CHEM Newsletter

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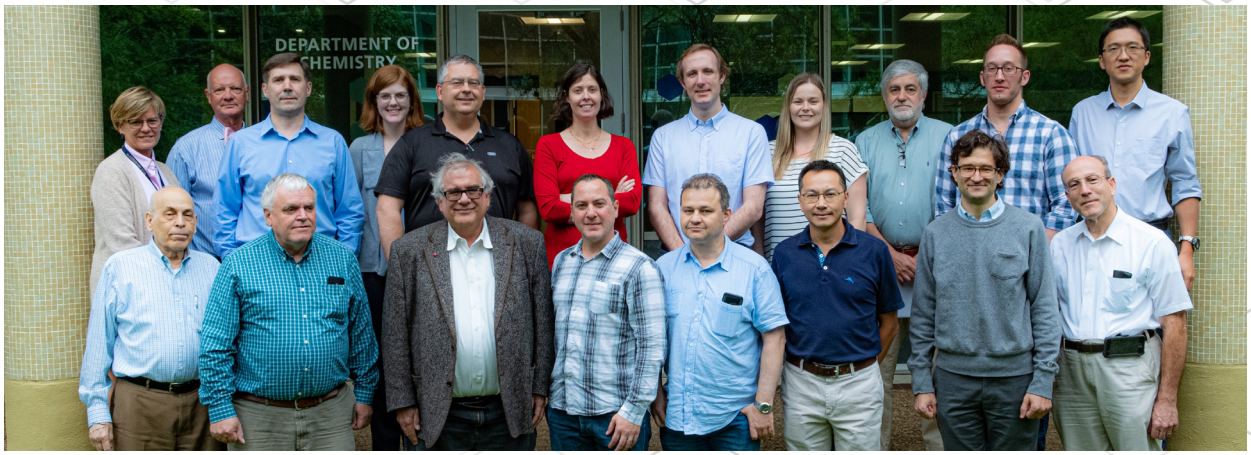
Where innovation meets collaboration. chemistry.rice.edu

Message from Chair

The Department of Chemistry continues to flourish with new opportunities and research endeavors. Please enjoy our second CHEM Newsletter, which will appear every 6 months, highlighting some of the recent accomplishments and several exciting news in the Department.

We are happy to announce that we have recruited a new assistant professor, Dr. Anna-Karin Gustavsson, an extraordinary talented researcher in the field of experimental physical chemistry and biophysics. She completed her Ph.D. degree with Prof. Mattias Goksör, University of Gothenburg, Sweden. She is currently at Stanford University where she holds an NIH K99 Postdoctoral Fellowship working for Nobel Laureate Prof. W.E. Moerner. Anna-Karin will join the Department of Chemistry at Rice University on August 1, 2020, as a recipient of a prestigious Cancer Prevention and Research Institute of Texas (CPRIT) grant. Dr. Gustavsson's arrival strongly increases our research capabilities and improves our diversity. We are very happy about this event since it shows that our program can attract the best scientists in the world!

Anatoly Kolomeisky, Chair,
Department of Chemistry



Faculty, from left to right: (Top Row) Michelle Gilbertson, Ken Whitmire, Eugene Zubarev, Kasey Leigh Yearty, Laszlo Kurti, Christy Landes, Julian West, Krista Kobylianskii, Gustavo Scuseria, Matthew Jones, Han Xiao (Bottom Row) Paul Engel, Bruce Johnson, Peter Wolynes, Angel Marti, Anatoly Kolomeisky, Mike Wong, Zach Ball, Larry Alemany

IN THIS ISSUE

Anna-Karin will join the Department of Chemistry at Rice University on August 1, 2020.

RICE NEWS *features*

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

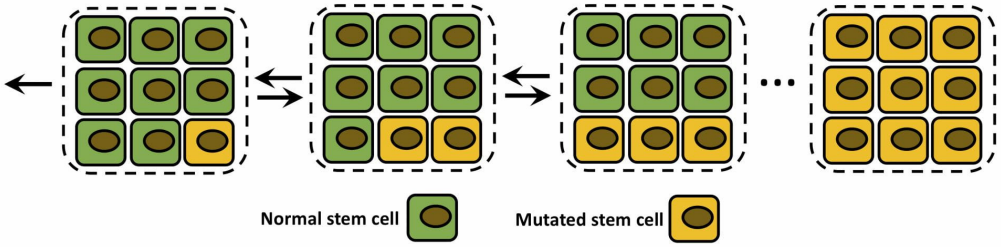
Chemists' calculations may advance cancer prediction

(Mike Williams, Rice News)

Rice scientists' approach to cell dynamics builds new view of lifetime risk

HOUSTON - (December 12, 2019) - Rice chemist Anatoly Kolomeisky, with postdoctoral research associate Hamid Teimouri and graduate alumna Maria Kochugaeva, directed their theoretical expertise in modeling random (stochastic) processes to the problem of why cancerous cells that are usually destroyed by the body's immune system sometimes overcome a gauntlet of defenses to become tumors.

The study in Scientific Reports is intended to clarify microscopic aspects of cancer initiation, the point at which random mutations become "fixed" in cells, which pass them on and eventually overwhelm tissue.



A schematic shows a single mutation fixation process in a tissue compartment. Normal stem cells are green, and mutated cells are yellow. Rice University researchers used a discrete-state stochastic model to see how cancer-leaning mutations affected the likelihood of cells turning tissue into a tumor, and how well the model correlates with widely used calculations of cancer lifetime risks. Illustration by Hamid Teimouri

Full article: http://news.rice.edu/2019/12/12/chemists-calculations-may-advance-cancer-prediction-2/

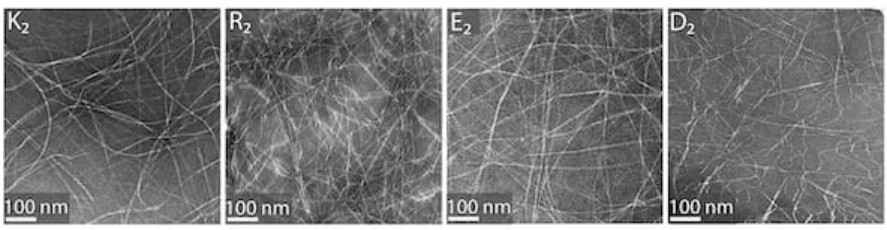
Hydrogels control inflammation to help healing

(Mike Williams, Rice News)

Rice, Texas Heart Institute scientists model how synthetic gels can tune body's inflammatory response

HOUSTON - (December 16, 2019) - Hydrogels developed at Rice are designed to be injectable and create a mimic of cellular scaffolds in a desired location. They serve as placeholders while the body naturally feeds new blood vessels and cells into the scaffold, which degrades over time to leave natural tissue in its place. Hydrogels can also carry chemical or biological prompts that determine the scaffold's structure or affinity to the surrounding tissue.

The study led by chemist and bioengineer Jeffrey Hartgerink and graduate student Tania Lopez-Silva at Rice and Darren Woodside, vice president for research and director of the flow cytometry and imaging core at THI, demonstrates it should be possible to tune multidomain peptide hydrogels to produce appropriate inflammatory response for what they're treating.



Researchers at Rice University and Texas Heart institutes tested a sampling of synthetic, biocompatible hydrogels to see how tuning them influences the body's inflammatory response. The hydrogels are being developed to help heal wounds, deliver drugs and treat cancer.

Full article: http://news.rice.edu/2019/12/16/hydrogels-control-inflammation-to-help-healing-2/

Gasification goes green

(Mike Williams, Rice News)

Rice's low-temp photocatalyst could slash the carbon footprint for syngas

HOUSTON - (January 10, 2020) - Rice University engineers have created a light-powered nanoparticle that could shrink the carbon footprint of a major segment of the chemical industry.

The particle, tiny spheres of copper dotted with single atoms of ruthenium, is the key component in a green process for making syngas, or synthesis gas, valuable chemical feedstock that's used to make fuels, fertilizer and many other products. Researchers from Rice, UCLA and the University of California, Santa Barbara (UCSB), describe the low-energy, low-temperature syngas production process this week in Nature Energy.

Naomi Halas, director of Rice University's Laboratory for Nanophotonics, is an engineer and chemist who's spent more than 25 years pioneering the use of light-activated nanomaterials. (Photo by Jeff Fitlow/Rice University)

Full article: http://news.rice.edu/2020/01/10/gasification-goes-green-2/

Deadly superbugs destroyed by molecular drills

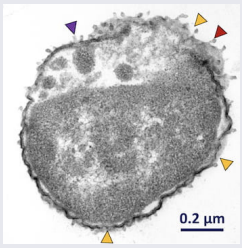
(Mike Williams, Rice News)

Rice, Texas A&M-led research shows motors kill bacteria, revive some antibacterial drugs

HOUSTON - (December 12, 2019) - Molecular drills have gained the ability to target and destroy deadly bacteria that have evolved resistance to nearly all antibiotics. In some cases, the drills make the antibiotics effective once again.

Researchers at Rice University, Texas A&M University, Biola University and Durham (U.K.) University showed that motorized molecules developed in the Rice lab of chemist James Tour are effective at killing antibiotic-resistant microbes within minutes.

"These superbugs could kill 10 million people a year by 2050, way overtaking cancer," Tour said. "These are nightmare bacteria; they don't respond to anything."



A Klebsiella pneumoniae bacteria exposed to motorized nanomachines invented at Rice and the antibiotic meropenem shows signs of damage in a transmission electron microscope image. The yellow arrows show areas of cell wall disruptions, the purple arrow shows where cytoplasm has escaped from the cell, and the red arrow shows cytoplasmic leakage. Image by Don Galbadage

Full article: http://news.rice.edu/2019/12/12/deadly-superbugs-destroyed-by-molecular-drills-2/

ACS ENERGY LETTERS

WOMEN SCIENTISTS AT THE FOREFRONT OF ENERGY RESEARCH

Christy Landes

"I need to feel like there is space for me to add value in order to be inspired and to have confidence that I can lead my students on a worthwhile scientific journey. There is an almost magical excitement when you discover a topic like reducing energy consumption in our separations industry and that you have a new way of looking at that problem that could push our fundamental understanding and, even in the smallest fashion, contribute to a greater good. At a time when as much as 15% of our domestic energy consumption is spent on separations, I am very excited about our group's work to develop a predictive theory of chromatography that would decrease our need for costly and energy-intensive empirical optimization. My advice to young researchers is not new advice: Never ever EVER give up on pursuing your passion.

FACULTY INTRODUCTIONS

Krista Kobylianskii

My name is Krista Kobylianskii (Vikse), and working with undergraduates to get them thinking like scientists is what I love to do. As a new lecturer in the Chemistry Department, I am thrilled to be surrounded by a group of like-minded people. I have taken a somewhat circuitous route to get here. I grew up in Canada where I completed my PhD at the University of Victoria on Vancouver Island. I studied with Dr. Scott McIndoe and used mass spectrometry to uncover the kinetic behavior of short-lived reaction intermediates in metal-catalyzed reactions. From there, I completed two postdoctoral appointments at the University of Melbourne (Australia) and ETH Zurich (Switzerland) with Dr. Richard O'Hair and Dr. Peter Chen, respectively. They taught me the art of "re-purposing" mass spectrometers as high-tech reaction vessels for gas-phase mechanistic studies.

In 2016, I accepted a faculty positon at San Francisco State University and began my own research program towards understanding the "birth" of metal nanoparticles using mass spectrometry (funded by an NSF RUI). Working at a primarily undergraduate institution fueled my passion for mentoring students at the very beginning of their scientific careers. When I had the opportunity to relocate to Houston, I knew Rice was the place that I wanted to be and, as luck would have it, there was an opening to help teach General Chemistry. I have thoroughly enjoyed my first semester here and moving forward I hope to pair my teaching with a new research focus in chemical education.

Kasey Leigh Yearty

I am a new non-tenure track faculty member serving as the Wiess Instructor of Chemistry. I am originally from Macon, Georgia. I earned my B.Sc. in Chemistry at the University of Georgia (UGA), where my research centered on nanocarrier-mediated delivery of metal-based drugs for cancer treatments. I continued at UGA to earn my Ph.D. with Prof. Richard Morrison. My doctoral research encompassed the development and implementation of multi-outcome experiments utilizing benchtop NMR technology in the undergraduate organic chemistry instructional laboratories.

During my first year at Rice, I've taught the discussion sections for both Organic Chemistry I and Organic Chemistry II. I have also taught two lab courses: the organic chemistry lab for chemistry majors (co-taught by Prof. Paul Engel) and the organic chemistry lab for chemical engineers. My additional teaching responsibilities include overseeing all of the undergraduate research conducted by chemistry majors both inside and outside of our department. The semester's culminating event for our undergraduate researchers is the Departmental Undergraduate Research Symposium. This event will be held on the afternoon of April 10, 2020. I hope that you are able to attend as we showcase the research efforts of our Chemistry majors!

STUDENT SPOTLIGHT

NIH, Ruth L. Kirschstein Predoctoral Individual National Research Service Award

Alyssa Pollard

"Measuing Tumor Acidosis with PET/MRI Contrast Agents"

Doctoral degrees, December 2019

Federico Bocci

"Phenotypic heterogeneity driven by cell-cell signaling: principles of pattern formation and implications for metastasis"

Samuel Cody Martin

"Rhodium and copper: chemical approaches to biological problems"

Macy L. Stavinoha

"Magnetic and Electronic Correlations in Rare Earth Intermetallic Compounds"

Alicia Mangubat-Medina

"Photocleavable approaches to reversible bioconjugation"

Meredith McDowell Ogle

"Photoactive inorganic molecules for the next generation of photoluminescent probes and materials"

Shu Tian

"Engineering Aluminum Nanocomposites for Sensing, Photocatalysis and Photothermal Conversion"

Arthur L. Draper Award

In recognition ofexceptional performance in undergraduate chemistry coursework.

Michelle Dai
Ruchi Gupta
David Yang
Elliot Ballato
Olivia Zhang
Kevin Gonzalez

COOPERATION IS KEY: A NEW, POTENT LIGAND FOR SH3 DOMAINS

MARY K. MILLER

One of the next frontiers in medicinal chemistry is a group of targets deemed "undruggable" until only very recently. These targets are known as protein-protein interactions (PPIs), and they play significant roles in a number of disease states, including many cancers. Targeting these interactions has been considered no easy feat. Traditionally, inhibiting protein function involves designing a small molecule that binds in a defined pocket in a protein of interest. In contrast, PPIs occur over large surface areas, making developing specific targets challenging. But recently, scientists have discovered methods for inhibiting PPIs, paving the way for new types of medical treatments.

SH3 domains are a prototypical PPI-involved protein domain present in a variety of different therapeutically relevant proteins. These domains present a challenge to inhibitor development due to structural similarities across a number of these domains. However, it has been found that many of the SH3 domains most closely associated with disease states contain nucleophilic (capable of donating electrons to form a new chemical bond) residues around the binding site, which can be targeted by researchers to develop specific inhibitors for protein-protein interactions.

Prof. Zachary Ball and Dr. Cody Martin from the Rice University Department of Chemistry are among those who have risen to this challenge. They recently disclosed a new strategy for inhibiting protein-protein interactions in SH3 domains using a known weak inhibitor modified with a rhodium metal center to strengthen its binding affinity. (ACS Med. Chem. Lett. 2019, DOI: 10.1021/acsmedchemlett.9b00309). The idea behind this strategy is that the electron-deficient metal center will interact strongly with nucleophilic residues surrounding the binding site of the small molecule, thereby lowering the binding energy and making a tighter association between the protein and small molecule.

SH3 domains are known to be inhibited by ligands derived from small molecule scaffolds called 2-aminoquinolines. In this report, several 2-aminoquinoline-rhodium(II) conjugates were synthesized with long, medium, and short length linkers between the small molecule inhibitor and metal center to analyze the importance of distance between the two. Interestingly, it was found that if the linker was too long or too short, the binding efficiency was negatively affected. An optimal mid-length "Goldilocks" linker was found that gave best results.

Researchers were pleased to note that the studies agreed with expected hypotheses. The data showed that if the SH3 domain did not possess a nucleophilic residue in the proximity of the binding pocket capable of interacting with the metal center, no enhancement in binding was observed. However, when a nucleophilic histidine residue was present, an increase in binding three orders of magnitude greater than the most potent inhibitor was observed.

This study provides an exciting example of combining metallic interactions with nearby residues to improve small molecule inhibitor binding. This method shows promise for selectively targeting other "undruggable" sites that could be used to study heretofore opaque human disease states.

STAFF CORNER

Greetings from the Department of Chemistry Administrative Staff. We continually strive to improve our services, to allow faculty to focus more on research and less on the administrative burdens. As a team, we manage research expenditures of $11M/per year, oversee the administrative activities of both graduate and undergraduate programs, plan numerous seminars and events throughout the year, as well as a host of other responsibilities. The team has successfully executed many undertakings during 2019, and we expect 2020 to be even more successful!

To highlight a few upcoming events, we have our graduate student-recruiting weekend (February 20-23, 2020), when we look forward to welcoming students from top schools all over the country and beyond, and our next departmental gathering (March 5, 2020), honoring Dr. Lon Wilson's upcoming retirement. We welcome all faculty, staff, alumni and friends of the department to join our gathering.

As we celebrate Dr. Wilson's long and successful career at Rice, we also look forward to welcoming our new faculty member, Dr. Anna-Karin Gustavsson, who will join us in August 2020.

"Every end is the beginning of something else…" (M.L. Stedman)

Please visit our website for news and upcoming events: chemistry.rice.edu

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We love to hear from you!

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

https://bit.ly/2Mezkwb

Giving to Chemistry

The global impact of Rice University is expanded and sustained by the accomplishments and support of its alumni and friends. The continued generosity of donors is paramount to the mission and goals of Rice Chemistry.

Graduate education and research are top priorities in the Department of Chemistry. Graduate student fellowships are of crucial importance to attract and sustain a strong body of doctoral students, an important component of our research programs. The department's research accomplishments would not be possible without the hard work of graduate students. Named endowment(s) for graduate student fellowships will 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.

We recommend that you give a donation to our Chemistry General Support Fund, which may be used for student support and other departmental needs. Please indicate your desired use. We also have several already established award and endowed funds to which you may make a specific donation. To learn more about our funds, please visit our website.

Your gift will tremendously help our research program in advancing science and in training new generations of educated specialists!

You may contact Department Chair, Anatoly Kolomeisky, for information about opportunities to give at chemchair@rice.edu.

https://riceconnect.rice.edu/donation/support-chemistry

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