

# KSU CHEMIST



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## From the Department Head

Dear Friends:

The afternoon of May 22, 2018 brought several fire trucks to the pedestrian mall in front of the CBC Building. Initially I worried that something serious had happened in our building that I had not yet heard about. A quick step outside made clear that the problem was actually at the library. My first thoughts were that a piece of equipment had overheated as is most often the case. But, as the afternoon went on, and more trucks and up to 70 fire fighters showed up, it became clear this was something much more significant. Needless to say, it was a very serious situation. The fire that occurred in the historic Farrell Library section of Hale Library has now shut down the entire library indefinitely, and for several days also shut down all regular phone and internet service on campus. The recovery from this fire will require a long time and has already involved a substantial amount of work by K-State staff and contractors. As with all projects at K-State, many

jumped right in to help where they could. In addition to difficulties with regular communications, Chemistry was directly impacted by a disruption in building temperature and humidity regulation. It turns out our building environment is monitored and controlled via the internet! As with the library, several faculty and staff moved quickly to locate or acquire and distribute dehumidifiers to help those doing moisture sensitive chemistry and to protect sensitive equipment. While relatively minor compared to the problems at the library, it's so very nice to work with people who are willing to drop what they are doing on short notice to help others in a time of need. The people are what brought me to K-State 22 years ago, and the positive, helpful environment survives to this day, making clear that no matter our current challenges, the future at K-State is bright! Best wishes to you all!

*David A. Higgins*

## Renovating Space in King Hall

Some of our space in the Chemistry Department is in real need of upgrades to help us fulfill our educational and research missions, and in some cases, these upgrades are required for safety reasons. We're thinking about starting our own cable TV series *Renovating Reactions*, focusing on renovations of chemistry lab space.... Anybody think it could be popular?

King Hall (1966) was renovated most recently in 1998. At the time, all the fume hoods and associated ducts and fans were replaced. The building also got new carpet and new paint, and two new technology classrooms. The lab benches also got fresh coatings of epoxy resin. The chemical storerooms used for our freshman labs were left largely unchanged. Recently, it was recognized that the dumbwaiter shaft, and some of the utilities chases were left open and would make for nice chimneys in the event of a fire. Under the original codes, some walls also were not extended fully to the ceiling.

The picture below shows progress on these renovations. The dumbwaiter is now gone and the openings are filled in. The storerooms will also get new fire rated ceilings in the process.



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## An Enhancement to Our Departmental Instrumentation

Chemists rely heavily on sophisticated instruments to verify that chemical compounds being synthesized are actually obtained, and to characterize chemical structures from small molecules to proteins. The instrument facility in the Department of Chemistry houses many such instruments, including two high-field NMR spectrometers. One of these is a new 600 MHz instrument that is sometimes used for routine experiments, but is primarily dedicated to magnetic resonance imaging (MRI) experiments on mice! The other is an aging 400 MHz instrument made by a company that no longer exists. It is slowly dying and is challenging to maintain, because replacement parts are hard to come by. In fall 2017, a group of faculty, led by Prof. Duy Hua, put together a proposal to the National Science Foundation, requesting funds to support the purchase of a new 400 MHz instrument capable of both liquid and solid-state experiments. Just recently, we heard our proposal would be funded, for \$416,212, with matching funds of \$178,372 provided by the Department and other offices on campus. We are now ordering the new instrument and are all very excited for its arrival. It will be used for both research and teaching, providing many students the opportunity to be trained on a state-of-the-art spectrometer. A good fraction of the matching funds have been provided through the generous contributions of our alumni and friends. Thanks to you all for your continued support of our programs!





## Transitions in the Chemistry Department

### New Arrivals



#### Dr. Simon Sham

Simon joined our department in late 2017, and serves as our Instrumentation Facility Manager. He is a skilled NMR spectroscopist with extensive experience in both solution-phase and solid-state NMR, and comes to us from a previous position as the NMR/EPR manager in the Department of Chemistry and Biochemistry at Utah State University. He is interested in teaching an NMR course sometime soon and enjoys interacting with students, and training them to use both our 400 and 600 MHz instruments. His days serving as nurse for our aging 400 MHz instrument will soon come to an end as our NSF proposal (led by Prof. Duy Hua) for a new 400 MHz NMR spectrometer was recently funded!

#### Dr. Elizabeth Ploetz

Elizabeth got her BS, MS, and PhD degrees at Kansas State University, working with Prof. Paul Smith. She subsequently moved on to a position as Visiting Scientist at the University of Groningen, before beginning postdoctoral work at the Johns Hopkins School of Medicine, where she was supported by a prestigious Ruth L. Kirschstein Postdoctoral Fellowship from the NIH. Her research interests are in molecular dynamics simulations of liquids. She will be teaching in our freshman program this fall.



#### Dr. James Townsend

Jamie got his M. Chem. From Nottingham Trent University and then completed his PhD at Kansas State University. Afterwards, he moved to Kansas Wesleyan University where he is currently an Associate Professor and the Department Chair. He will be on leave from Kansas Wesleyan this next year and will be teaching organic chemistry courses in our department while Prof. Mark Hollingsworth is on leave. He has also recently been teaching organic courses at K-State during the summer.

#### Dr. Kanika Sharma

Kanika received her BS, MS, and M.Phil degrees at the University of Delhi, and then completed her PhD at Kansas State University. Her research at K-State was performed under the direction of our former Head, Prof. Eric Maatta. Afterwards, she taught at Humboldt State University before recently returning to Manhattan. She will be teaching our Environmental Science class and lab this fall and will be teaching in the freshman program during the spring term.



### Departures

Sadly, a few of our faculty and staff have decided to pursue other opportunities. Each had been making vital contributions to our educational and research missions, to the positive atmosphere in our program, and each of them will be greatly missed! After several successful years here, Assistant Professor Emily McLaurin announced early in the year that she would be leaving academics to explore a different career path. Assistant Teaching Professor Laura Fox also announced she would be leaving K-State to move back to Minnesota and a better opportunity to fulfill her life plans outside of work. Most recently, our long-term Organic Laboratory Director and general chemistry lecturer, Associate Teaching Professor Lou Wojcinski announced he had accepted a position as an Instructor at Oregon State University. Finally, after two years of service to the Chemistry Department, our Accountant Yvonne Bachura accepted a promotion that required she move elsewhere on campus. She continues to help us out regularly, largely by providing our accounting staff with access to custom-designed accounting software that she wrote. This software has greatly increased our operational efficiency while also providing our faculty and staff with more up-to-date information on the status of their extramural funding and state accounts!

## Chemistry Research Experiences for Undergraduates (REU)

During each of the previous several years, the Department of Chemistry has hosted a number of undergraduate researchers recruited from primarily undergraduate institutions (PUIs) across the U.S. and Puerto Rico. Our REU program is funded by the National Science Foundation and is led by Professors Chris Culbertson and Stefan Bossmann. This year we are finishing the second round of funding for our program. Over the last 8 years, we have provided the opportunity for 62 undergraduates to spend 10 weeks each performing research in our labs. Fifty percent of our participants have been female and 50% are from under-represented minority groups. Last year 8 of our 10 students presented posters about their research at the Midwest Regional ACS Meeting and 3 presented posters at a national ACS meeting. Almost two-thirds of our REU students have gone on to graduate school in Chemistry. We have convinced 5 of these to attend graduate school in Chemistry at K-State! We will be applying for a renewal of the program this fall.

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### Recent Graduates

#### Bachelor of Science

Kyle Daryl Apley  
 Riley Nicole Bowen  
 Morgan Nicole Fortunski  
 Patrick James Gillespie  
 Jacob Forrest Iverson  
 Sarah Nicole Lamm  
 Lydia E. Lawlor  
 Mechelle Catherine McCoy  
 Logan Michael McGinley  
 Alex Hale Peterson  
 Celesta Elyse Robinson  
 Dalia Cecilia Sanchez  
 Theresa Marie Vail  
 Kellie Weeks

#### Graduate Degrees

##### **Stefan Nirasher Lorenzso Andree, Ph. D.**

Major Prof: Christer Aakeröy  
 Title: From Supramolecular Chemistry to Crystal Engineering using Hydrogen and Halogen Bonds.

##### **James Emery Brown, Ph. D.**

Major Prof: Jun Li  
 Title: Advances in Electrical Energy Storage Using Core-Shell Structures and Relaxor-Ferroelectric Materials.

##### **Medha Jaimini Gunaratna**

##### **Anhettigama Gamaralalage, Ph. D.**

Major Prof: Duy Hua  
 Title: Design, Synthesis and Bio-Evaluation of Piperidines and CGRP Peptides; Synthesis of Substituted 6-(dimethylamino)-2-phenylisoindolin-

1-ones for the Inhibition of Luciferase.

##### **Bo Hao, Ph. D.**

Major Prof: Duy Hua  
 Title: Microscale Analysis Systems for the Study of Proteins and Proteases.

##### **Natalia Vladimirovna Karimova, Ph. D.**

Major Prof: Christine Aikens  
 Title: Theoretical Study of the Optical Properties of Noble Metal Nanoparticles: CD and MCD Spectroscopy.

##### **Kathleen Ann Sellens, Ph. D.**

Major Prof: Christopher Culbertson  
 Title: Identification of *In-Vivo* Protein-Protein Binding Partners in *Anopheles Gambiae* by Immunoaffinity Chromatography and Mass Spectrometry.

##### **Ravithree Dhaneeka Senanayake, Ph. D.**

Major Prof: Christine Aikens  
 Title: Electron-Nuclear Dynamics in Noble Metal Nanoparticles.

##### **Ruben Shrestha, Ph. D.**

Major Prof: Ping Li  
 Title: Molecular Mechanism and Enzymological Studies of Dye-Decolorizing Peroxidases (DyPs) from *T. Curvata* and *E. Lignolyticus*.

##### **K. L. Dimuthu M. Weerawardene, Ph. D.**

Major Prof: Christine Aikens  
 Title: Optical and Luminescence Properties of Noble Nanoparticles.

##### **Manomi Dharshika Perera, Ph. D.**

Major Prof: Christer Aakeröy  
 Title: Hydrogen and Halogen Bonding in

Co-Crystallization from Fundamentals to Applications.

##### **George Valentin Podaru, Ph. D.**

Major Prof.: Viktor Chikan  
 Title: Exploring Controlled Drug Release from Magneto Liposomes.

##### **Bo Wang, Ph. D.**

Major Prof: Mark Hollingsworth  
 Title: Synchrotron Studies of "Self-Compression" in Urea Inclusion Compounds.

##### **Chamitha Janani Weeramange, Ph. D.**

Major Prof: Ryan Rafferty  
 Title: Inhibition of UDP Glucose Dehydrogenase by 6-Thiopurine (6TP) and its Oxidative Metabolites: Possible Mechanism for its Interaction within the Bilirubin Excretion Pathway and 6TP Associated Toxicity.

##### **Chelsea Nicole Weese, M. S.**

Major Prof: Ryan Rafferty  
 Title: Synthetic Efforts Toward Lagunamide C: Route Development and Implementation upon a Model System.

##### **Jing Yu, Ph. D.**

Major Prof: Stefan Bossmann  
 Title: Structure Determination, Mechanistic Study, and Safe Delivery of an Anti-Cancer Peptide.

##### **Xingao Zhang, M. S.**

Major Prof: Emily McLaurin  
 Title: Charge Transfer between TCNQ and Different Sizes of InP Quantum Dots.

## Giving to the Chemistry Department

A Hearty **THANK YOU** to all who have given to Chemistry this past year!

Total giving to the Department of Chemistry from July 1, 2017 to June 30, 2018, in each of four general areas is shown below. These represent both expendable funds and contributions to our permanent endowment by many individual, corporate, and foundation donors. We are grateful to all our faithful alumni and friends for their continued support!

**Undergraduate Student Scholarships: \$322,600**

Undergraduate scholarships are awarded directly to our individual students majoring in Chemistry. The funds are commonly used by the students to pay tuition, room and board expenses, and to purchase textbooks.

**Graduate Student Fellowships: \$799,700**

Graduate student fellowships help pay student stipends so that they may concentrate on their research projects.

**General Departmental Support: \$157,300**

General departmental support is critical to the operation of our department, and is used to pay for seminar speakers, faculty travel to conferences, startup funds to our new faculty, and matching funds for large equipment grants.

**Chemistry Instrumentation Support: \$20,100**

These funds are used to help maintain our chemical instrumentation for use in both teaching and research. Due to recent budget challenges, they are now also used to help pay the salaries of our skilled instrumentation support staff.

## News from Our Research Groups

### Analytical

Jun Li's group is working on developing nanotechnology for cancer diagnosis (supported by a National Cancer Institute grant with Duy Hua), and next-generation batteries and fuel cell catalysis (supported by two NSF grants). A patent on nanoelectrode array based protease biosensors has been awarded and is in negotiation for licensing. Prof. Ito was awarded a NSF grant with researchers at Indiana University to design nanopores for chemical sensing in aqueous media. Chris Culbertson and Stefan Bossmann are developing a point of care microfluidic device for early (stage 0 and 1) diagnosis of lung, pancreatic, prostate and breast cancers in research supported by two NSF grants and a Johnson Cancer Center grant from Eric Stonestreet. Dan Higgins continues his work in single molecule detection and spectroscopy and was recently awarded a new NSF grant to study aldol condensation reactions at the single molecule level with Keith Hohn (Chemical Engineering).

### Inorganic

Tendai Gadzikwa was awarded an NSF grant for her work on "Enzyme-Inspired Catalysis in Multifunctional Metal-Organic Framework Materials". Peter Sues set-up his lab and started two new projects on olefin metathesis and small molecule activation with two new graduate students. The Aakeroy group's work on improving urea as a fertilizer was published in ChemComm and was highlighted by two 'general interest' publications/websites (Chemistry World and Chemistry Views). Emily McLaurin's group is wrapping up research on their indium phosphide quantum dots.

### Organic

Over the past year, 24 papers have been published by our six faculty, numerous (>30) papers were presented at conferences, and several major grants were funded. Ping Li has continued his work in lignin degradation and was recently awarded an NSF grant to support this work. Duy Hua has continued his work in synthetic methodology and the construction of new bioactive agents. He was recently awarded NIH and NSF grants for these projects. Sadly, Prof. Hua will begin four years of phased retirement this coming fall. While he will continue to mentor graduate students in his laboratory, future students will miss out on his amazing lectures in the classroom. Stefan Bossmann continues his active, productive research in the development of "liquid biopsies" and other nanomaterials-based methods for early-stage detection of breast, lung, pancreatic, and thyroid cancers. He also has the distinct honor of being the only(?) active researcher in a Chemistry Department with funding from the National Endowment for the Arts, in collaboration with Jason Scuille (Art).

### Physical

Christine Aikens and Paul Smith received an NSF Major Research Instrumentation grant to enhance computational chemistry at KSU through upgrades to the Beocat supercomputer. Paul Smith gave a Plenary Lecture at the *International Conference on Computational Modeling and Simulation*, in Colombo, Sri Lanka. Ryszard Jankowiak delivered multiple invited lectures in venues around the world, include at the *International Conference on Quantum Effects in Biological Systems*, in Vilnius, Lithuania. Viktor Chikan continued his work in helping establish the ELI-ALPS research facility in Szeged, Hungary.

## Recognition and Awards

Faculty	Graduate Students
<p><b>Christer Aakeröy:</b> 2017 Midwest Regional Award, American Chemical Society</p> <p><b>Christine Aikens:</b> Commerce Bank and WT Kemper Foundation Distinguished Graduate Faculty Award</p> <p><b>Stefan Bossmann:</b> Ervin W. Segebrecht Distinguished Faculty Achievement Award, 2017</p> <p><b>Stefan Bossmann:</b> Named one of the 50 Kansans You Should Know, Ingram's 2018</p> <p><b>Christopher Culbertson:</b> Promoted to Professor</p> <p><b>Ryszard Jankowiak:</b> Elected a Distinguished Fellow of the Collegium, Kosciuszko Foundation</p> <p><b>Jun Li:</b> Ervin W. Segebrecht Distinguished Faculty Achievement Award, 2018</p>	<p><b>Bhupinder Sandhu (Aakeröy):</b> PLU Award</p> <p><b>Nilusha Kariyawasam (Smith) and Zi Li (Higgins):</b> Graduate Research Award</p> <p><b>Jing Yu (Bossmann):</b> Mitsugi Ohno Award</p> <p><b>Jay Sibbitts (Culbertson):</b> Meloan Award in Analytical Chemistry</p> <p><b>Herman Coceancigh (Ito) and Govinda Chimire (Ito):</b> Chemistry Alumni Award</p> <p><b>Amila Abeysekera (Aakeröy):</b> PLU Classroom Performance Award</p> <p><b>Olivia Hull (Aikens):</b> Department of Energy Computational Science Graduate Fellowship</p> <p><b>Bhupinder Sandhu:</b> 2018 Graduate Award for Leadership and Service, K-State Alumni Association</p> <p><b>Tuyen Nguyen:</b> Scott Fateley Memorial Award</p> <p><b>Herman Coceancigh:</b> Fateley-Hammaker Collaboration Award</p> <p><b>Tuyen Nguyen (Aryal):</b> John Berschied and Donna Derstadt Fellowship</p> <p><b>Mahboobe Jassas (Jankowiak)L</b> Jerry and Judy Reed Fellowship</p> <p><b>Kaimin Jia (P. Li):</b> Dane G. Hansen Fellowship</p>
Undergraduate Students	
<p><b>Kyle Apley (Hua) and Annie McLean (Aakeröy):</b> PLU Undergraduate Research Award</p> <p><b>Kyle Apley and Annie McLean:</b> Senior PLU Classroom Performance Award</p> <p><b>Erin Meyers and Makena Utech:</b> Junior PLU Classroom Performance Award</p> <p><b>Abigail McCormick and Mikaela Moore:</b> Sophomore PLU Classroom Performance Award</p> <p><b>Douglas Farleigh and Joseph Kempin:</b> Freshman PLU Classroom Performance Award</p> <p><b>Kyle Apley:</b> National Science Foundation Graduate Fellowship</p>	<p>Cover Photo: Students attending the 2<sup>nd</sup> Annual Chemistry Undergraduate Research Poster Session, hosted by the American Chemical Society Student Affiliate. Photo Credit: Olivia Haney.</p>