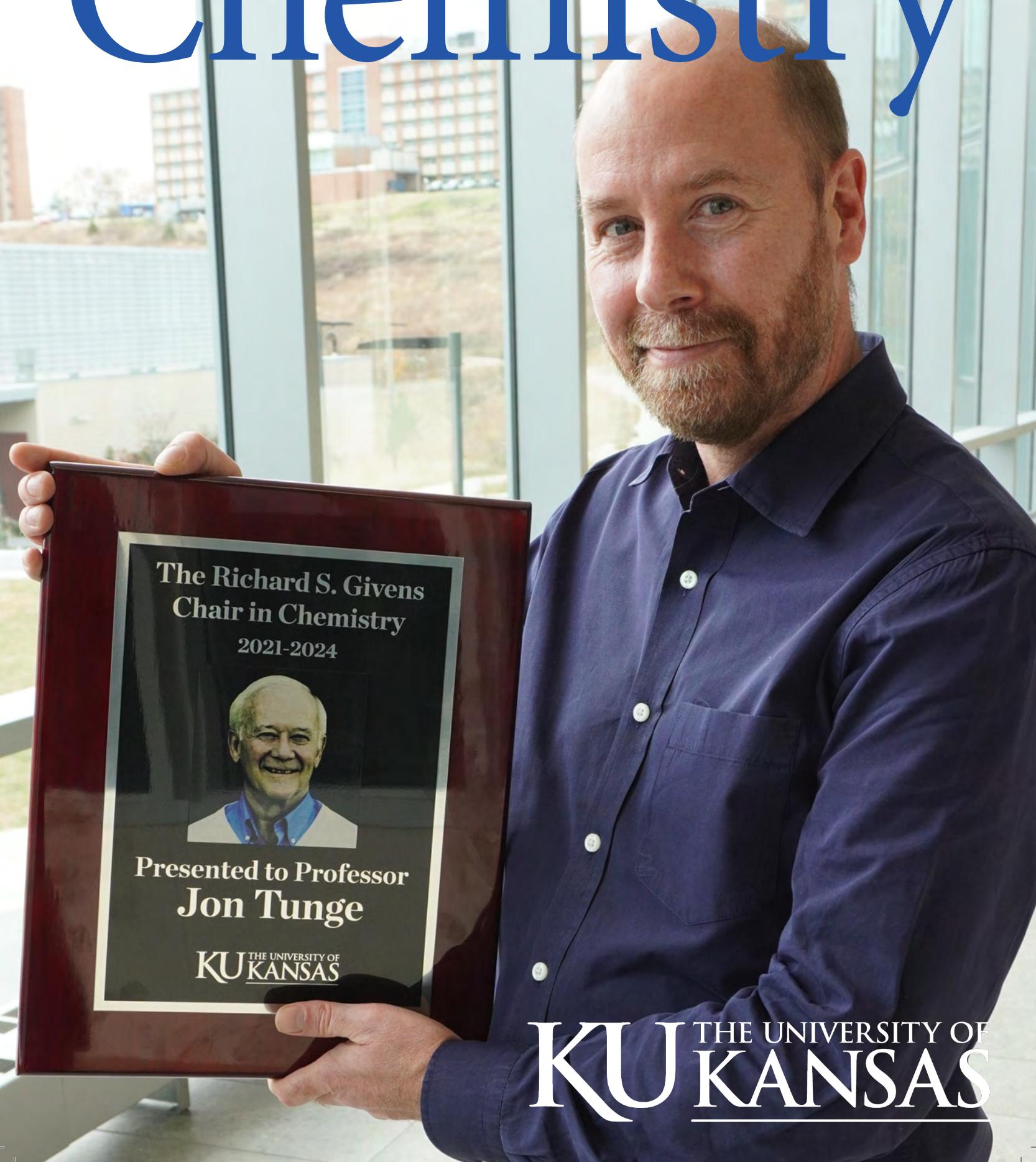


2021

Chemistry



KU THE UNIVERSITY OF
KANSAS

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Greetings from the Department of Chemistry! We hope this newsletter finds you healthy, happy, and excited for the new year. It has been an eventful year for chemistry at KU and we are pleased to share some of that with you in these pages. We have welcomed several new faculty members to KU and are currently searching for another. As the pandemic thankfully winds down, life on campus is slowly returning to normal. While we currently remain under an indoor mask mandate, social distancing guidelines have been lifted and all chemistry lectures and labs were taught in-person, at full capacity this fall. Throughout the pandemic, our faculty, students, and staff have adapted admirably to the ever-changing landscape; maintaining our high level of rigor in our instruction and productivity in our research.

Last year on the cover of this newsletter we announced a fundraising effort to establish the Richard S. Givens Chair in Chemistry (see pg 10). With the cover of this newsletter, we are pleased to announce that we have met our initial fundraising goal and selected our first recipient, Professor Jon Tunge. We want to sincerely thank everyone who donated to establish this new Chair; your generosity and support makes a significant difference in what we can accomplish. As you will see from the accompanying article, Prof. Jon Tunge is highly deserving of this honor and sets a very high bar for future recipients of the Givens Chair. The rotating chair model also inspired a former Jayhawk and generous donor, Dr. Keith Wilner, to accelerate his plans to establish a chair in chemistry, as discussed on page 5.

As highlighted throughout this newsletter, our faculty and students continue to be recognized for their outstanding accomplishments. We are particularly proud of our three Goldwater Scholars shown on the opposite page.

We place a high value on undergraduate research and this national scholarship recognizes students with exceptional promise for becoming leaders in the field. Only six Goldwater Scholars were selected from the state of Kansas, three came from the KU campus, and all three are chemistry majors!

Going forward, your generous donations and support have enabled us to initiate several new programs this year. We established the Sutton Family Research Impact Award, given monthly to recognize a high-profile paper published by a chemistry faculty member. We also initiated the Berger Student Travel Award, which provides up to 10 awards of \$750 each to support the travel of graduate students to present at national meetings. The Summer Scholars Program, discussed on page 3, was initiated this year to support the research of exceptional graduate students over the summer. We supported 14 graduate students this summer and, with your help, hope to expand it to 20 students next year with the introduction of the Richard and Barbara Schowen Summer Scholars. Also discussed on page 3 is the newly introduced Clark E. Bricker ChemScholars. This 4-year scholarship program has several goals, but one main focus is to recruit underrepresented minorities, first generation students, and women to KU as chemistry majors. None of these programs could have been possible without your generous support and we look forward to expanding their impact with your help!

We hope you enjoy the newsletter. On behalf of all of us here in Chemistry, we wish you and your families the very best in the new year. ROCK CHALK JAYHAWK!

Sincerely,

Robert C. Dunn
Professor and Chair



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Director
Graduate Studies
tunge@ku.edu



Prof. David Benson
Director
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Nicole-Marie Konopelko
Communications Assistant
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Three Chemistry Majors Named Goldwater Scholars

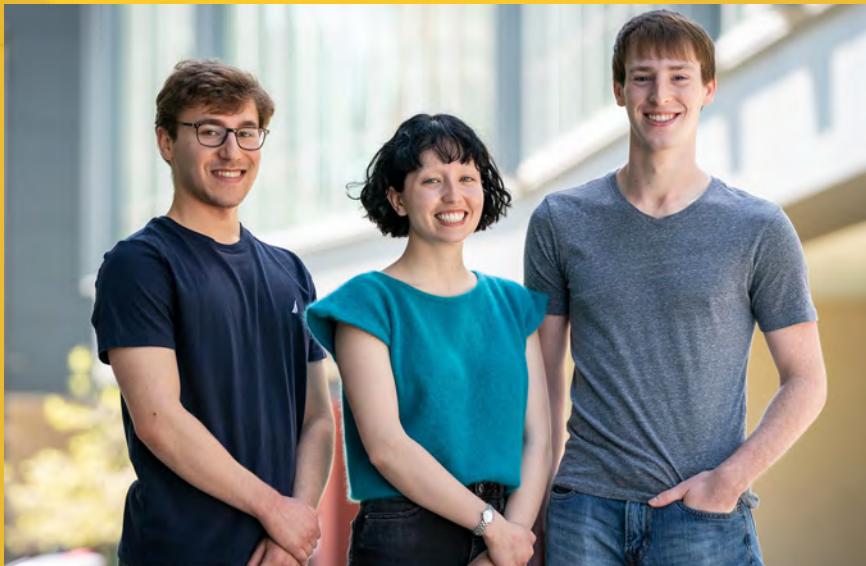


Photo by Steve Puppe | Goldwater Scholars pictured from left to right: Senior Chemistry Majors Anton Barybin, Emma Cosner, and Jonah Stiel.

In Spring 2021, three KU Chemistry juniors were named 2021-22 Barry M. Goldwater Scholars. Anton Barybin, Emma Cosner, and Jonah Stiel were among 409 US college sophomores and juniors selected by the Goldwater Scholarship Program for their "exceptional promise of becoming this Nation's next generation of research leaders" in the natural sciences, engineering, and mathematics. Emma, Jonah and Anton earned this prestigious national recognition through a rigorous two-tier competition. Earlier this year, 438 academic institutions nominated 1256 finalists (a maximum of four per college/university) from a pool of about 5,000 applicants. All three of our newly minted Goldwater Scholars are members of the KU Chemistry Club executive board, the University Honors Program, and the Department of Chemistry Honors Program. Jonah, Emma, and Anton will be writing and defending their Honors undergraduate research

theses next semester. The trio is now working on preparing and submitting graduate school applications as they all seek admissions to prominent doctoral graduate programs in chemistry or a chemistry-related field. Upon earning his Ph.D., Jonah ultimately aims to conduct research in the field of environmentally beneficial catalysis at a research-intensive academic institution or a national laboratory. After receiving her Chemistry doctorate, Emma aspires to engage in chemical and particle physics research at a national laboratory. She is also eyeing the career of an astronaut. Anton is targeting doctoral studies pertaining to chemical origins of neurodegenerative diseases followed by a career in translational research in an academic or private sector setting.

Both Jonah Stiel and Emma Cosner are undergraduate researchers in the group of Professor James Blakemore who won the 2021 K. Barbara Schowen Undergraduate Research Mentor Award.

It is extremely unusual, if not unheard of, to have two Goldwater Scholarship recipients hail from the same research group in a given annual nomination cycle. Jonah's research focuses on chemical systems capable of storing renewable energy in chemical bonds, with his major project aimed at the development of CO₂ reduction catalysts supported by unusual analogues of the 2,2'-bipyridyl ligand. This work is currently submitted for publication. More recently, Jonah has completed syntheses and full characterization of two new rhodium complexes supported by rare mono-substituted bipyridyl ligands.

Emma's research under the umbrella of energy conversion lies in the domain of redox chemistry. She endeavors to understand how changes in metal formal oxidation state can be controlled by ligand environments. Emma's study on the oxidation-induced reactivity of a novel rhodium hydride complex supported by the redox-active ligand bis(diphenylphosphino)ferrocene will soon be submitted for publication. More recently, she has prepared intriguing heterobimetallic complexes of samarium and europium and is now attempting to access the uncommon +II oxidation states of these more exotic elements. Anton Barybin is an undergraduate researcher in the group of Distinguished Professor Sue Lunte. Anton designs separation-based sensors to probe the role of catecholamine neurotransmitters in aberrant neurochemical processes. His recently co-authored publication introduced a microfluidic lab-on-a-chip device for in vitro monitoring the conversion of levodopa to dopamine and for evaluating stimulated dopamine release in vivo in a rat. Anton is currently expanding the cohort of his target analytes to include neurotransmitter metabolites.

We are all proud of our talented Goldwater Scholars and their incredible research mentors, and wish Anton, Emma, and Jonah success in securing admission to their dream graduate programs!

2021 DEPARTMENTAL SNAPSHOT

\$8,700,000 IN RESEARCH EXPENDITURES

97 - PAPERS PUBLISHED

92 - GRADUATE STUDENTS

145 - UNDERGRADUATE CHEMISTRY MAJORS

13 - RISING SCHOLAR CHEMISTRY MAJORS

14 - PH.D. DEGREES CONFERRED

3 - M.S. DEGREES CONFERRED

23 - BS AND BA DEGREES CONFERRED

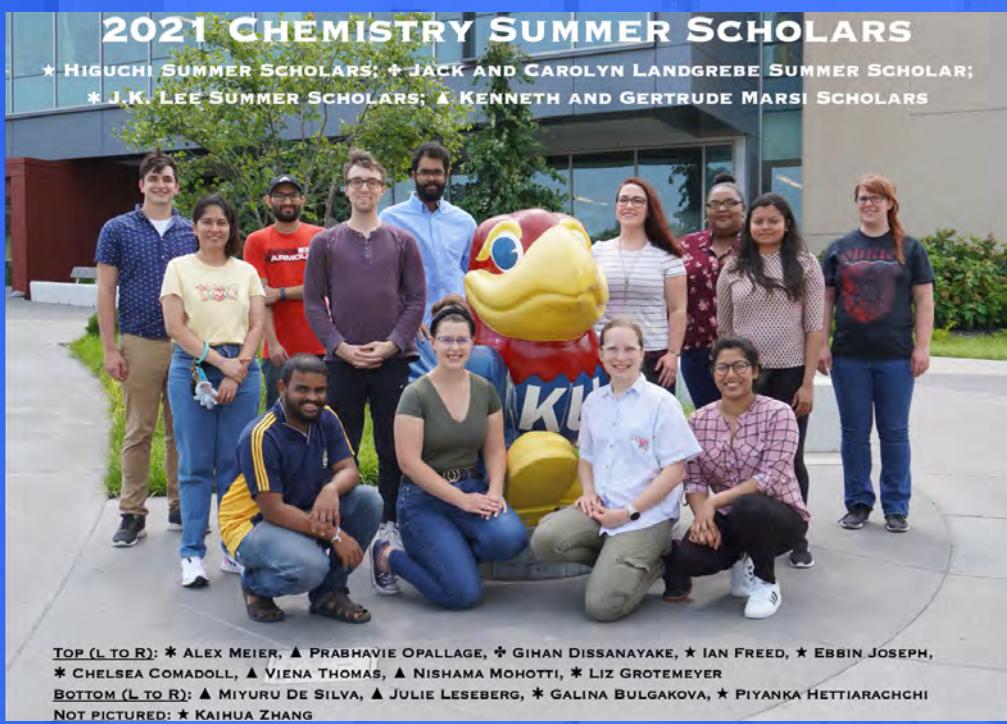
20,145 STUDENT CREDIT HOURS TAUGHT



Opportunities for Giving

1 The Summer Scholars Program

The Chemistry Department is excited to announce the Summer Scholars Program, which recognizes and supports the research of exceptional graduate students over the summer semester. The accompanying picture shows the first 14 recipients of our inaugural 2021 class. Each student received tuition and fees, along with a generous stipend to support their research activities over the summer. The support for this program came from generous donations to our endowment, using the funds acknowledged in the picture. Awardees were selected by our graduate affairs committee, based on letters of recommendation and the strength of the student's CV. Galina Bulgakova, an advanced student working with Prof. Sue Lunte, commented that: "Getting the Summer Scholarship was very motivating. On top of providing generous support through the summer semester (including health insurance!) it also was a very clear message that my research efforts are being recognized and appreciated by the Department." She went on to say: "I also took my J.K. Lee Summer Scholarship as an opportunity to learn more about the history of our department and the contributions Dr. Lee made to making it the place it is today." Nishama Mohotti, a second-year student working with Prof. Meredith Hartley, wanted to convey her thanks to the donors: "Thank you for enabling me to reach my fullest potential on performing research over the summer by your generous contributions...your generosity has helped me get one step closer to my future success."

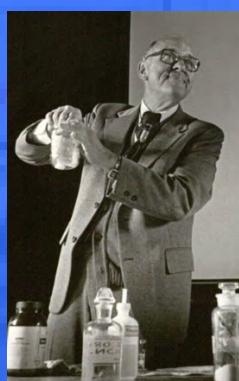


2 The Clark E. Bricker ChemScholars Program

As then Chair of the Department, Prof. Craig Lunte established the ChemScholars program in 2002. This program committed four years of scholarship support (\$500 per year) to talented undergraduates entering KU as chemistry majors. This program, however, never had a dedicated source of funding. That all changed this year when we introduced the Clark E. Bricker ChemScholars program! The Bricker family, along with George and Bev Wilson, helped us consolidate two endowment funds named in honor of Prof. Bricker to support this worthy program. With significant additional support from Glendon and Karen Cox, the Clark E. Bricker ChemScholars program can now provide \$2,000 of scholarship support for 8 deserving students.



While all students are strongly encouraged to apply, applications from underrepresented minorities, first generation students, and women are particularly sought. In spring 2022, we are initiating a mentorship program that pairs our graduate students with local high school students. It is hoped that these relationships will strengthen our ties with local high schools and increase the diversity in our program. If you are interested in helping us expand this worthy program, we ask that you donate using the envelope included or contact KUEA using the information on the back page. Rock Chalk!



Please support...

The Barbara and Richard Schowen Summer Scholars

Our students are our top priority, so the Chemistry Department has set an ambitious goal of expanding this program to support 20 students in 2022. It takes approximately \$200k of invested funds in our endowment to generate sufficient income to support one summer scholar. We have already identified additional funds to partially expand the program next year, but we need your help to reach our goal. We are starting a fundraising drive to add two additional scholars to the program named in honor of Barbara and Richard Schowen. The Schowens are well known for their care and support of our students, so it seems natural to name summer scholars in their honor. With your help, our goal is to raise \$400k which will enable us to support two Schowen Summer Scholars every year in perpetuity. If you would like to contribute to this effort, please use the enclosed envelope or contact KUEA using the information on the back page. Rock Chalk!

Welcome!

The Department is thrilled to welcome these new faces to Gray-Little Hall.



**Dr. Erin
Burger-Dunn**

Teaching Assistant
Professor



**Dr. Aaron
Teator**

Assistant
Professor



**Nicole-Marie
Konopelko**

Communications
Assistant



**Avery
Meadows**

Graduate Program
Coordinator



**Lindsey
Roe**

Administrative
Associate

After completing her B.S. in chemistry at the University of Nebraska-Lincoln, Erin joined the Department of Chemistry at KU as a Madison and Lila Self Graduate Fellow. Upon her arrival at KU she joined the Tunge group, graduating in 2007. After a short time away from Kansas, during which she worked in the laboratory of Prof. John Hartwig at the University of Illinois at Urbana-Champaign, Erin returned to Lawrence to begin her career as a Senior Scientist at Deciphera Pharmaceuticals. As a chemistry tutor for Kansas Athletics Student Athlete Support Services, she was excited to find herself back on the KU campus. When the opportunity to rejoin the Department of Chemistry as an Assistant Teaching Professor presented itself, she was happy to find herself back among so many familiar faces and grateful for the opportunity rejoin the KU community.

Prior to joining the Chemistry Department at KU as an Assistant Professor, Aaron attended the University of Texas at Austin where he worked under the co-mentorship of Prof. Jennifer Brodbelt and Prof. Christopher Bielawski. His dissertation work centered on the design of photochromic N-heterocyclic carbene scaffolds and their subsequent application in the development of switchable transformations. Aaron then joined the lab of Prof. Frank Leibfarth at the University of North Carolina at Chapel Hill. As a Cottrell Postdoctoral Fellow, his research focused on the development of stereoselective ionic polymerizations as a new approach to polar thermoplastics. Research in the Teator Lab at KU resides at the interface of organic chemistry, polymer chemistry, and materials science, and is centered on expanding the diversity of structures available through controlled polymerization. The materials developed here will have wide-ranging applications that address current limitations in diverse fields, including engineering, medicine, and biotechnology.

Nicole-Marie Konopelko joined the Department in November 2020 as a Social Media & Communications Assistant. She is a senior at KU majoring in journalism and Russian. Nicole-Marie runs our departmental social media accounts and website (chem.ku.edu), which she redesigned and migrated to the University's new Drupal 8 format. Nicole-Marie has extensive communication and journalism experience from her time as a University Daily Kansan News reporter. She was also named the 2019 Kansas Student Journalist of the Year and was a 2019 National High School Student Journalist of the Year Runner-Up. Nicole-Marie would like to remind our followers to follow our social media accounts (see first page of this newsletter). Outside of work, Nicole-Marie enjoys playing piano and spending time with her family.

Avery Meadows attended KU for a brief time as an undergraduate but ended up graduating from Truman State University with a B.S. in Mathematics. During her time at Truman, she gained experience working with incoming STEM undergraduates as a study skills seminar instructor and academic trainer, which helped to prepare her for working with our graduate students. Before joining the Department of Chemistry, she was most recently underwriting flood insurance policies as a contractor for FEMA's National Flood Insurance Program. While the change from insurance to education may seem vast, she's found that her experience in insurance helped her to develop a knack for understanding policy that has proven useful while helping our program to coordinate with University policy. Outside of work, she likes to relax with her partner and their cat by watching old movies, reading, playing guitar, and spending time with her nephews.

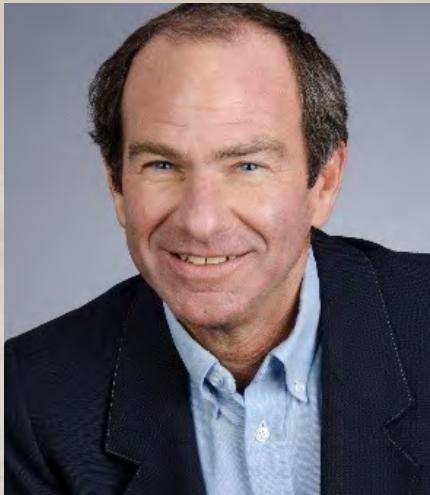
Lindsey Roe joined the Chemistry office in October 2021 as an Administrative Associate. She graduated from KU with a B.A. in Human Biology and worked as a laboratory technician in Molecular Biosciences for 10 years, before joining Chemistry as an Administrative Assistant for Prof. Steven A. Soper's NIH-funded Center of BioModular Multiscale Systems for Precision Medicine in 2016. Lindsey is administrator for the Chemistry Undergraduate program and Alumni Relations. She is very excited to be part of the Chemistry family, and looks forward to assisting the undergraduates through their degree program as well as planning departmental and alumni events.

Scan for a full
faculty list!



The Chemistry Department presents:

The Keith D. Wilner Chair in Chemistry



Pictured: Keith D. Wilner

The Chemistry Department is thrilled to announce the establishment of the Keith D. Wilner Chair in Chemistry. Keith earned his B.A. in chemistry from KU in 1978 and carried out undergraduate research in the labs of Prof. Rich Givens and Prof. Ralph Christofferson. After graduation, he earned a Ph.D. in pharmacology from the University of Texas Health Science Center at Houston followed by postdoctoral studies at UC San Diego. He joined Pfizer Global Research and Development in 1986 and worked his way

up to his current position of leadership as Oncology Clinician Leader and Global Clinical Lead.

Keith originally signed estate plans to establish an endowed professorship in 2007, when Professor Joe Heppert was leading the Department. Keith liked the model we recently developed for the Richard S. Givens Professorship, so he decided to put his bequest to work now! Keith is generously funding an endowment that will support the Keith D. Wilner Chair in Chemistry. Like the Givens Chair, this will be a rotating chair awarded to a faculty member excelling in all three areas of research, teaching and service. When the invested endowment grows to a sufficient level, the Wilner Chair will be converted to a permanent endowed professorship and used to attract a faculty member at the Distinguished Professor level.

In 2007, when Keith originally established his bequest, he said he wanted to "...pay KU back for setting him on the path to a successful career." Keith, who grew up in St. Louis, was attracted to KU by the campus and the knowledgeable and approachable professors, especially Prof.

Richard Givens whom Keith described as a "great lecturer." "His influence was one of the reasons why I am doing a named professorship at KU." Keith credits his undergraduate research experience with opening his eyes to the opportunities in

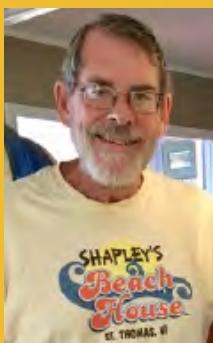
My experience at KU certainly provided me with the initial path for my career.

-Keith D. Wilner

pharmacology, leading to his Ph.D. in neuropharmacology and career at Pfizer. "My experience at KU certainly provided me with the initial path for my career. I have been very fortunate to work in an area that is amazingly rewarding and having an impact on patients' lives." The Chemistry Department is truly fortunate to have alumni like Keith and we look forward to announcing our first recipient of the Wilner Chair in 2022. Rock Chalk!

Introducing...

The John R. Shapley Award for Excellence in Research by an Undergraduate in Chemistry.



A new award recognizing excellence in undergraduate research has been established through a generous donation from Dr. John Shapley, who received his B.S. in chemistry in 1967. Upon graduating from KU, John earned his Ph.D. from Harvard and carried out postdoctoral studies at Stanford, before joining the faculty at the University of Illinois in 1972. While at KU, John carried out undergraduate research under the direction of Professor Richard Schowen, which had a lasting impact on him. "Prof. Richard Schowen

opened a portal to the research lab for me as an inexperienced but enthusiastic sophomore, and I began a journey that fascinated me for nearly fifty years." John went on to say that: "KU Chemistry has a long-term, outstanding record of involving undergraduates in research activities" and that he is pleased to establish an award that, "...highlights the passion, commitment, and promise..." of exceptional undergraduate researchers. Now retired, John and his wife Patricia live off-the-grid in the U.S. Virgin Islands.



Pictured: Dr. Misha Barybin in his lab and classroom. This year, Barybin was awarded with the title of "Chancellor's Club Teaching Professor." Dr. Barybin will receive an annual honorarium of \$10,000 for the next five years, as part of the award.

Mikhail 'Misha' Barybin 2021 Chancellors Club Teaching Professor

Professor Mikhail 'Misha' Barybin has been awarded a prestigious Chancellors Club Teaching Professorship. This campus wide honor recognizes "sustained excellence in teaching and is awarded to persons who have demonstrated outstanding teaching competence over an extended period of time." Misha was one of only four awardees in the 2021 class, which

comes with a generous honorarium for 5 years. Misha's dedication to our students and effectiveness in the classroom are legendary. His teaching creativity is exemplified by offerings such as his Honors Freshman seminar on "Exploring parallels between Chemistry and Music." He has taught at all levels from introductory General Chemistry to advanced level graduate courses and

recently developed a University Scholars Seminar course on "Nuclear chemistry in the modern society." Misha was an Honors Faculty Fellow from 2013 to 2020 and his research program has been funded continuously by NSF since 2006. On behalf of our Department, congratulations Misha on this very well-deserved recognition!

Dr. Paul Hund Goes "Back to School"



Dr. Paul Hund earned his B.S. degree in chemistry in 1971, went to dental school at UMKC, and spent 45 years in dental practice before retiring. He is a generous donor to the department and fondly remembers taking introductory chemistry from the legendary Prof. Clark Bricker, where he learned "how to think". Interested in seeing how things are done today, Paul went "back to school!" He monitored Prof. Misha Barybin's Honors General Chemistry course remotely through

the fall semester of 2020. At the end of the semester, Paul even gave the CHEM 190 "gang" some sage advice from his Bricker days. He reminded the students about the critical importance of learning "how to think" and praised the efforts of Prof. Barybin in helping them develop this important skill. Professor Barybin has subsequently been named a Chancellors Club Teaching Professor. Thank you Paul for your generous support and for taking the time to interact with our students!

Dr. Glendon and Karen Cox

with friends like these....



We are very fortunate to have friends and supporters like Dr. Glendon and Karen Cox. With a very generous gift, they were able to help us reach our initial fundraising goal for the Givens Chair. They gave generously to the Bricker ChemScholars fund, increasing the number of students we can support in this very worthy program. Finally, they established a new student scholarship in chemistry focused on attracting and retaining

students from diverse backgrounds.

Both Kansas natives, Karen received her bachelor's degree from the KU School of Business in 1982. After serving in the business offices of several Kansas City firms, she moved to volunteer activities with organizations like CASA, which helps abused and neglected children. A native of southeast Kansas, Glen received his BA degree in chemistry from KU in 1977. During his time he carried out research in the lab of Prof. Burgstahler, who Glen describes as an "...immensely patient research mentor...". When asked about KU Chemistry, he said that "Most of my memories are about the people that I worked with and learned

from, particularly Clark Bricker, Albert Burgstahler, Richard Schowen, Peter Hierl, and Kristin Bowman." He continued, "Not much that I can say about Brick other than he was a master teacher..."

Following graduation, he attended medical school and received his MD from the KU School of Medicine in 1980. After residency and several prestigious visiting fellowships, he joined the faculty as an assistant professor in the De-

partment of Radiology. He was quickly promoted through the ranks and after a brief period in private practice, returned as Professor of Radiology and Director of Thoracic Radiology and Imaging. He has served on the Board of Directors of Kansas University Physicians, and as the Associate Dean of Graduate Medical Education, Senior Associate Dean of Medical Education and Vice Dean of the School of Medicine. He was appointed the Director of the Institute for Community and Public Health in 2008 and Chair of the Department of Health Policy and Management the following year. Among other awards, he received a "Special Services Award" from the Kansas Public Health Association in 2010, a Chancellor's Award for Outstanding Classroom Teaching from KU in 2011, and the Leadership Luminary Award from the Radiology Leadership Institute in 2016.

Glen and Karen give generously to several philanthropic causes. When asked about giving to Chemistry, Glen said: "The work with the department and its faculty set me up for my success in the remainder of my undergraduate career, my acceptance to medical school and whatever professional accomplishments I have enjoyed." Their investment in Chemistry has already had a tremendous impact and we are very grateful for their generous support.

Research Highlight: The Search for Extraterrestrial Life

Emily Kurfman, a graduate student in Prof. Susan Lunte's research group, is a Fellow in the NASA Space Technology Graduate Research Opportunities (NSTGRO) program. She and Dr. Lunte are collaborating with Dr. M. Fernanda Mora and Dr. Peter Willis at the NASA/Caltech Jet Propulsion Laboratory in Pasadena on the development of analytical instrumentation and methods to look for extraterrestrial life on Europa (one of Jupiter's moons) and Enceladus (one of Saturn's moons), which are known to contain water. The project involves the development of methodology to look for chemical signatures that indicate the presence of cells in samples



collected *in situ* on these ocean worlds. Emily is working on the development of an apparatus for cell enrichment and lysis, as well as methodology to

analyze the resulting samples online by capillary electrophoresis with mass spectrometry. This project was inspired by an internship that Emily carried out in Dr. Willis's group at JPL in 2019 as a participant in the NIH Graduate Training Program in Dynamic Aspects of Chemical Biology. Emily greatly enjoyed her internship and learned much about astrobiology and spaceflight instrumentation during the four-and-a-half months she was there. This experience sparked her interest in a research career at NASA in the field of astrobiology and, with encouragement from her mentors at JPL, an application to NSTGRO in 2020.

Degrees (Spring, 2021)

Elaena Barney, B.S.
Bailey Boswell, B.S.
Ming Chen (December, 2020), B.A.
Madeline Devries, B.S.
Jack Dingle, B.A.
Logan Forshee, B.S.
Matthew A. Gadberry, B.S.
Lexi Gambill, B.S.
Ashley Grande, B.S.
Megan Hegarty, B.S.
Zuyu Jin (December, 2020), B.A.
Morgan Johannesen, B.S.
Alexyss Lambert, B.S.
Jeehyun (Janet) Lee, B.A.
Shawn Mikeska, B.S.
Kaley Muir, B.S.
Nick Murphy, B.S.
Thy Nguyen, B.A.
Zachary Panther, B.A.
Seungbin (Sarah) Park (December, 2020), B.A.
Cole Sherrill, B.A.
Bowen Tang, B.A.
Josh Wade, B.S.

Goldwater Scholars

Anton Barybin
Emma Cosner
Jonah Stiel

Rhodes Scholar Nominee

Anton Barybin

Marshall Scholar Nominee

Anton Barybin

Landgrebe Summer Scholar

Emma Cosner

Beckman Scholars

Claire Dopp

Bricker ChemScholars

Brian Faintich
Trisha Nair
Tommy Nguyen
Maria Matulis

Kansas ChemScholars

Anton Barybin
Emma Cosner
Jonah Stiel

Rise Fellow

Jonah Stiel

Undergraduate Research Awards

Emma Cosner
Claire Dopp

Degrees (2020 - 2021)

Kaitlyn Chase Cartwright, Ph.D.
Jennifer Doolin, Ph.D.
H.M. Emranul Haque, M.S.
Amy Jystad, Ph.D.
Michael Kim, Ph.D.
Seth Curtis Martin, Ph.D.
Xavier Ortiz, M.S.
Yun Peng, Ph.D.
Ezekiel Ashe Piskulich, Ph.D.
Sijin Ren, Ph.D.
Kelci M. Schilly, Ph.D.
Tu Vu, M.S.
Milani Rasangika Wijeweera Patabandige, Ph.D.
Pubudu N. Wimalasiri, Ph.D.
Pavel Yamanushkin, Ph.D.
Xin Zhou, Ph.D.

NIH Chemical Biology Training Grant Program

Hayley Blockinger
Gihan Dissanayake
Wade Henke
Esther Holt
Emily Kurzman
Jaycee Mayfield
Ian McBride
Jacob Theismann
Dimuthu Vithanage
Matthew Zupan

Self Fellowships

Madeline Haga (2021-2025)
Patrick Connelly (2020-2024)
Shaun Kelsey (2019-2023)
Michael Wrigley (2018-2022)

Kansas Academy of Sciences Grant

Wade Henke

NASA Fellowships

Emily Kurzman

2021 Chancellors Club Teaching Professor

Misha Barybin

Ralph Adams Award in Bioanalytical Chemistry

Steve Soper

2021 ACS Award, Inorganic Chemistry

Kristin Bowman-James

2021 ACS Roland F. Hirsch Award

Sue Lunte

K. Barbara Schowen Research Mentor Award

James Blakemore

American Thyroid Association Early Career Research Grant Award

Meredith Hartley

Innovation Award from Center for Teaching Excellence

Shuai Sun

Steven F. Warren Research Achievement Award

Maggie Witek

2021 Class of Influential Researchers - I&EC Research

Marco Caricato

College of Fellows American Institute for Medical and Biological Engineering

Sue Lunte

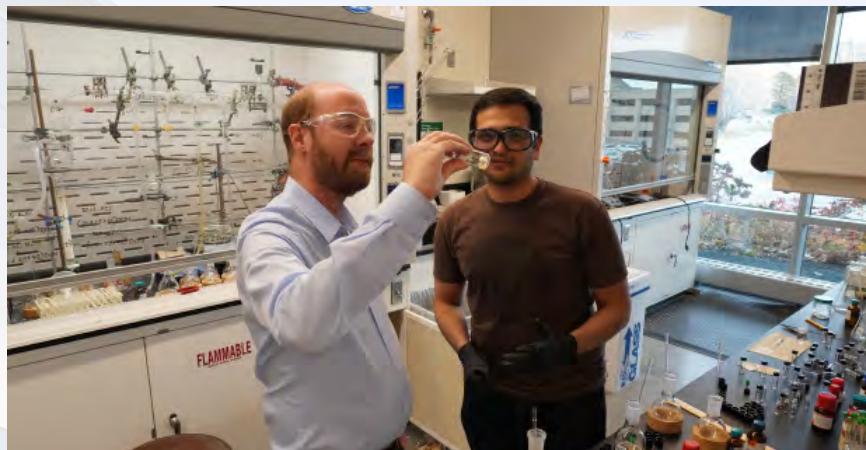
KU Office of Research New Faculty Research Award

Meredith Hartley

Sabbaticals

Misha Barybin (sp 2021)
Marco Caricato (sp 2021)

OUR
CHANT
RISES



Professor Jon Tunge

The Richard S. Givens Chair in Chemistry

Jon Tunge grew up in a small town on the Missouri River in South Dakota. He earned his B.S. degree in Chemistry from the University of Idaho where he performed undergraduate research in analytical chemistry. The research merged organic chemistry with surface chemistry and fluorescence spectroscopy to detect high explosives. The synthesis of new fluorophores for surface modification was particularly exciting, cementing his interest in synthetic chemistry.

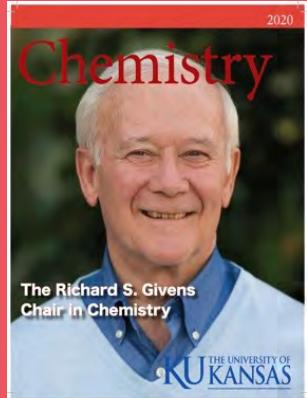
Jon went on to perform dissertation research under the direction of Prof. Jack Norton and received his Ph.D. from Columbia University in 2000. His research involved the development of new strategies for the synthesis of amino acids as single enantiomers and the study of organometallic mechanisms. One day he was asked to assist a visiting professor by synthesizing a trifluoromethyl mercury compound for protein labelling. The synthesis was difficult, potentially dangerous, and the cleanup was horrific. Nonetheless, the method he used – decarboxylation – would stick in his

mind and subliminally influence his future independent career direction. Following graduation, Jon joined the lab of Charles P. Casey at the University of Wisconsin-Madison. Since Prof. Casey had recently been elected President of the ACS, Jon had a lot of freedom to drive the direction of his research on olefin polymerization catalysts. Using the mechanistic skills developed in his Ph.D. studies, he performed NMR spectroscopic studies at -150 °C to observe and study the reactivity of a key intermediate in olefin polymerization for the first time. Just weeks prior to leaving Wisconsin, Jon's wife Kelly Jones graduated from the University of Wisconsin and their daughter Stella was born.

Jon arrived in Lawrence, sleep-deprived but ready to start his independent career. Initially he was studying new methods for halogenation that was supported by an NSF EPSCoR First Award and mechanisms of C-H activation that was supported by the ACS-PRF. However, the decarboxylation experiment he had performed as a graduate researcher still loomed. Thus, he began developing catalytic methods

that could utilize the loss of carbon dioxide to drive the formation of very reactive organometallic intermediates without the need for hazardous or high-energy reagents. Early aspects of this work were supported by the National Institutes of Health and an NSF CAREER Award, and is still supported today by NSF. The methods that he has developed rely on the use of carboxylic acids and esters, which are widely available, inexpensive, and non-toxic. Under the action of catalysts, carbon dioxide is released. The formation of this stable (likewise non-hazardous) small molecule energetically drives the formation of reactive intermediates that can be used for C-C bond forming reactions.

Prof. Tunge's group extended the synthetic capabilities of that strategy to the edge of its limitations. His research group learned that the energy derived from loss of CO₂, while large, significantly limited the carboxylic acids that could be used in his synthetic coupling chemistry. More recently, these limitations have been overcome by merging photocatalysis with decarboxylation catalysis. Such dual catalytic activation harnesses



Pictured: (upper left) Shrikant Longhe, Ebbin Joseph, Jon Tunge, Rafa Diaz Hernandez, and Andrea Altamira. (bottom left) Ebbin in the dry box. (right) Jon and Rich Givens after the award presentation.

both the energy of CO_2 loss and the energy of photons to allow nearly any carboxylic acid to be synthetically useful.

More recently, the Tunge group has utilized vitamin B12 mimics as catalysts for the functionalization of organic molecules. Once again, merging these catalysts with photocatalysts allows synthetic “editing” of molecules like amino acids and peptides through decarboxylation and hydrogen evolution. While such hydrogen evolution catalysts have been used for decades for water oxidation, only recently have they been used for complex synthesis.

In addition to his independent research, Prof. Tunge has been involved in many collaborations since arriving at KU. This began early on with his involvement as a founding member of both the NSF Center for Environmentally Beneficial Catalysis (CEBC) and the NIH Center for Chemical Methodologies and Library Development (CMLD). He continues to be active with the CEBC and has recently become leader of the Synthetic Biology Core that provides

synthetic expertise to the COBRE Center for Molecular Analysis of Disease Pathways and the center for Chemical Biology of Infectious Disease, for which he is also co-PI. In addition to working in these exciting collaborations, Jon has had the pleasure of conducting research alongside 17 Ph.D. graduates who have gone on to careers at places like Merck, Catalent, Haliburton, the University of Florida, Oklahoma State University, and even the University of Kansas (Rock Chalk)!

Prof. Tunge was promoted to Associate Professor in 2007, to Professor in 2011, and has been an adjunct faculty member with the Department of Medicinal Chemistry since 2007. He has received a number of awards including a W.T. Kemper Fellowship for Teaching Excellence, the University Scholarly Achievement Award, and was named a Kansas Bioscience Authority Rising Star. Most recently, Prof. Tunge was delighted to be named the first Richard S. Givens Chair in Chemistry. When asked about it, Jon simply stated - “To be given a recognition that carries the name of a friend, colleague, and mentor that I deeply admire and respect is an honor to which words cannot do justice.”

The Richard S. Givens Chair in Chemistry is a rotating Chair that will be awarded every three years to a deserving faculty member in recognition of their outstanding contributions in research, teaching, and service. During the 3-year term, each awardee will hold the title of the Richard S. Givens Chair in Chemistry and receive \$15,000 a year in support for their scholarly activities. We announced the fundraising effort to establish the Givens Chair on the cover of last year’s newsletter and were heartened by your overwhelming response. With your generosity, we quickly reached our endowment goal to establish the Chair and sustain the associated support. We are continuing to invest and encourage donations to grow the endowed funds. Once the endowment reaches a sufficient level, the Givens Chair can be converted to a Distinguished Professorship in the Department. Professor Givens came to KU as an Assistant Professor in Chemistry in 1967 and helped shape the collegial and productive department we have today. We are very grateful for your support in honoring his legacy with the establishment of this Chair.

Steve Soper: 2022 Ralph N. Adams Award



The Chemistry Department is thrilled to announce that Professor Steve Soper has been selected for the 2022 Ralph N. Adams Award in Bioanalytical Chemistry. This national award was established in 2005 by friends and former students of Ralph Adams, and has a special significance here at KU given Ralph's influence and impact on our department. Steve is one of 10 Foundation Distinguished Professors at KU and he leads an internationally recognized program developing exciting new tools for discovery and medical diagnostics. In particular, he and his group are at the

forefront of developing highly integrated microfluidic platforms for the analysis of complex, biological samples. Awardees of the Ralph N. Adams Award are selected by an anonymous committee comprised of former students and past awardees. Steve will officially receive his award at the next Pittcon meeting, during a scientific session organized in his honor. With this award, Steve deservedly joins a very select group of past winners including Chad Mirkin (2018, Northwestern), Robert Kennedy (2017, U. of Mich.), and David Walt (2016, Tufts).

Research Highlight - Weis Research Group

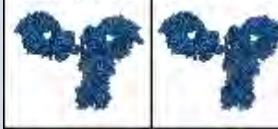
Weighing up biosimilars with mass spectrometry

Protein-based pharmaceuticals, particularly those based on monoclonal antibodies are revolutionizing the treatment of many diseases, making drugs like Humira, Embrel, Leuentis, and Herceptin into household names. An antibody drug's function derives from its higher-order structure, the three-dimensional positioning of its roughly 150,000 atoms, based on a complex network of weak intermolecular forces that causes the molecule to adopt a complex, well-defined structure. Grown in living cells, antibody drugs require complex manufacturing processes and are inherently unstable, making them expensive to manufacture and deliver.

The Affordable Care Act established a potential lower-cost approval pathway for biosimilars, essentially the generic biologics. A comprehensive package of analytical data can be used to obtain approval without expensive clinical trials. The producer must demonstrate

that the biosimilar is "highly similar to" the patented biologic. While the traditional tools of structural biology, X-ray crystallography and NMR, and the emerging tools of cryo-electron microscopy and computational methods are quite successful in determining protein structures, they are quite limited in their utility in such pharmaceutical contexts.

Hydrogen exchange-mass spectrometry (HX-MS) is a widely-accepted technique that probes protein structure based on the H/D exchange kinetics of proteins in heavy water. Relative rates of HX, measured by MS, provide a structurally-resolved map of protein structure. Thus, HX-MS can define a "structural fingerprint" that can be used to support claims of similarity between patented and biosimilar proteins. However, a typical HX-MS study of an antibody yields approximately 10,000 data points, rendering traditional statistical

| Equivalence testing of higher-order protein structure | | |
|---|---|---|
| Reference material | Biosimilar candidate | Process change |
|  |  |  |
| Statistically equivalent HX-MS? | ✓ | ✗ |

approaches invalid. Recent work in the Weis Lab, published in Analytical Chemistry, has established statistical methods and frameworks for these kinds of studies. Collectively, these papers established that even small amounts of a structural variant could be reliably detected using the newly-established statistical methods and that a modified form of statistical equivalence testing could be used to demonstrate structural equivalence between biosimilar antibodies and their reference products.

Research Highlight

Minae Mure Research Group

In the Mure lab, we have been studying the molecular functions of lysyl oxidase-like 2 (LOXL2) to gain insight into its roles in promoting tissue/organ fibrosis and tumor invasion/metastasis. The ultimate goal of our research is to identify methods to selectively inhibit LOXL2, as such methods can be further developed into a LOXL2-targeted therapy. LOXL2 is a copper (II) and lysine tyrosylquinone (LTQ) dependent amine oxidase and catalyzes the conversion of peptidyl lysines to allysines via an LTQ-mediated oxidative deamination reaction. LOXL2 promotes crosslinking of the extracellular matrix (ECM) proteins (e.g. collagen and elastin) leading to remodeling of the ECM. The LTQ cofactor is post-translationally derived from conserved lysine and tyrosine residues in the active site. The molecular mechanisms of LTQ biogenesis and the LTQ function in amine oxidation

remain elusive. We have been conducting biochemical and biophysical characterization of our recombinant LOXL2 (rLOXL2) that contains nearly stoichiometric amount of LTQ and is catalytically active. We just submitted a full manuscript concerning biophysical characterization of LOXL2, entitled "Oligomeric states and hydrodynamic properties of lysyl oxidase-like 2." We collaborated with Dr. Krzysztof Kuczera (KU, Chemistry) on molecular modeling of LOXL2, with Drs. Ronald Toth and C. Russel Middaugh (KU, Vaccine Analytics and Formation Center) on analytical ultracentrifugation, and with Dr. Ewa Folta-Stogniew (Yale, W. M. Keck Biotechnology Resource Laboratory) on multi-angle light scattering with size-exclusion chromatography. Alex Meier, a 5th year graduate student is the first author of this paper as well as the following three full papers (in preparation)



Pictured: Alex Meier, a 5th year graduate student and member of Dr. Minae Mure's lab.

we hope to submit all within this year. Alex was supported by the Charles and Beatrice Kulier scholarship, the Chemistry Scholarship Fund, the Elmer McCollum research Scholarship and the J.K. Lee Summer Scholar Program from the Department of Chemistry, KU and that helped him greatly to focus on research.



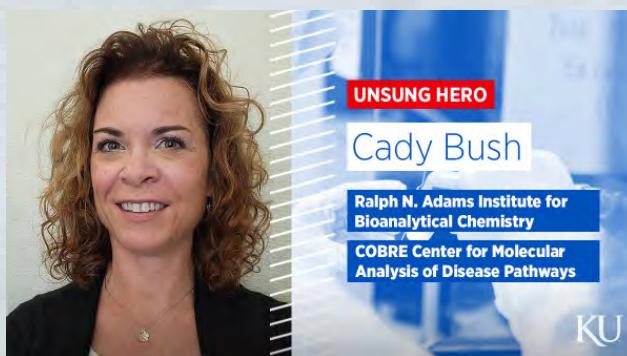
Pictured: Chem GSO held the first research poster session in two years at the beginning of the semester.

A message from CHEM GSO

2021 has been a roller coaster of a year! As the Chemistry Graduate Student Organization, our mission remains to (1) facilitate communication between graduate students and the chemistry department, (2) promote professional development for chemistry graduate students, and (3) build social ties within the department while advocating for science within our community. We started off the year with a free professional headshot event for graduate students in February, followed by a T-shirt design contest where we later partnered up with a local screen printer and sold ChemGSO shirts to the department. Throughout the summer, we hosted Nicole Reiz, Director of Professional Development in the Office of the Vice Provost for Graduate Studies at KU, for an outstanding professional development seminar series covering topics from networking to interviews to resumes.

Two highlights of the year included some summer cookouts and a research poster session. As we eased back into some in-person events during the summer, it was great to reconnect with old friends and make some new ones over food, softball, and volleyball. Then, at the beginning of the semester, we held the first research poster session in two years with excellent participation from almost every research group in the department! If you would like to receive more information on how to get involved with ChemGSO and our current graduate students, please contact us at kuchemgso@gmail.com and/or follow us on Facebook (@KUChemistryGSO).

Cady Bush: An 'Unsung Hero'



Kudos to Cady Bush who was recently recognized as an unsung hero by the Office of Research at The University of Kansas for her role as the Program Manager supporting the Ralph N. Adams Institute for Bioanalytical Chemistry and the COBRE Center for Molecular Analysis of Disease Pathways (CMADP). In 2021, Cady was instrumental in submitting the application for

the third round of NIH funding for the COBRE CMADP. "Her positive attitude and willingness to work 12 hours a day during the month of May to get the proposal in were inspiring," said Susan Lunte, Ralph N. Adams Distinguished Professor of Chemistry & Pharmaceutical Chemistry and director of both the institute and the CMADP. Thanks, Cady, for all you do!

NSF Undergraduate Research Program

35 years of excellence

Nothing better exemplifies the KU Chemistry Department's dedication to providing quality research experiences to its majors than its long running, NSF-sponsored Research Experiences for Undergraduates (REU) program. Currently co-directed by Dave Benson and Misha Barrybin, the program has been in nearly continuous operation ever since Barbara Schowen and Marlin Harmony brought the first cohort of REU students to Lawrence in the summer of 1988. Throughout that 35-year time span well over 300 students from around the nation have participated in the program, the vast majority from Primarily Undergraduate Institutions (PUIs). The total number of undergraduate students who have benefitted from this program is closer to 600, since each summer's cohort is expanded through participation of KU Chemistry majors and, in recent years, a student from Dublin City University in Ireland (via an exchange program initiated by Craig Lunte). Participants

the summer 2020 offering. Our NSF-REU funds supported ten non-KU students, including five who had been selected to participate in summer 2020. Two additional non-KU students were supported through individual faculty NSF grants. Rounding out the cohort were five KU students, a group that included 2020 KU Beckman Scholar Claire Dopp and the inaugural Jack and Carolyn Landgrebe Summer Research Scholar, Emma Cosner. The ten-week program began on May 24th with masking and social-distancing in place. While those restrictions were soon lifted, concerns about the Delta variant led us to don masks once again for the closing poster session on July 30. Despite these restrictions (or perhaps because of them!) the summer 2021 cohort was as interactive and enthusiastic as any we've had in recent years. Professional development activities included two oral presentations, one at the beginning of week three in which participants outlined the goals of their research projects, and another in week ten in which they described their accomplishments. The program concluded with a poster session in the main floor hallway of Gray-Little Hall that was held jointly with the Chemical and Petroleum Engineering REU program. Many of the participants in this outstanding group will be

presenting their posters at an ACS regional meeting or at the Spring 2022 ACS national meeting in San Diego, CA. As in previous years we are hoping that some of these participants will return to KU for graduate studies.

engage in ten weeks of full-time research, along with educational and professional development activities.

The program was back in operation in summer 2021, after the pandemic forced cancellation of



Caricato Research Group

Heterogeneous catalysts based on metal-doped amorphous silicates are characterized by quenched disorder and dynamical disorder. The first refers to the disordered siloxane network that is locked-in by strong bonds that do not rearrange on the time scale of the catalytic reactions. The second refers to the hydrogen bond network of the silanol groups that can rearrange quickly during the reactions. However, in quantum mechanical (QM) simulations of these materials, there is a third type of disorder that is often overlooked: the procedural disorder. This refers



RESEARCH HIGHLIGHT

to differences in energy and barriers of the active sites that are solely induced by the computational protocol used to create the supermolecular cluster models often used in these simulations. KU investigators Amy Jystad and Marco Caricato, along with collaborators from Univ. of Illinois, present a detailed investigation of this procedural disorder for the grafting of CrO_2 on the silica surface and propose a strategy to minimize it (Ind. Eng. Chem. Res., 2021, 60, 12834-12846). Specifically, starting from a silica structure obtained from classical molecular dynamics (MD) simulations, they demonstrate that relaxing a large portion of the cluster at the QM level before grafting minimizes the effects of procedural disorder, and the effect smoothly decreases with the size of the relaxed region. Therefore, this protocol allows accurate simulations of the active sites free of computational artifacts from the creation of the atomistic models. As part of this work, Marco was named to "I&EC Research's 2021 Class of Influential Researchers Award".

Dr. Michelle Buchanan (BS 1973)

*Senior Technical Advisor to the Deputy for Science Programs at the DOE Office of Science
Former Deputy for Science and Technology Oak Ridge National Laboratory*



Dr. Michelle Buchanan was the Deputy for Science and Technology at Oak Ridge National Laboratory (ORNL) until recently and is now on special assignment to the Department of Energy as the Senior Technical Assistant to the Deputy for Science Programs for the Office of Science. Michelle received her B.S. in Chemistry from KU in 1973. She is a first-generation college student who grew up in Independence, Missouri and originally came to KU for our Russian program. Having discovered a passion for chemistry, she quickly corrected course and flourished. Unsurprisingly, Michelle was first drawn to chemistry in the freshman course of Dr. Clark Bricker. "It was Dr. Bricker who inspired me - he was phenomenal." Michelle studied the electrochemistry of transition metal complexes in the labs of Prof. Reynold Iwamoto and Prof. Jacob Kleinberg. Our department has always valued and encouraged undergraduate research and Michelle said that, "...this experience is definitely what really convinced me to pursue chemical research as a career." "Conducting research doesn't always go the way that you expect, but the anticipation of a new observation or discovery is simply addicting." She went on to say that, "My mentor, Reynold Iwamoto, told me that you should always give a student a first research assignment that

you know will work—with the first taste of success, the student would be hooked on research." Now hooked, Michelle went on to be the first woman to earn a Ph.D. in analytical chemistry from the University of Wisconsin in 1978.

Michelle joined ORNL that same year and has been promoted through the ranks to her current position of leadership. As Deputy for Science and Technology, she reported directly to the Director of ORNL and managed the entire research portfolio of the lab. As the ORNL site stated "... Dr. Buchanan oversees one of the nation's most extensive portfolios of research and development, spanning physical and materials sciences, energy and engineering sciences, computing and computational sciences, biological and environmental sciences, neutron sciences, and global security, for the U.S. Department of Energy and other sponsors." That is a

Chemical Biology training grant program, which Tim leads. As Tim noted, "Graduate students do not often hear from scientists who have had such accomplished careers at a National Lab, and they found Michelle's story compelling." He went on to say that the students were most interested in "...how Michelle has worked both with teams of researchers to tackle big problems and has also interacted with government officials to help define the grand scientific challenges faced by the U.S." Having an impact in both science and policy is appealing to many students and in a subsequent Q&A session, "Michelle was able to provide some insight into how to get involved in these fields."

Her broad background led her to be named co-Director of the National Virtual Technology Laboratory (NVBL, <https://science.osti.gov/nvbl>), which brought together scientists from all 17 national laboratories to address issues in the fight against COVID 19. "It was incredible to see how the expertise and the capabilities of DOE's national laboratories could rapidly pivot to support a national emergency—this is what labs are meant to do." Based on this leadership, she was asked to join the DOE Office of Science to continue to support inter-disciplinary programs at DOE. After a 42-year career at ORNL, she sees this position as another way to serve the greater scientific community.

"It was Dr. Bricker who inspired me - he was phenomenal"

-Dr. Buchanan

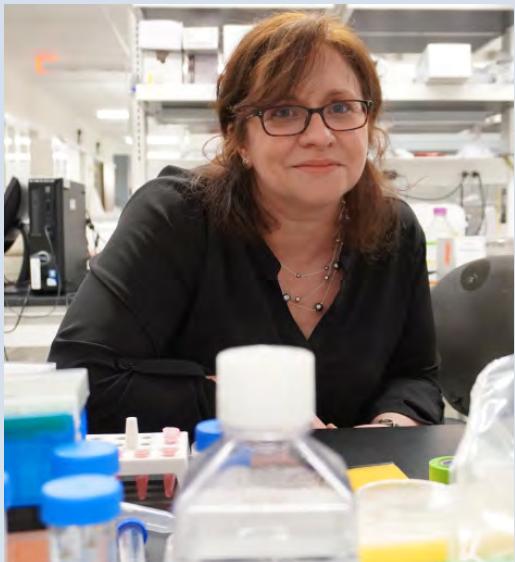
lot of "sciences"! How does one manage all of that? By being well-versed in many areas. Michelle has published on protein-protein interactions in bacteria, forensic chemical fingerprint analysis, small angle neutron scattering, materials in extreme environments, and the hydrogen economy, to name a few.

This past year, Michelle generously volunteered to share her experiences with the students taking Prof. Tim Jackson's graduate-level "Careers in the Biomedical Sciences" class. This course is part of the curriculum for the NIH

When asked about her time at KU, Michelle said that it was, "...enriched by a group of professors who really cared for their students and wanted them to succeed. From encouraging me to persevere in pursuing a career in chemistry to having a group of six professors sit around a conference table with me to help select which graduate school offer to accept—it was the dedication of the professors that really inspired me. I have endeavored to continue their tradition of mentoring staff and students, which has been the most enjoyable aspect of my career."

Maggie Witek:

2021 Steven F. Warren Research Achievement Award Recipient



Research Associate Professor Maggie Witek was one of three recipients of a 2021 Steven F. Warren Research Achievement Award. This award was established in 2006 to recognize outstanding academic staff researchers and comes with a \$10,000 prize for research. Maggie is an Associate Research Professor of Chemistry and team leader in the Center of BioModular Multi-Scale Systems for Precision Medicine. She received her master's degree in chemical technology from Silesian University of Technology in Poland and Ph.D. in analytical chemistry

from Michigan State University. Working with Professor Steve Soper, she is developing new liquid biopsy approaches for the early detection of disease and creating enabling technologies for isolating and analyzing circulating tumor cells and exosomes. For the past few years she has been teaching our undergraduate analytical chemistry laboratory course and is actively involved in organizing workshops and public outreach activities to highlight the role of chemists in advancing developments in precision medicine. Congratulations, Maggie!

In the summer of 2021, Betsy Carlson, our former Program Coordinator for the department, reached out with an opportunity to apply online to represent the American Chemical Society at the United Nations Framework Convention on Climate Change (UNFCCC) 26th Conference of the Parties (COP26). Needless to say, this was the opportunity of a lifetime. Since being accepted into the program and attending COP26 in Glasgow, Scotland, I could not be more thrilled to continue to communicate the amazing experiences I had at these climate change talks and to express my gratitude to the Department of Chemistry for their support of my journey.

My team of four undergraduates and I had the privilege of obtaining status as accredited observers, allowing us to

attend a range of discussions spanning from new innovative climate technologies to the implementation of science-centered policies in corporations and government. My goal in attending was to better understand the mechanisms for adopting alternative energy techniques and the policies that support such work. My research in the Blakemore Group seeks to contribute to the improved sustainability of nuclear fuel technologies. After careful research on these new scientific methods for the mitigation of harmful climate effects, along with my participation in an extension conference, I am very excited to be presenting this combined work at the ACS Spring 2022 Meeting in San Diego, California. Expanding my knowledge on such topics has broadened my view

of the field of chemistry and the ways in which understanding science can be made accessible for all. In addition, the dissemination of such important information to young students has a role in building climate literacy. I am incredibly fortunate to be involved with this and will continue working in the months and years to come. I am thankful that at the University of Kansas, particularly in the Department of Chemistry, such opportunities for young researchers to grow are abundant. Thank you for the support. Rock Chalk!

-Claire Dopp

Note: Claire's travel was supported by a Robert G. Carlson Travel Award. Thank you to everyone who has contributed to this worthy fund.





Pictured: Dr. Abraham Opalade, 2021 PhD Graduate

Research Highlight

Imitation is the Sincerest Form of Flattery

The pathogenic fungi *G. graminis* and *M. oryzae* can decimate crops such as wheat and rice. The growth of each of these fungi depends upon a lipoxygenase (LOX) enzyme, which catalyzes the formation of cell-signaling molecules. While LOX enzymes are found in nearly all organisms, these fungi use a form of the enzyme that has a manganese ion in the active site. Abraham Opalade's PhD dissertation project in the Jackson Lab was to create and study chemical reactions that mimic key steps in the mechanism of manganese-dependent LOX enzymes.

In a recent publication in *J. Am. Chem. Soc.*, Abraham generated a manganese(III)-hydroxo adduct that mimics a key intermediate in the LOX enzyme. While manganese(III)-hydroxo adducts had been generated before, Abraham used some clever synthetic techniques to position a hydrogen-bond acceptor adjacent to the hydroxo ligand. The resulting hydrogen

bond mimics interactions observed in the LOX active site. The hydrogen bond also made the synthetic manganese(III)-hydroxo unit significantly more reactive than a control complex lacking this interaction.

In a separate study in *Chemical Science*, Abraham described the formation and characterization of a manganese(III)-alkylperoxo adduct, another intermediate proposed to form in LOX enzymes. In this study Abraham built off initial observations made by a previous graduate student (Josh Parham; PhD 2019). While previously reported manganese(III)-alkylperoxo were thermally unstable, the complex Abraham and Josh reported was stable at room temperature, allowing its properties to be studied in detail.

Dr. Opalade successfully defended his PhD dissertation this July (graduating with Honors) and is currently a Research Scientist at Gilead Sciences.

NSF Grant

KU Chemistry Leads Successful Effort to Enhance High-Performance Computing at KU

Thanks to a recent grant from the National Science Foundation, a high-performance computing cluster will be built at KU. This cluster, nicknamed *BigJay*, will become a major part of the KU Community Cluster housed in the state-of-the-art Advanced Computing Facility. *BigJay* represents a million-dollar effort led by Prof. Brian Laird with co-investigators from chemistry (Ward Thompson), computational biology (Yinglong Miao), and electrical engineering/computer science (Suzanne Shontz). The new cluster will benefit 24 research groups spanning 11 different academic departments and programs at KU. Select undergraduate institutions from across the country were also included and will have access to *BigJay* to support their undergraduate research efforts. The advanced cluster will enable the development of exciting new computational methods, impacting important areas from energy storage to medical diagnostics. *BigJay* will help expose our graduate and undergraduate students to advanced computing techniques and foster collaborative research efforts across the campus. Chemistry led the way on this effort and obligated significant matching funds to acquire *BigJay*. The matching funds came from generous donations made to the department through our endowment association. Thank you again for all your support!



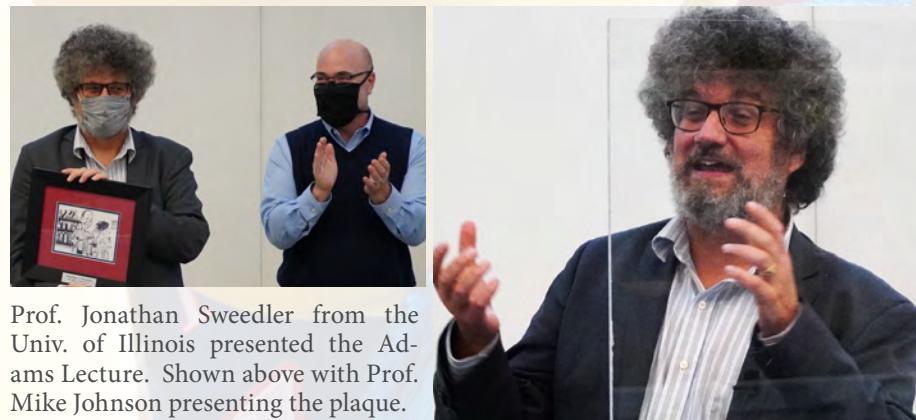
KU Advanced Computing Facility where *BigJay* will be housed.



In-person graduate ceremonies resumed this year. Newly minted Ph.D. students, Achala Punchi Hewage and Thilanga Pahattuge, enter the stadium. Prof. Steve Soper greeted graduates in full regalia.



Combined poster session from the NSF-REU programs held in the hallway of Gray-Little Hall. (Left) Anthony Gideon from Clayton State University explains his results from the summer spent in the lab of Prof. Misha Barybin.



Prof. Jonathan Sweedler from the Univ. of Illinois presented the Adams Lecture. Shown above with Prof. Mike Johnson presenting the plaque.

Artist Marty Gibson and her daughter Demaree drove a U-Haul from Arizona to donate her art. Now available for sale with proceeds to benefit Chemistry!



Prof. Dave Benson surprises Janet Lee with a student award during class. We adopted a roving prize patrol to replace our canceled Awards Banquet.



Graduate students Prabhavie Opallage and Piyanka Hettiarachchi enjoy a cookout organized by the GSO. Among other activities, some enjoyed a spirited game of volleyball away from the lab!



In Memoriam



Dr. Shih-I Chu passed away peacefully in Taipei, Taiwan on August 7, 2021. He was 78 years old and lived a long, happy life including 41 years as a professor at KU. A fervent Jayhawk basketball fan, he is survived by his wife, Wen Wen Chu, and three adult children, Emmeline Wong (Greg), Kim Bramel (Jeff), and Alexander Chu (Michelle). He was a beloved grandpa to six grandchildren. Dr. Chu cared about his family very much and would do anything for them. He enjoyed traveling on family vacations to see National Parks throughout the USA including Yellowstone, Yosemite, and the Rocky Mountains.

Dr. Chu was a prominent figure in the fields of quantum science and computational science. By developing numerous theories and computation methods, Dr. Chu made pioneering contributions in atomic, molecular, and optical physics; intense and ultrashort laser fields; chemical physics; many-body resonances; time-dependent density functional theory; quantum chaos and fractals; and scattering theory and reaction dynamics. After receiving his Ph.D. in chemical physics from Harvard University in 1974, Dr. Chu taught at the Department of Physics at Yale University and the Department of Chemistry at the University of Kansas, where he became a Distinguished Professor in 1990.

In addition to his outstanding scholarly achievements, Dr. Chu dedicated himself to nurturing young scientists, founding the Kansas Institute for Theoretical and Computational Chemistry and the Kansas Center for Advanced Scientific Computing at the University of Kansas to support research in these fields. During his distinguished career, Dr. Chu received numerous honors, including election as Fellow of the American Physical Society and member of the World Academy of Science. Dr. Chu was elected Academia Sinica Academician in 2006.

After returning to Taiwan in 2007, he continued to support scientific developments in quantum science and engineering. Dr. Chu was a talented theoretician and respected colleague; he will be greatly missed at KU.

Emeritus Distinguished Professor Daryle H. Busch passed away on May 19, 2021 at the age of 93. Professor Busch was a prominent leader in the field of transition metal coordination chemistry and one of the founding fathers of synthetic macrocyclic chemistry. He is survived by his wife, Geraldine Barnes (Jeri) of 70 years and their children Michael C. Busch, Steven J. (Becky) Busch, Cheryl A. (John) Rome, Kristina M. (Eric) Rodriguez, plus eleven grandchildren and ten great-grandchildren. He was predeceased by a sister, Robbie Joanna and Derek H., a son.

Prof. Busch began his teaching and research career at The Ohio State University (OSU), where he served on the faculty from 1954 to 1988. During that time, he established himself as an international leader in inorganic chemistry. Dr. Busch joined the faculty at KU in 1988 as the Roy A. Roberts Distinguished Professor of Chemistry, where he continued to make significant scientific contributions until his retirement in 2013. Dr. Busch was the first to devise an intentional strategy that resulted in the synthesis of molecules that were initially known as synthetic macrocycles, first published in the early 1960s. Over the next several decades macrocyclic chemistry exploded into many areas of chemistry including applications in biomedicine, catalysis and materials science.

While at KU, Dr. Busch proactively encouraged collaborative research and worked with Professor Bala Subramaniam (Chemical and Petroleum Engineering) to establish KU's Center for Environmentally Beneficial Catalysis (CEBC). In 2000, he was elected President of the American Chemical Society (ACS) and was also active in the American Association for the Advancement of Science (AAAS) and the International Union of Pure and Applied Chemistry (IUPAC). Among his many awards include the ACS Award in Inorganic Chemistry; ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry; the Dwyer Medal in Coordination Chemistry; and the Izatt-Christensen Award in Macroyclic Chemistry. He had over 400 publications, including five books and 14 patents.

Professor Busch was a highly creative scholar, with incredible instinct and understanding of chemistry at the molecular level. He was a dedicated teacher and mentor to his many students both in the classroom and in his research enterprise. Finally, he was a valued colleague and friend that will be greatly missed by all of us here at KU.

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PLEASE SUPPORT CHEMISTRY AT KU

The mission of Jayhawks Rising, KU's strategic plan, is to educate leaders, build healthy communities and make discoveries that change the world. KU Chemistry is meeting each of these goals through our exceptional community of scholars, but we need your support to help us rise to this challenge. Scholarship support helps make a KU degree possible for students from underrepresented minority populations. Support for research advances great ideas and

helps find answers to complex questions. Faculty support provides a lift for those working hard to teach, mentor, and do research in an exceptionally difficult budget environment. We welcome your support of the department and appreciate your investment in KU Chemistry. The easiest way to make a gift is to go to www.kuendowment.org/givenow.



There will be a field for you to designate that you'd like your gift to support KU Chemistry. If you'd like to know more about how you can make a difference in the lives of our students or faculty, contact Dan Simon, Team Lead & Senior Development Director at KU Endowment (dsimon@kuendowment.org or 785.832.7378). Thank you for your support and Rock Chalk!



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