RICE NATURAL SCIENCES
Chemistry

CHEM NEWSLETTER

SPRING 2022

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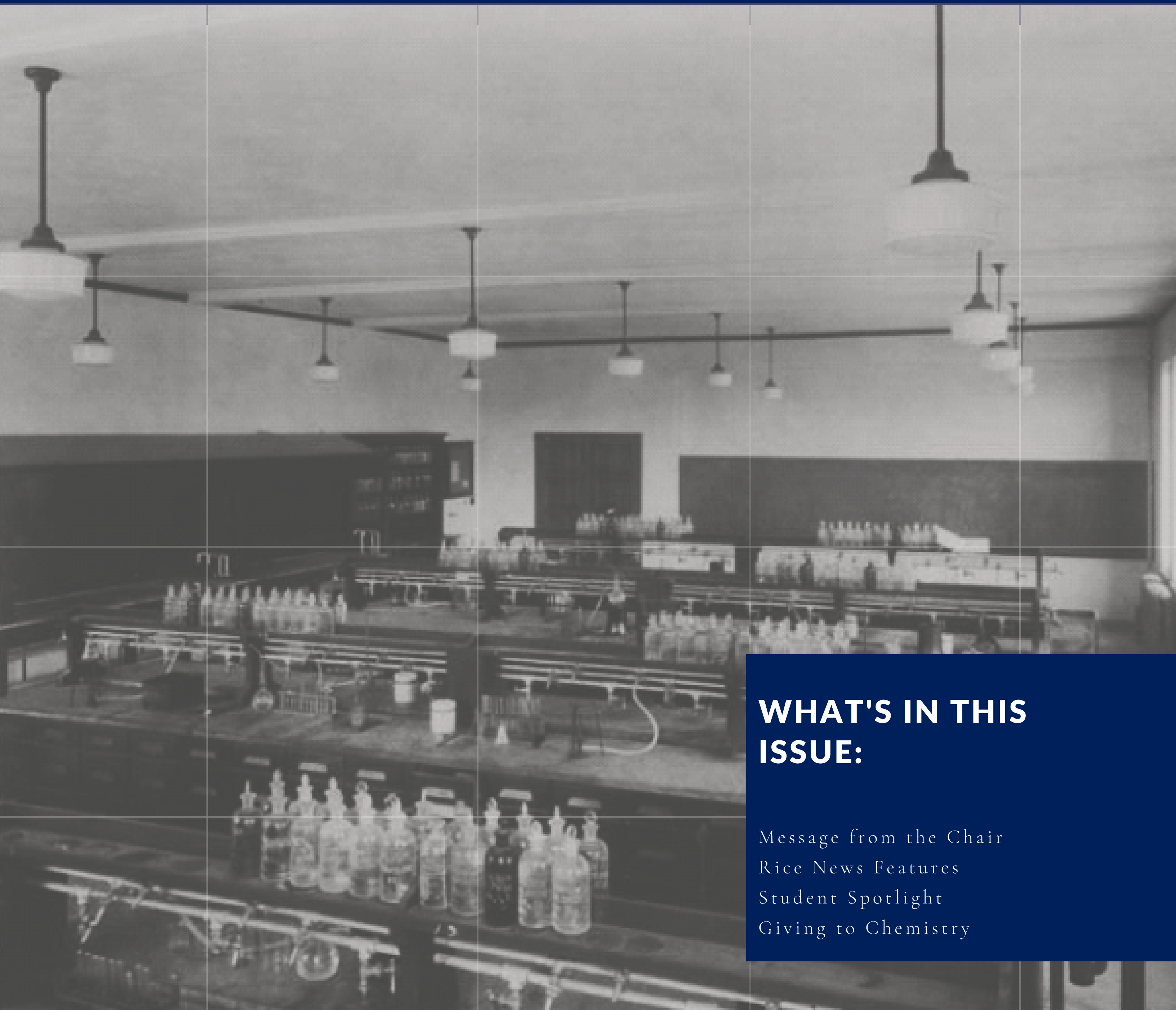


WHAT'S IN THIS ISSUE:

Message from the Chair

The Department of Chemistry at Rice University continues our endless endeavor in research and educational fields. Please enjoy our CHEM Newsletter, which appears every 6 months, highlighting some outstanding recent accomplishments and news from the department.

We are excited to share our research successes that resulted in multiple research grants and awards. Jeff Hartgerink has been awarded a 2022 George R. Brown Award for Superior Teaching, and Kasey Leigh Yearty has received a 2022 Nicholas Salgo Distinguished Teacher Award. The department has also been awarded a new REU program from the NSF, and we thank Angel Marti and Michelle Gilbertson for carrying this important task.

We are also very excited to announce that three new faculty members are joining our department beginning July 1, 2022. Sam Yruegas, coming to us from Princeton University and Raul Hernandez Sanchez from University of Pittsburgh join us as assistant professors working in the area of inorganic/materials chemistry. Hans Renata, a specialist in organic chemistry from Scripps Research Institute in Florida joins us as associate professor. We wish them all the best in their new career at Rice!

In addition, please enjoy a few write-ups by some of our graduate students, written for your enjoyment.

We are looking forward to have more exciting news and research accomplishments from people at the Department of Chemistry!

Anatoly Kolomeisky, Chair
Department of Chemistry

Rice News Features

Our faculty, students and researchers are doing outstanding work in the classroom and in the lab. Catch a glimpse of a few of their stories featured on Rice News this cycle.

Rice lab improves recipe for valuable chemical

Skipping ahead in a line is rude, but sometimes it's acceptable. Especially for salt.

The Rice University lab of materials theorist Boris Yakobson shows why in its follow-up to a 2018 study that demonstrated how salt simplifies the formation of valuable 2D molybdenum disulfide (MoS_2) with a first-principles analysis of the process that could refine it even further.

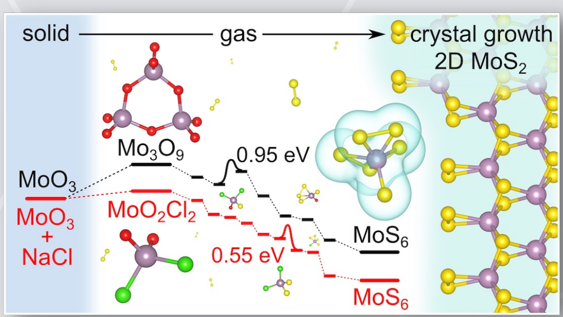
The theoretical study by Yakobson and colleagues Jincheng Lei, Yu Xie and Alex Kutana, all alumni of his lab, and researcher Ksenia Bets shows through the simulation of atom-level energies why salt -- particularly iodized salt -- lowers the reaction temperature in a chemical vapor deposition (CVD) furnace necessary to form MoS_2.

It does so by helping to skip some steps and leap high energy barriers in conventional CVD growth to yield far more MoS_6, an essential precursor to 2D MoS_2.

Their study in the Journal of the American Chemical Society focused on how salt lowers activation barriers to enhance the sulfurization of molybdenum oxyhalides, the gas feedstock in MoS_2 crystallization.

MoS_2 is a natural compound known in bulk form as molybdenite, and in 2D form is highly coveted for its semiconducting properties, which promise advances in electronic, optoelectronic, spintronic, catalytic and medical applications.

Full Article: news.rice.edu/news/2022/rice-lab-improves-recipe-valuable-chemical



Antibody with engineered peptide targets bone metastasis

A moderate amount of a peptide-enhanced, biological cancer drug goes a long way in treating breast cancers that metastasize to the bone.

A study by scientists at Rice University and Baylor College of Medicine demonstrated the effective treatment of such cancers in rodent models, bringing hope for new therapies to treat bone metastases.

The open-access study, to appear on the cover of the American Chemical Society journal ACS Central Science, advances techniques pioneered by Rice chemist Han Xiao and his co-author at Baylor, biologist Xiang Zhang.

They discovered through extensive testing that engineering "bone-homing" peptides and attaching them to a common breast cancer drug, the antibody trastuzumab, effectively targets and attacks bone tumors.

The researchers reported their surprise that injecting more of the drug compound doesn't make it better. The drug contains an engineered peptide that finds and binds to bone, but worked best when a moderate amount was delivered.

"The negative charge of the peptide has an affinity for the positively charged bone cancer niche," said Xiao, whose lab created a library of modified antibodies for testing. "We found the therapeutic efficacy is best with the antibody that has mediocre affinity. That's a really big discovery."

As many as 40% of breast cancer survivors eventually experience metastases to distant organs, most often to the bone. Xiao noted bone tumors are notoriously difficult to treat, given the hard nature of the material and its limited vascular network. Delivering a low amount of a drug, he said, can also help tumors develop resistance.

Full Article: news.rice.edu/news/2022/antibody-engineered-peptide-targets-bone-metastasis

Rice chemists skew the odds to prevent cancer

Theory shows mutations have few easy paths to establish themselves in cells and initiate tumors

The path to cancer prevention is long and arduous for legions of researchers, but new work by Rice University scientists shows that there may be shortcuts.

Rice chemist Anatoly Kolomeisky, lead author and postdoctoral researcher Hamid Teimouri and research assistant Cade Spaulding are developing a theoretical framework to explain how cancers caused by more than one genetic mutation can be more easily identified and perhaps stopped.

Essentially, it does so by identifying and ignoring transition pathways that don't contribute much to the fixation of mutations in a cell that goes on to establish a tumor.

A study in the Biophysical Journal describes their analysis of the effective energy landscapes of cellular transformation pathways implicated in a variety of cancers. The ability to limit the number of pathways to the few most likely to kick-start cancer could help to find ways to halt the process before it ever really starts.

"In some sense, cancer is a bad-luck story," said Kolomeisky, a professor of chemistry and of chemical and biomolecular engineering. "We think we can decrease the probability of this bad luck by looking for low-probability collections of mutations that typically lead to cancer. Depending on the type of cancer, this can range between two mutations and 10."

Calculating the effective energies that dictate interactions in biomolecular systems can predict how they behave. The theory is commonly used to predict how a protein will fold, based on the sequence of its constituent atoms and how they interact.

The Rice team is applying the same principle to cancer initiation pathways that operate in cells but sometimes carry mutations missed by the body's safeguards. When two or more of these mutations are fixed in a cell, they are carried forward as the cells divide and tumors grow.

Full Article: news.rice.edu/news/2022/rice-chemists-skew-odds-prevent-cancer

Matthew Jones wins NSF CAREER Award

Rice University chemist Matthew Jones has won a National Science Foundation (NSF) CAREER Award to discover how metallic nanoparticles find their sizes and shapes and ultimately control the process.

CAREER Awards, among the most competitive offered by the NSF, are typically given to fewer than 400 young scientists and engineers each year across all disciplines. According to the agency, they support "early career faculty who have the potential to serve as academic role models in research and education and to lead advances in the mission of their department or organization."

The five-year grant for more than $650,000, administered by the NSF's Macromolecular, Supramolecular and Nanochemistry program, will support his exploration of the fundamental processes of nanoparticle formation.

Nanoparticles have been well characterized by labs around the world, including those at Rice, for how they handle light and heat and catalyze chemical reactions. Famously, plasmonic gold nanoshells developed at Rice have enabled successful trials to obliterate prostate cancer in patients.

Full Article: news.rice.edu/news/2022/matthew-jones-wins-nsf-career-award

Closer look helps Rice lab ponder when a protein's prone to wander

A surface that feels smooth to human touch could be pretty rough to a protein. That can be good or bad, depending on what you want that protein to do.

Exactly how proteins interact with solid surfaces is a concern for health care manufacturers who design drugs, make biosensors or develop anti-fouling materials.

The mechanisms that control these interactions are hard to see, but researchers at Rice University are changing that with a microscopy technique to assess the effects of surface roughness as well as water-repelling properties (hydrophobicity) and electrostatic charge. The ability to tune those parameters will lead to more predictable materials.

"The main idea is to understand the how the combination of these properties influences protein dynamics," said Anastasiia Misiura, lead author of a study in the Journal of Chemical Physics and a graduate student in the Rice lab of chemist Christy Landes. "It turned out that roughness and hydrophobicity are opposite forces, but proteins get stuck on areas that are very rough."

The paper, an "editor's choice," is part of the journal's "Ever-Expanding Optics of Single Molecules and Nanoparticles" collection.

How molecules interact at surfaces is important at every scale in the physical realm, from grinding planetary plates to brakes grabbing the wheels in your car to the invisible molecular transactions that make life possible. Understanding these mechanisms at the very smallest level is the focus of Landes' lab as its members attempt to clarify what's actually happening down there.

On that end, the lab develops sophisticated microscopes that see things smaller than visible light and the best of lenses will allow. In this case, the lab used single molecule fluorescence microscopy, a technique that allows them to watch how proteins interact with the surfaces they design.

The team discovered two modes of transport that influence whether and how proteins attach themselves to a surface, travel along it or release their grip, never to return. The two distinct interaction mechanisms they found ranged from the quicker localized adsorption/desorption, associated with less hydrophobic surfaces, and an unpredictable continuous-time random walk observed in interactions with rough, more hydrophobic surfaces.

For experiments, the researcher placed a "well-studied model protein," fluorescent-labeled a-lactalbumin, on a surface with bare glass alternating with stripes in various concentrations of a self-assembled monolayer (SAM) commonly used to purify proteins via chromatography. Each stripe contained a different balance between hydrophobicity and surface roughness.

The bare glass showed plenty of localized action with proteins taking a longer time on the surface, while the degree of roughness in the SAM-covered regions (due to the concentration of octadecyltrichlorosilane, or ODTS) promoted longer flights. The degree of "stickiness" is associated with a greater concentration of long alkyl chains on the surface.

Full Article: news.rice.edu/news/2022/closer-look-helps-rice-lab-ponder-when-proteins-prone-wander

Student Spotlight

Rice Science Policy By: Jordin Metz

Science policy is a field that I knew nothing about when I entered Rice, but I did care about how my research would impact the world. That potential for impact, and the excitement of describing the big picture ideas of my research to others, is what led me to this field. Science policy is both how policy affects research and science and how science affects policy, and requires skills in scientific writing, communication, and advocacy. People who work in science policy must bridge the gap between technical expertise and policy. This is inherently interdisciplinary and can have wide-reaching effects on research funding and the implementation of research findings on laws and regulations. Appropriating NSF and NIH funding is one aspect, while writing laws about, for example, greenhouse gas regulations, is another.

In Spring 2020 I took a class with Rice's Baker Institute for Public Policy, which launched me on this path. The graduate students in the course later formed the Rice Science Policy Network, a student organization that has written op-eds, engaged in local advocacy and science communication, and hosted events. In April 2022, I co-hosted the Rice Science Policy Symposium, bringing the Rice community together for a hybrid event featuring speakers including Texas State Senator Carol Alvarado and President of the National Academy of Sciences Dr. Marcia McNutt. It was a great opportunity to learn about science policy —I highly recommend you watch Dr. McNutt's talk!

I'm excited that I will continue my journey in science policy and be able to apply my scientific expertise in a new, interdisciplinary way after I graduate. This Fall, I will serve as an AIP Congressional Fellow, part of the AAAS Science & Technology Policy Fellowships (STPF), working in Congress for a year as a science policy staffer.

Margrave Thesis Awardee

Xun Chen

Harry B. Weiser Research Awardee

Kuan-Lin Wu

Harry B. Weiser Teaching Awardees

Sarah Hulgan
Caroline Peterson
Nima Soltani
Hana Jaafari
Nahima Saliba

Harry B. Weiser Leadership Awardees

Jacob Beckham
Sam Castro
Michelle Duran-Chavez
Jesse Shooter
Vanessa Espinoza
Tracy Yu

Distinction in Research and Creative Works Awardees

Alex Berlaga
Robert Carter
Pearl Fernandes
Maia Helterbrand
Sohyun Lim
Hallie Trial

Arthur L. Draper Awardees

Pearl Fernandes
Hallie Trial
Nikhil Gattu
Michael Nevins
Alex Berlaga
Robert Carter
Maia Helterbrand
Sohyun (Alexandra) Lim

Spring 2022 Graduates

Graduate Degrees:

Xun Chen
Yuda Chen
Thasneem Frousnoon
Sarah Hulgan
Axel Loredo Pineda
Alicia Mangubat-Medina
LaurenMcCarthy
Alyssa Pollard
Zhe Wang
Lauren Warning
Lin Yuan

Undergraduate Degrees:

Ryan Armijo
Alexander Berlaga
Roberto Carcamo
Robert Carter
Andrew Cui
Pearl Fernandes
Elizabeth Fontana
Nikhil Gattu
Isaac Goforth
Maia Helterbrand
Eddie Jackson
Minjun Kim
Caroline Koester
Jared Lee
Sohyun (Alexandra) Lim
Sarah Mozden
Michael Nevins
Sanjay Pandiri
Ziyana Samanani
Emily Sierra
Hallie Trial
Kathryn Wall
Daniel Wang
Joseph (Tre) Williams
Aaron Wyderka
Ashley Zhou

RICE NATURAL SCIENCES
Department of Chemistry

GIVING TO CHEMISTRY

The global impact of Rice University is expanded and sustained by the accomplishments and support of our alumni and friends. The continued generosity of our donors is paramount to the mission and goals of Rice Chemistry. Graduate student education and research are top priorities in the Department of Chemistry. Graduate fellowships attract and sustain a strong body of doctoral students, an important component of our research programs and accomplishments. Endowments for graduate student fellowships provide an opportunity to complement and improve our chemistry graduate program, thereby contributing to educating and training the next generation of scientists to improve our healthcare, protect our environment, develop new and clean energy sources, and create the novel materials of the future—for all intents and purposes, for a better world.

Giving to Chemistry means supporting our academic efforts. Gifts to the General Support Fund have significant student impact by providing student stipends or other education needs of our students. Additional awards and endowed funds in the Chemistry Department are also established to support various aspects of teaching, learning, and research. To learn more about our funds, please visit our website: https://chemistry.rice.edu/give-chemistry Your gift will tremendously help our research program in advancing science and in training new generations of educated specialists. If you would like to know more about how you can support the Department of Chemistry please contact the Wiess School of Natural Sciences Director of Development Jackie Macha at jackie.macha@rice. edu or 713-348-4268. We are grateful for your support. Thank you!

The Department of Chemistry thanks you very much for your continued support!

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Let us know what you've been up to since leaving Rice by filling out our alumni form:
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