Highlights 2018

Our core mission is research/education
It’s about the science!!
Here are some highlights...
Pete Padolik and Kristina Ament

- Devotion to providing high quality education to many many (thousands of) undergraduate students at UC!!
- We honor you both for your efforts
- Kristina we wish you all the best
New Research Instrumentation

- 2x NSF-MRI
- X-ray (here, thanks Jeanette et al!)
- NMR (on the way)
- Mass Spec proposal submitted
Dear William Connick,

I’m pleased to inform you that you have been selected as a recipient of the Award for Faculty Excellence. This award is designed to honor faculty who have done an outstanding job in teaching, research, and/or service. You will receive $2000 in discretionary funds to support teaching or research efforts. The Office of the Provost will transfer funds to the appropriate business administrator for distribution to you.

Congratulations on your award!

Regards,

Keisha Love, PhD.
Associate Provost for Faculty Development and Special Initiatives
Amie Norton and collaborators at NIOSH developed a Roomba robot having unprecedented combination of indoor positioning, telemetry, and real-time chemical vapor sensing capabilities, thereby allow for complete remote mapping of VOC levels in laboratories.

She also conducted a study that demonstrated that flammable storage cabinets are significant points sources for VOCs in laboratories and identified key countermeasures to protect laboratory workers.

Our publication "Shape memory polymer foams prepared from a heparin-inspired polyurethane/urea" was published in the Royal Society of Chemistry journal 'Polymer Chemistry' (Current IF = 5.375) as part of the “Pioneering Investigators” Special Issue--Qinyuan Chai, Yongshun Huang, Terrence Kirley, and Neil Ayres, Polymer Chemistry, 2017, 8, 5039-5048.

This work demonstrated that heparin-inspired polymers could be used to prepare shape-memory foams with tunable materials properties and remarkably low adherent platelets in human plasma, this indicates these materials are exciting candidates for blood contacting applications such as small diameter vascular grafts.
Mack Lab Publications/Highlights

**Mechanochemical Innovations**

![Graph showing conversion vs temperature](image)

**Green Chemistry In Education**


**Soon to Be New Faculty Member!**

Becca Haley Accepted a Position as Assistant Professor of Organic Chemistry at University of Wisconsin - River Falls!

A. Javidialesaadi and G. Stan, GPU-Accelerated Molecular Dynamics Simulations of Protein Remodeling Mediated by AAA+ Biological Nanomachines
Top 5 Finalist NVIDIA GPU Award, COMP Division, ACS National Meeting Fall 2017
In-Kwon Kim

• Project: Structural biochemistry of human poly(ADP-ribose) turnover proteins (obtained new crystal structures of complexes!)

• Summary: We are working on mechanism and function of PARG and ARH3 with an aim to develop new cancer therapeutics.
Ryan White

Research in our group combines themes at the forefront of nanoscience, biomolecular engineering, and electrochemistry, for the development of innovative analytical tools and their application in both the physical and life sciences. Examples include the development of sensitive, nanometer scale chemical and biological sensors that will probe materials and biological systems with unprecedented temporal and spatial resolution. Researchers in the group will gain a highly interdisciplinary background electrochemistry, biochemistry, nanotechnology and biomolecular engineering pushing the frontiers of basic science while also narrowing the gap between laboratory-bound research and real-world applicability.

**BIO-SCANNING ION CONDUCTANCE MICROSCOPY**
We are developing a bio-inspired, scanning ion conductance microscope that uses protein channels as sensing elements to provide specific molecular flux.

Learn More

**SENSORS FOR THE CHEMISTRY OF THE BRAIN**
We are developing electrochemical, aptamer-based (E-AB) sensors for the detection of a variety of targets including the gliotransmitter ATP.

Learn More

**APTAMER-HYDROGEL HYBRID SENSORS**
We have developed a biocompatible interface of hydrogel membranes with our E-AB sensors that enables compatible sensing in complex media and an ideal environment for cellular measurements.

Learn More

**RANDOM WALK MODELS FOR BETTER BIOSENSORS**
We are developing random walk models to better understand the electrochemical response of our aptamer-based sensors.

Learn More
Bio-Inspired Electrochemical Sensing and Imaging

Conformation Switching Sensors.

We develop electrochemical, aptamer-based sensors to provide rapid, sensitive, specific, and selective detection to meet the challenges of several different bioanalytical applications.

Monitoring Brain Chemistry

Rational Sensor Design

We have developed a quantitative framework for rational sensor design including strategies in biomolecular engineering and electrochemistry.

Protein Nanopore Sensors

We develop nanopore based sensors and imaging platforms that enable extremely sensitive sensing at the single molecule level.

Bio-Inspired Scanning Ion Conductance Microscopy

We have developed a bio-inspired imaging platform. This chemical imaging platform could allow for imaging of the cellular microenvironment. We employ two different probe types including pulled pipettes to support lipid bilayers and protein channels and etched gold nanopores modified with PEG monolayers.
Julio Landero

“I am pleased to inform you that you are the recipient of an “Outstanding Undergraduate Research Advisor” Award to be presented at UC’s Undergraduate Scholarly Showcase, Monday, April 16 in the Great Hall of TUC. One of your students submitted an endearing nomination for this award and it is clear that you are well-deserving.”

Thank you for your service to the scholarly development of undergraduate students.

Sincerely,
Megan Lamkin

Plus 8 peer-reviewed publications in ICP-MS etc!
Noe Alvarez

I have published papers on carbon nano materials applications in sensors and electrically conducting water membranes to eliminate biofouling and energy storage.

We are currently working with a company (AOSmith) interested in heavy metal sensor technology.

Three-dimensional, free-standing polyaniline/carbon nanotube composite-based electrode for high-performance supercapacitors

Rachit Malik a, Lu Zhang a, Colin McConnell b, Michael Schott c, Yu-Yun Hsieh a, Ryan Noga b, Noe T. Alvarez b, Vesselin Shanov a, b, *

a Department of Mechanical & Materials Engineering, University of Cincinnati, Cincinnati, OH, 45221, USA
b Department of Biomedical, Chemical and Environmental Engineering, University of Cincinnati, Cincinnati, OH, 45221, USA
c Department of Physics, University of Cincinnati, Cincinnati, OH, 45211, USA

Carbon Nanotube Thread Electrochemical Cell: Detection of Heavy Metals

Daoli Zhao, † David Siebold, ‡ Noe T. Alvarez, ‡ Vesselin N. Shanov, ‡ and William R. Heineman *; † ©
We have expanded the structure types of our alpha-hydroxy acid-containing chelates that form photochemically active complexes of Fe(III) and other metals to include the tripodal amine motif. These new chelates from both monomeric and dimeric Fe(III) complexes, depending on the anion used, which allows us to better understand the electron stoichiometry of the photolysis reaction.

Ruxandra Dima’s group

Nan Jiang, Megan Bailey, Jessica Burke, Jennifer L. Ross, and R. I. Dima, "Modeling the effects of lattice defects on microtubule breaking and healing", *Cytoskeleton, 74*, 3-17 (2017)

The mechanism of the reaction at room temperature between an unactivated 2-benzyl aziridine and carbon dioxide to generate the corresponding oxazolidinone has been studied. Kinetic studies show that the reaction displays a zero-order dependence with respect to aziridine, indicating that free aziridine is not involved in the rate-determining step. An ammonium salt generated in situ acts as a catalyst.
Tom Beck

Re-examining the tetraphenyl-arsonium/tetraphenyl-borate (TATB) hypothesis for single-ion solvation free energies

Travis P. Pollard, and Thomas L. Beck


FIG. 2. Visualization of solvation structure at the boundary (white surface) of the 9 Å radius cavity used to compute solvation free energies. The ion is at the center of this void and is shown in purple. The solvents from left to right are as follows: water, dimethyl sulfoxide, and 1,2-dichloroethane.
The Ross lab has developed an electrochemical method to detect subsecond changes of melatonin signaling with low nM limits of detection. This method was successfully validated in live lymph node tissue, which represents the first millisecond detection of a chemical messenger within intact immune tissue.
Pat Limbach

LETTER

doi:10.1038/nature21396

Editing and methylation at a single site by functionally interdependent activities

Mary Anne T. Rubio1, Kirk W. Gaston1,2, Katherine M. McKenney1, Ian M.C. Fleming1, Zdeněk Paris1,3, Patrick A. Limbach2 & Juan D. Alfonzo2

Nature (2017) 454 494-497

Figure 3 | LC-MS/MS analysis confirms the in vitro formation of m'U. a-e, tRNA trimethyl transcript incubated with various enzymes analysed by LC-MS/MS. The extracted ion chromatogram (XIC) of m/z 127.08 ((B + H)⁺ for m'U) of an MS/MS scan targeting m/z 239 (M + H)⁺ ion for m'U) is shown. f-j, Same as a-e showing inosine (XIC m/z 269) and the inosine standard eluting at 20.8 min. k, MS/MS spectra of m/z 259 at 25.8 min from e produced the expected product ion of m/z 127.08, also observed with the m'U standard. l, Mass spectrometry at 20.8 min showing the spectra for inosine with m/z 269.09 (M + H)⁺ and m/z 137.05 ((B + H)⁺) in all samples.
In this collaborative project led by Prof. Juan Alfonzo at Ohio State, Kirk Gaston – a post-doc in the group at the time – helped demonstrate that cytosine 32 in the anticodon loop of *Trypanosoma brucei* tRNA-Thr is methylated to 3-methylcytosine (m\(_3\)C) as a pre-requisite for C-to-U deamination. Formation of m\(_3\)C in vitro requires the presence of both the *T. brucei* m\(_3\)C methyltransferase TRM140 and the deaminase ADAT2/3. Once formed, m\(_3\)C is deaminated to 3-methyluridin (m\(_3\)U) by the same set of enzymes.

Hard to imagine, but this was a collaboration that took nearly six years to obtain all the evidence to prove this mechanism actually occurs in nature.
Guan: Earth-Abundant Metal Based Catalysts for Energy and Chemical Applications

The Sagle Group: Plasmonic Platforms Enabling Biological Measurements

The First Single Molecule Vibrational Spectroscopy In A Cell-Like Environment

The First Vibrational Spectroscopy Of A Fluid Solid Supported Lipid Bilayer
Peng Zhang
Phase 2 UC Technology Accelerator Award

Photoactivated nanoparticles to photodynamically kill bacteria efficiently without involving antibiotics
Anna’s research group accomplishments 2017

Determining reaction mechanisms in crystals using transient spectroscopy

- Identifying excited states and reactive intermediates within crystal lattices

New Directions: Developing sustainable synthesis - Using visible light for selective solid state reactions

- Converting vinyl azides into heterocyclic compounds with green laser pointer

- No solvent, no purification, 100% yields


Hot paper
Capturing Conformation-Dependent Photoreactivity of Crystalline 3-Azido-1,3-diphenylisobutyrophenone. Karthik et al. ChemPhotoChem, 2017, 1 (9), 408-414

Wavelength-Dependent Photochemistry


Professional Development updates in Anna’s Research group in 2017

**Sujan Sarkar**, PhD 2015 obtained **JSPS fellowship** to do research at Hiroshima University for 2 years.

**Dushanee Sriyarathne** got her PhD 2017, was a postdoctoral fellow at Rice University and is currently a R&D chemist with **Firmenich NJ**.

**Anushree Das**, PhD 2017, is a postdoctoral fellow at **Stanford Research Institute International, CA**.

**Breyinn Loftin**, REU student 2014, was awarded **NSF graduate fellowship**.
A range of RNA photoproducts and post-transcriptional modifications that arise due to UVR-induced cellular stress are documented in this study.
Statement of Research in the Jiang Group

Our research interests center on the development of advanced materials with novel properties to address the main question in the renewable energy field: What are the guiding principles for the design of well-defined materials as platforms for energy capture, conversion and storage? Leveraging synthetic and molecular engineering techniques, we will design and synthesize a series of model materials (i.e., multifunctional organometallic compounds and (bio)polymers) and evaluate their performance in various applications, so as to elucidate the materials structure-function relationships and to understand the molecular interactions underpinning renewable energy storage. Our research is focused in two areas: catalysis for renewable fuel production and rechargeable battery for energy storage, as briefly described below.
In the Sun group, we are particularly interested in the following catalyst systems:

(i) Metallic catalysts decorated with nonmetal elements on the catalyst surface
(ii) Ultrathin two-dimensional nanosheets of earth-abundant elements with thickness less than 1 nm
(iii) MOF-derived single-atom catalysts bridging the concepts of solid-state and molecular catalysts
(iv) Molecular transition metal catalysts with redox inactive cations in the secondary coordination sphere
I am sorry if I missed any information that was sent to me… Please send again if so (or if you want to add something) and I will insert and we can post the information as an informal record of the year.
Bill Heineman

--500+ publications
--Extraordinary funding level over 45+ year career
--World leader in electrochemistry and the development of chemical sensors
--Department Head, leader of UC sensors effort etc.
--National ACS Award Analytical Chemistry, many others
--We have been very lucky to have Bill on our faculty during his superlative career
--His career is ongoing; he has 10+ papers to write and ongoing grants
--This last year at the age of ?? Bill published 10 papers in top journals!! Some APR!
--While we have very promising new faculty, we will never replace Bill Heineman
Shirmir Branch – last PhD student graduating next week (# 97)

Thanks to ALL for your contributions this first year for me as Head. I greatly appreciate how people step up in this Department!

Let’s take a breath, and spend some time deepening the work we do this summer.