.

Laura Serbulea, Ph.D.

2023 Undergraduate Student Awards

Rohan Parikh – Oscar R. Rodig Alpha Chi Sigma Chemistry Award

Nina Jannatifar – ACS Student Chapter Award

Brigitte Meyer – Hugh Miller Spencer Scholarship Award

Abhishek Bazaz – Hugh Miller Spencer Scholarship Award

Olivia Hathaway – Department of Chemistry Service & Community Award

Sarah Newkirk – Carl O. Trindle Award for Excellence in Chemistry

Catherine Delcommenne – Frederick S. Richardson Award for Excellence in Chemistry

Claire Piczak – Robert G. Bryant Award for Excellence in Chemistry

Matthew Wilcox – Chemistry Departmental Award for Excellence

Kristina Prioleau – Chemistry Departmental Award for Excellence for a Transfer Student

Rohan Parikh – Francis Carey Undergraduate Teaching Award

Shreya Vundela – Robert Bryan Undergraduate Teaching Award

Cole Faggert – Robert Burnett Undergraduate Teaching Award

Celeste Costa – Richard J. Sundberg Undergraduate Teaching Award

Sam Hanser – Chemistry Departmental Undergraduate Teaching Award

Andrew DiSanto – Chemistry Departmental Undergraduate Teaching Award

Patrick Scolese – Chemistry Departmental Undergraduate Teaching Award

Kamil Stelmach and Drew Christianson Awarded NASA FINESST Fellowships

The FINESST (Future Investigators in NASA Earth and Space Science and Technology) award is a training grant provided by NASA to fund graduate students to design and lead their own research projects. The awardees are called future investigators (FIs) to emphasize their role as future leaders in Earth and space science. Proposals are evaluated on scientific merit, relevance to NASA's goals, research readiness of the applicant, and cost reasonableness. There are five divisions one can apply to (astrophysics; earth science; planetary science; heliophysics; and biological and physical sciences).

Kamil Stelmach

Kamil Stelmach's funded work uses crystalline quartz as a model chiral surface for testing the enantioselectivity of that surface for amino acid enantiomers through preferential sublimation. The heating process would be monitored using an X-ray photoelectron spectrometer, which allows him to track the decrease of the amino acid enantiomer. One enantiomer is predicted to sublimate before the other due to a small difference in adsorption energies between the enantiomers. Separate angle-resolved X-ray photoelectron experiments will allow us to test how the amino acid enantiomers bind to the surface. Experimental data will be compared with density functional theory calculations utilizing periodic boundary conditions conducted through the Vienna ab initio Simulation Package (VASP). VASP has the capability of both predicting the adsorption energy differences and informing on the preferred binding sites of the amino acid enantiomers. The award pays for stipend, tuition, health insurance, and some experiment time to utilize the X-ray

Continued on page 7

"The awardees are called future investigators to emphasize their role as future leaders in Earth and space science."

Department Staff

Seth Matula, Business Administrator
Cecelia Cropley, Scientific Program Administrator
Cindy Knight, Undergrad Prgms. Coord. & Asst. to Chair
Sage Bradburn, Grad. Prgms. Coord.
Victoria Beamer, Finance Specialist
Cameron Hawley, Storeroom Manger
Amy Adams, Inventory Line Lead
David Johnson, Inventory Line Lead
Ed de Bary, Infrastructure Manager
Jerry Shiflett, Service Technician
Jarrad Reiner, Computing Services
Chuck Arrington, Org. Chem. Lab Coord.
Jan Dean-Clemmer, Gen. Chem Lab Coord.
Carol Price, Biochem. Lab Coord.
Earl Ashcraft, Instrument Technician

Undergrad Spotlight: Celeste Costa

Celeste Costa is a fourth-year undergraduate student studying chemistry with a concentration in biochemistry. Costa is heavily involved in the department. She was previously a member of the Yan Lab in the School of Medicine at UVA, a group that studied metabolomics.

For the past year, she has served as a Teaching Assistant for Professor Charles Grisham. She has also assisted Grisham with his teaching project PSAFE, or Protein Structure and Function Exploration. In the past year, Costa has been remodeling the PSAFE website, as well as building a Cengage course for the project so that it may be shared with other Universities.

Celeste Costa

Costa shared that she has been passionate about chemistry since she first began studying the subject in high school. "I just really enjoyed it," Costa said. "It was challenging, but I got it. Junior year, I took AP Chemistry — I still loved it and did well… and then I got here, and I stuck with it."

This passion only grew when she joined the UVA Chemistry Department. When she got to the University, Costa had not planned on studying biochemistry. However, after taking Professor Landers's Biochemistry II course, she realized the concentration was for her.

"It was just such a phenomenal class. It was so interesting," Costa said. "The way he taught it had a very clinical perspective. And I was like, that's it — this is what I'm doing."

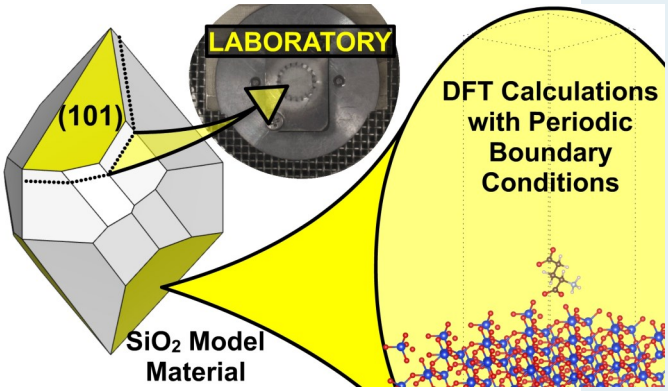
Costa also cited her biochemistry lab class as a highlight of her experiences as a Chemistry major.

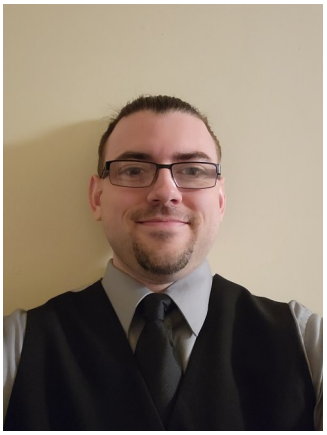
"I wish all chemistry majors had to take it," she said. "It's just a fantastic course — it teaches so much that you can actually use in a lab. I wish we [could take] it earlier."

Costa's hard work and commitment to the Chemistry Department will surely be missed after she graduates this Spring. After graduation, she plans on taking a gap year in Charlottesville and working in either a hospital or a research lab. Following that, Costa hopes to attend medical school.

NASA FINESST Fellowships *Continued*

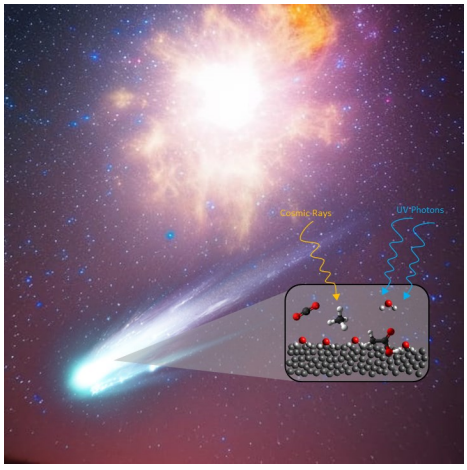
photoelectron spectrometer at the Nanoscale Materials Characterization Facility (NMCF) at UVA. Stelmach says," I hope to continue working on space-related research in the future and maybe tie in a practical aspect to it as well by studying potentially commercializable reactions that could occur in the vacuum of space. Blue Origin recently demonstrated that they could synthesize solar cells from lunar regolith analogs, and I think the market for useful space chemistry will only continue to grow in the coming years."





Drew Christianson

Drew Christianson's work is being funded over a two-year period. Comets are balls of ice and dust formed in the early solar system and preserve much of their initial content in the cold outer reaches of the solar system up to the modern day. Still, even out in the Kuiper Belt and Oort Cloud, chemistry still proceeds within the ices over its several billion-year lifespan. Rare highly energetic events such as nearby supernovae and close passes of hot stars can affect the chemistry in the cometary nuclei as well. This project aims to find what impacts these extrasolar energetic events have on the ice composition of comets and how impactful each event or a series of such events would have on cometary nuclei. Further, the project will also determine the impacts such events have on modern comets in their active phases as well as any implications such events might have for early comets and the origins of life on earth. The award pays for stipend, tuition, fees, health insurance, and travel. Christianson says, "The NASA fellowship gave me the opportunity to further my research on comets here at UVA. After graduating, I intend to continue doing computational astrochemistry, though I also have an interest in branching out to other astrochemical fields as well."



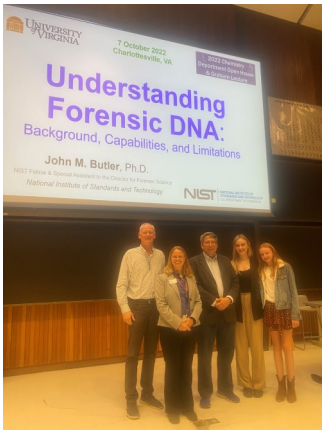
Comets are continuously being bombarded with ultraviolet (UV) photons and cosmic rays. Cosmic rays are highly energetic particles, usually protons, traveling at relativistic speeds, originating from outside the solar system. Other lower energy protons may also originate from the Sun. UV photons can originate from both galactic sources as well as solar. All of these events allow chemical reactions to occur within the bulk ice on the comet and on the surface. Sublimation of ice species into the gas phase is included as well. Nearby highly energetic events such as a passing hot star or a local supernova enhance these factors which may result in different chemistry and chemical abundances during its long lifetime.

Department of Chemistry

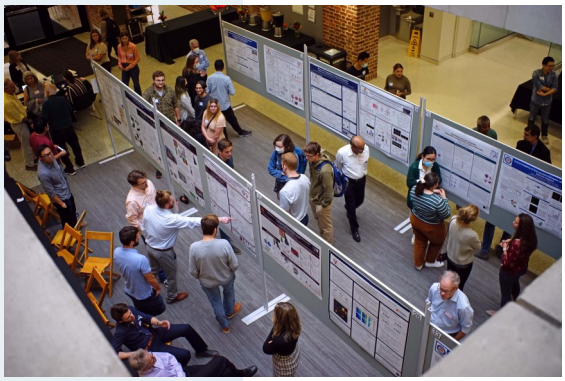
University of Virginia

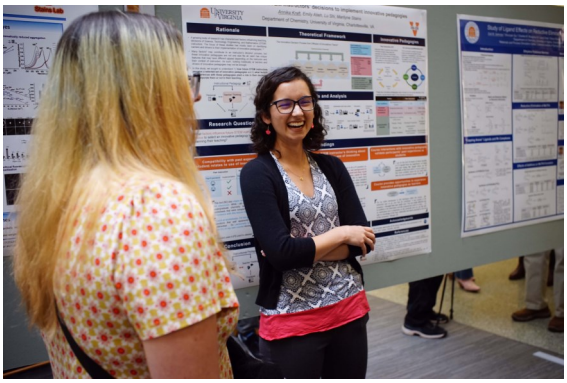
Open House and Graham Lecture

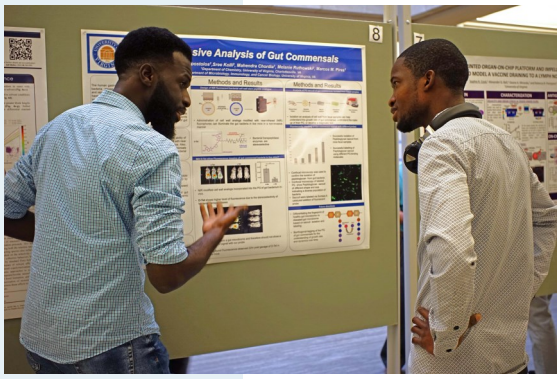
On October 7, 2022 the UVA Chemistry Department held an Open House for students, faculty, alumni, and friends of the Department to show off the recently completed $100M renovations of the main chemistry building. The open house included tours and poster sessions from both graduate and undergraduate students.
The night was topped off with the annual Marie Payne Graham Lecture. The invited speaker was Dr. John M. Butler who is a Fellow and Special Assistant to the Director of Forensic Science at the National Institute of Standards and Technology. In addition to faculty, students and alumni, the Graham Lecture was attended by family of Mary Graham Payne.



Photos below of the activities by Jacque Moon Yee







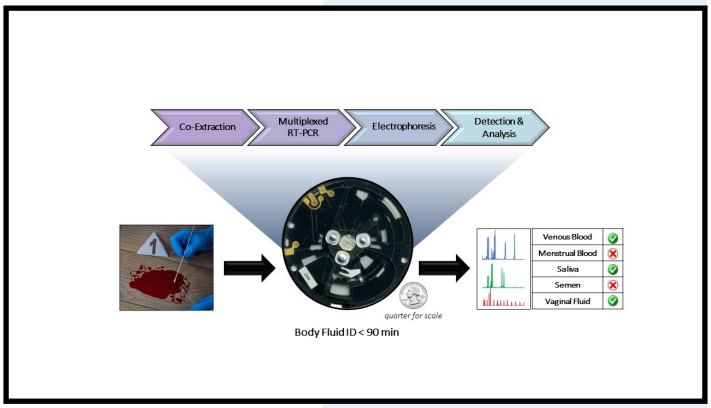
The Chemistry Department would like to thank the family of Marie Graham Payne for their continued support of this lecture.

Department of Chemistry
University of Virginia

Grad Student Profile: Renna Nouwairi

UVA Chemistry graduate student Renna Nouwairi of the Landers Group was awarded a 2023 Jefferson Scholars Foundation Dissertation Year Fellowship which will allow her to continue her work towards her Ph.D. in the area of microfluidics. Her research projects all have the goal of optimizing standard, commercialized assays for translation into portable, automated, sample in—answer out microfluidic systems with the potential for commercialization and real-world implementation. One main project aims to integrate mRNA extraction, amplification, and electrophoretic separation on a microfluidic disc and develop a fully-enclosed mechatronic system that automates all on-disc processes to perform body fluid identification in under 1 hour at a crime scene, as opposed to 10+ hours in a lab. Another primary project focuses on optimizing a microfluidic amplification instrument to perform sub-15 min real-time analysis of nucleic acids with comparable sensitivity and specificity to gold standard instrumentation, which traditionally consumes multiple hours. Furthermore, she will expand the capacity of the system to perform high resolution melting for epigenetic analysis. James Landers says of Nouwairi, "Renna's ability to think critically, be productive experimentally, and lead while being part of a team, are testimony to her deserving a Jefferson Dissertation Year Fellowship. She has redefined microchip electrophoresis for us, while leading the NIJ body fluid project with collaborators in New Zealand. Her creativity will serve her well in whatever career she chooses to pursue."

Renna Nouwairi



The figure illustrates the steps for body fluid identification that we are integrating onto a microfluidic disc that will be operated by an automated instrument so the user can simply add a swab containing an unknown fluid to the disc, place the disc in the instrument, press start, and return in 90 mins to have present fluids identified.

"She has redefined microchip electrophoresis for us" - James Landers

Grad Student Profile: Kelly Dunham

Kelly Dunham is a Ph.D. candidate in the Venton Group. She was recently awarded a Jefferson Fellowship for 2022-23. This fellowship funds a dissertation year and one post-doctoral year where she will continue research in the Venton lab and also teach an Empirical Engagements course to 1st year undergraduate students. The course is entitled "Can a pill make you happy?" and will dive into the history of antidepressant research, as well as discussions on controversial new micro-dosing scheduled drug therapies and the roles of antidepressants in current society. Students will get the opportunity to learn recent scientific advancements and ask questions like a scientist. She was also given a research fund to buy equipment and software to finish her dissertation work and design her course. This fund also pays for travel/fees for conferences.

Dunham says, "I'm very honored that this grant will allow me to stay an additional year at UVA to work in my lab and continue my research measuring serotonin and investigating different antidepressant and genetic effects in fruit flies. I am excited to get the opportunity to design and teach my dream course to undergraduate students, and this award will afford me invaluable experiences to teach and mentor new students about chemistry and neuroscience, and also hopefully spark interest in chemistry and advertise the great work we do in the Chemistry department to new students."

Carbon fiber microelectrode placement in fruit fly larva ventral nerve cord to measure serotonin with fast-scan cyclic voltammetry (FSCV)

Kelly Dunham

UVA Receives $3.7M DOE Grant

From left: Charlie Machan, UVA President Jim Ryan, Brent Gunnoe, Sen Zhang, ang Huiyuan Zhu

In August of 2022, the Chemistry Department learned that a $3.7 million grant from the Department of Energy was being awarded to Associate Professor Sen Zhang as the principal investigator and UVA Chemistry faculty co-investigators Brent Gunnoe, Charles Machan and Huiyuan Zhu. Other co-investigators include Jingguang G. Chen from Columbia University, William A. Goddard III from the California Institute of Technology, and Yushan Yan of the University of Delaware.

The grant is titled, *"Fundamental Studies of Catalytic Sites and Catalyst/Membrane Integrations for Advanced Hydroxide Exchange Membrane Electrolyzers"* and is funded for three years. The idea is that hydrogen can become a plentiful and efficient source of energy when produced by using solar energy. The electrolysis process of separating the hydrogen molecules from the oxygen molecule in water is a viable option if the process can be done cheaply. That is the team's goal: to research and develop the process of producing hydrogen in a way that is economical and can be scaled-up and industrialized. The four UVA Chemistry research groups will be developing the molecules used in water splitting reaction (Gunnoe and Machan), and the materials being used as the catalyst in the electrolyzer (Zhang and Zhu). The collaborators outside UVA will play other roles in helping the research to develop a prototype.

Deep decarbonization of the energy sector needs green hydrogen (H_2) from water electrolysis that utilizes electricity from carbon-free sources. H_2 is a clean fuel, and a valuable chemical used in a variety of large-scale industrial processes including the production of ammonia (i.e., fertilizer). Currently, the majority of H_2 is produced from fossil resources, which is responsible for over 900 million tons of carbon dioxide emissions per year. An exciting advance in water electrolysis technologies in recent years is the development of hydroxide exchange membrane electrolysis (HEMEL), which allows the potential use of inexpensive electrocatalysts and low-cost membranes and ionomers. Despite this progress, the cost of H_2 (at ~$5/kg) from state-of-the-art HEMEL is still 5-fold higher than the Department of Energy's target for possible commercial viability. The key limitations that need to be addressed to establish advanced HEMEL for scaled use include: (1) electrocatalysts based on inexpensive metals with limited activity and durability under realistic operating conditions and insufficient atomistic and molecular understanding of catalyst design principles; (2) limited understanding of the complicated interfaces between catalysts, ionomers, and hydroxide exchange membrane that govern membrane electrode assembly (MEA) performance and longevity.

The goal of the proposed research is to develop a deep understanding of how atomic structures and molecular environments of catalytic sites affect catalyst properties and how chemically-tailored catalysts/ionomers/membrane interfaces can be steered toward optimized MEA performance. By leveraging the diverse and complementary expertise of the research team, they will unravel catalyst and interface design principles through a combination of computational and experimental approaches, and understand how to improve MEA performance by ligand-tailoring catalyst/ionomer/membrane interfaces. The new knowledge and experimental/theoretical tools developed in this project will enable the continued design of increasingly efficient and inexpensive catalysts as well as predictive models for water electrolyzers. Professor Zhang says, "We are excited about the

Charles Machan, an associate professor of chemistry, tells Secretary of Energy Jennifer Granholm and Asmeret Asefaw Berhe, the department's director of the Office of Science, about the molecular portion of the research. (Photo by Dan Addison, University Communications)

Department of Chemistry

University of Virginia

Continued on page 11

UVA Receives $3.7M DOE Grant *Continued*

inter-disciplinary and cross-institution collaboration opportunity to address this challenge for future hydrogen economy. The success of this project will contribute to clean H_2 production using electricity produced from carbon-free sources (e.g., solar), potentially transforming the U.S. energy portfolio. It aligns with the Department of Energy's mission of reducing the H_2 production cost using water electrolyzers to $1 per 1 kg in 1 decade."

Storeroom Hires Amy Adams

In February of 2021 Storeroom Manager Cameron Hawley took over from longtime manager Danny Via. Roughly a year and a half later, he was tasked with "restocking" the staffing of the storeroom. The Fall semester of 2022 was a time of change for staffing in the UVA Chemistry Stockroom as Amy Adams started. Cam aligned the two positions to have identical duties in order for a more efficient service model. Training on the new Workday financial system and the iLab software in addition to learning the purchasing, and shipping & receiving needs of customers has kept Amy extremely busy. Amy, a 23-year UVA employee, began in November-2021, coming over from Comparative Medicine. The second position has recently become vacant again and the department has initiated an immediate search.

Amy Adams

"The Chemistry Storeroom team is looking forward to a fantastic 2023 and beyond!" - Cameron Hawley, Storeroom Manager

Staff Spotlight: Sage Bradburn

Sage Bradburn

In June of 2022, Sage Bradburn came to UVA Chemistry as the new Graduate Programs Coordinator, replacing longtime UVA and Chemistry GPC Susie Marshall. Sage came to Chemistry from a similar role in the Economics department where she had been since 2017. Prior to Economics, Sage worked for the UVA Center for Teaching Excellence, the UVA French Department, as a High School and Middle School English teacher, and an English as a Second Language instructor. Sage has a BA in English from the College of William & Mary and a MA in English from the University of Florida.

Department of Chemistry

University of Virginia

University of Virginia
Department of Chemistry

If you would like to make a donation to the Chemistry Department of the University of Virginia please send to:

UVA Fund – Chemistry Department
Account FASCH103
University of Virginia Fund
P.O. Box 400331
Charlottesville, VA 22904

For other giving options please visit:

https://alumni.virginia.edu/uvafund/give-uva-fund-clients/

All gifts for the Chemistry Department need to reference **Account FASCH103**.

Keep In Touch

We love to hear updates from our alumni on your life and career. You can join our alumni group on

LinkedIn: https://www.linkedin.com/company/uva-chemistry

Follow us on Twitter: https://twitter.com/chemistryuva

Or Facebook: https://www.facebook.com/UVAChemistry/

Or send us an update by email to chem@virginia.edu

Also, would you consider a donation to our mission. Donations may be targeted to any program you have read about, but the vast majority of our donations are not targeted and are used to finance our summer undergraduate research fellowships. We appreciate your support of the department!

University of Virginia
Department of Chemistry

McCormick Road
P.O. Box 400319
Charlottesville, VA 22904-4319

Phone: 434-924-3344
E-mail: chem@virginia.edu

PLEASE
PLACE
STAMP
HERE

Mailing Address Line 1
Mailing Address Line 2
Mailing Address Line 3
Mailing Address Line 4
Mailing Address Line 5

Department of Chemistry
UNIVERSITY of VIRGINIA