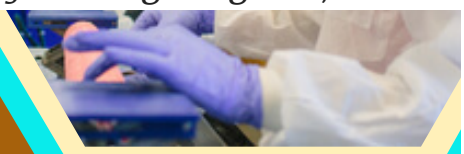
MUDD IN YOUR EYE

Fall 2021 Newsletter

No. 51

Great importance is given to chemistry as an elementary branch of learning – Lehigh Register, 1866.



MEET THE PEOPLE OF THE LEHIGH UNIVERSITY DEPARTMENT OF CHEMISTRY

LEHIGH UNIVERSITY | DEPARTMENT OF CHEMISTRY

Achieving Forward Progress Even Through Global and Educational Pandemic-Related Challenges

Research advancement attains new heights as a result of dedicated efforts of outstanding faculty, staff and students

We're back on campus and classes are in person! Like the rest of the country, Lehigh has worked to weather the pandemic, raising and lowering restrictions to follow the ever-evolving circumstances. After a surge of cases of the "beta variant" at the start of the semester, the number of infections has fallen to near zero on campus. Nonetheless, cases in the local community remain at a high level, so we're still wearing masks indoors and almost everyone is vaccinated. It will undoubtedly take years to understand the full impact of this period on teaching and research, but we have new capabilities we didn't have in 2019. Zoom ... Docusign, anyone?

New faces in the department abound, with a new General Chemistry Lab Manager (Dan Prendergast), Visiting Assistant Professor (Dr. Hannah Cronk), and a large incoming class of graduate students. This installment of Mudd-In-Your-Eye will introduce you to some of these new members of the Lehigh Chemistry department, and celebrate some of the successes our colleagues have enjoyed. Of particular note, it also contains a tip-of-the-hat to Professor Kamil Klier, whose intellect and friendship helped shape the department and inspire generations of students.

This year we also said goodbye to two good friends. Professor Dmitri Vezenov passed away in late October and our former colleague, Professor Jim Sturm (see Mudd-in-Your-Eye 50th Edition, Page 17), passed away at the end of November. These two people shared a lot in common —both were accomplished physical chemists, known also for their friendly and supportive dispositions, eagerness to help others, and sense of humor. We are indeed fortunate for them having been part of our Lehigh family, and our wince for their loss is accompanied by smiles for their memory.

Gregory S. Ferguson
Professor and Chair
Department of Chemistry
Lehigh University

In This Issue

Department of CHEMISTRY

LEHIGH CHEMISTRY

Stay in Touch

Lehigh Chemistry alums can be found all across the globe--using their degrees to address universal issues that impact the world community.

Your Lehigh Department of Chemistry would like to stay in touch. We love hearing about where your degree has taken you! Send your stories--professional or personal--to mwr217@lehigh.edu

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ON THE COVER: Clockwise from top center: Graduate students (L to R) Fatema Amin and Gisselle Rojas at the Chemistry Club Fall 2021 Coffee; (L to R) Muhammad Imran, Caleb Wehrmann, Dmitri Vezenov, and Xiaoji Xu at Fall 2018-2019 department "Welcome" picnic; Dr. Damien Thévenin advising doctoral student Kelly Burns (PhD '13); Academic Coordinator Kerry Livermore assisting Graduate Student Aarshi Singh with her General Exam preparations; Dr. Xiaoji Xu explaining the intricacies of a spectroscopic process to Graduate Student Le Wang.

THEVENIN AWARDED TWO MAJOR RESEARCH GRANTS

Funding from the NIH and the Kaufman Foundation will facilitate next-generation cancer research and treatment

The Thévenin group has been awarded two major research grants: A $1.6 million Project Research Grant (R01) from the National Institute of General Medical Sciences of the National Institutes of Health (NIH), and a $300,000 New Initiative grant from The Charles E. Kaufman Foundation.

The NIH grant titled "Promoting Receptor Protein Tyrosine Phosphatase Activity by Targeting Transmembrane Domain Interactions" is led by Damien Thévenin and co-principal investigator Matthew Lazzarra (Associate Professor of Chemical Engineering at the University of Virginia). They are joined by collaborating investigator Forest White at the Massachusetts Institute of Technology.

The protein at the center of the project is known as protein tyrosine phosphatase receptor type J (PTPRJ), a member of the family of receptor-like protein tyrosine phosphatases (RPTP), which target and dephosphorylate, or deactivate, proteins involved in cell proliferation and survival. The main goal of the project is to understand how to promote the activity of PTPRJ—and eventually other RPTPs—by interfering with the ability of the phosphatase to bind to itself, a process called homodimerization in which two identical proteins form a structure. The Thévenin group has identified a set of mutations and designed small peptide binders that disrupt PTPRJ homodimerization to promote phosphatase activity. Because the phosphatase acts on, and effectively turns off, certain receptors that can promote tumor growth, they think this could eventually lead to a new method to interfere with signaling in cancer cells in a way that would not be circumvented by the common forms of drug resistance seen in cancer treatments. The team also anticipates that their work on the PTPRJ protein will yield insights that are relevant across the receptor-like protein tyrosine phosphatase family.

"Mutations in growth hormone receptors within cancer cells can blunt the effectiveness of cancer drugs. . . This development of resistance happens in most cancers and drugs become ineffective after a relative short period, resulting most often in patient relapse. Since our peptides do not target directly those receptors that are the most susceptible to mutations in cancers, we expect that our strategy will bypass the development of resistance."

-- Damien Thevenin, Lehigh News - May 5, 2021 (Read more)

The work funded by the Kaufman Foundation grant ("Full sail ahead: How do cells sense and decode flow?") is in collaboration with Aurelia Honerkamp-Smith (Assistant Professor of Physics at Lehigh University) and is aimed at understanding how cells from the inner surface of mammalian blood vessels respond to flow, which influences biological processes, such as cardiovascular health and embryonic development. Honerkamp-Smith and Thévenin hypothesize that flow-mediated reorganization of proteins at the surface of cells (similar to sailboats responding to wind) not only encodes information about flow speed and direction, but also initiates intracellular signaling. The two groups will be combining fundamental fluid mechanics and lipid physics with cell signaling and membrane protein biochemistry to quantitatively define the physical and molecular mechanisms that cells use to sense flow and translate this mechanical stimulus into intracellular molecular responses. They anticipate that these studies will not only be applicable to multiple cell lines and flow conditions, but also provide relevant physiological insights into different cardiovascular pathologies and cancers.

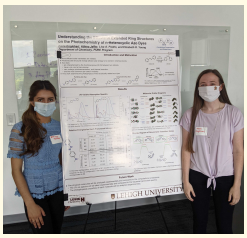
FREDIN AND YOUNG ESTABLISH IMMERSIVE RESEARCH PROGRAM

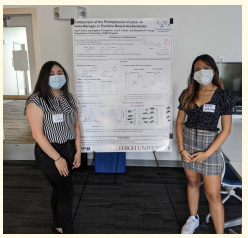
THROUGH KAUFFMAN FOUNDATION INTEGRATED-RESEARCH EDUCATION GRANT

Photochemistry Undergraduate Research Experience (PURE) provides a unique long-term project to develop undergraduate researchers' chemical intuition and expand academic and career success

In order to build a clean energy economy, new photochemically-driven reactions are important for efficient solar energy capture and conversion. While driving reactions with light is less conventional than the typical heating of a beaker, it provides unique opportunities to initiate and control chemical reactions. For the past 50 years, physical chemists, especially spectroscopists and theorists, have built their so-called "chemical intuition" or understanding of how electron and proton transfer reactions occur primarily in the lowest energy states of molecules. However, when driving reactions with light, molecules necessarily become excited. The complex nature of excited states makes them more difficult to predict and understand, and thus we must develop a new chemical intuition for their reactivity. Profs. Fredin and Young received a Kaufman Foundation Integrated Research-Education Grant to establish a program for undergraduates to build chemical intuition of light-initiated electron and proton transfer in model azo dyes by combining spectroscopy and quantum mechanics.

Long-term undergraduate research participation has been proven to increase the academic performance, enhance the confidence, and lead to successful careers for undergraduate students. The newly established **Photochemistry Undergraduate Research Experience (PURE)** provides a unique long-term project for each undergraduate researcher that combines experimentation and computation.





This summer four Lehigh undergraduates, Kiera Engelhart '22, Athina Jaffer '23, Keyri Sorto '24 and Ing Angsara Thongchai '24, participated in an immersive, research-intensive, summer experience. The students worked for ten weeks learning how to model electronic structure of molecular dyes using Gaussian in the Fredin Lab, as well as how to measure steady-state and time-resolved spectroscopic properties in the Young Lab. They took part in dedicated workshops on the theory and hands-on training in each experimental or computational method. They learned about the scientific process and developed career skills. The students engaged the material with Profs. Fredin and Young, two graduate student mentors, and each other. This academic year (Fall 2021-Spring 2022) each student is continuing their research into the proton-coupled photophysics of their dyes through the combination of extensive density functional theory and spectroscopic studies. Together the trends the students are seeing, provide new chemical intuition of the photoexcited states of azo dyes.

Top left: Sorto and Thongchai; Top right: Engelhart and Jaffer (left to right) Bottom: Graduate student Zach Knepp, Young, Engelhart, Jaffer, Sorto, Thongchai, graduate student Gil Repa and Fredin (left to right)

CONGRATULATIONS GRANT AWARD RECIPIENTS

GLOVER LAB

RECEIVES NIH AWARD TO FURTHER CAVEOLIN PROTEIN RESEARCH

The Glover Lab is very elated about receiving a $475K National Institutes of Health grant award to continue their research on the caveolin protein. The caveolin protein is critical for cellular homeostasis--and aberrant caveolin behavior has been implicated in a number of human maladies including cancers and heart disease.

Specifically in this award, they aim to take a multi-faceted approach utilizing NMR, molecular dynamics simulations, and fluorescence spectroscopy to determine the three-dimensional conformation of caveolin in a bilayer. In addition, unique experiments are planned to explore the oligomeric state of caveolin using the lipid cubic phase.

The Glover Lab is also enthused to be collaborating with Drs. Wonpil Im of Lehigh University and Kyle Root of Lockhaven University on this important, far-reaching, and exciting project!

FISHER LAB >> FISHER LAB >> FIS

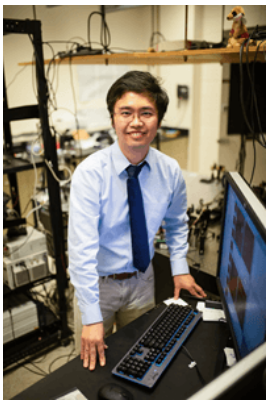
A recent recipient of a $250K National Science Foundation grant award, Professor Oriana Fisher and her students will study the behavior of copper ions in bacteria using a wide range of chemical and biochemical techniques. The research will provide a detailed understanding of how bacteria process copper and this will help lead to a better understanding of the chemistry of antibiotic resistance.

Dr. Fisher's plan to pilot a summer research program that will recruit students from groups underrepresented in science will broaden participation in chemistry at Lehigh and will provide long-term mentoring of a cohort of underrepresented minority students as they navigate the transition from undergraduate to graduate school.

Professor Fisher will biophysically and structurally elucidate proteins that orchestrate copper acquisition in Bacillus subtilis, with the aims of elucidating how Cu is recognized and chaperoned extracellularly--and investigating the structural and biophysical basis for transcriptional control of the ycn operon, which may hold a key to understanding bacterial copper acquisition and regulation. While copper export proteins are highly conserved throughout evolution, copper importers in bacteria appear to be completely distinct from their eukaryotic counterparts. Previous studies have focused on this problem primarily from a biological perspective; research under this award will provide new insight into a molecular level understanding of proteins that govern these processes.

This award is funded under the American Rescue Plan Act of 2021 and reflects NSF's statutory mission. The Fisher Lab project has been deemed worthy of support through evaluation using the Foundation's intellectual merit and broader impacts review criteria.

FISHER LAB'S NSF AWARD FUNDS COPPER IONS IN BACTERIA RESEARCH--AND OFFERS SCIENTIFIC RESEARCH OPPORTUNITIES FOR UNDERREPRESENTED MINORITY STUDENTS



Xiaoji Xu Recognized as Outstanding Teacher-Scholar

The Camille & Henry Dreyfus Foundation

Selected by the Camille & Henry Dreyfus Foundation as one of the 2021 Camille Dreyfus Teacher-Scholar award recipients, Dr. Xiaoji Xu is one of only 16 individuals chosen to receive this prestigious and highly competitive award. Xu's research focus on "Development of the Next Generation of Multimodal Chemical, Optical, and Electrical Scanning Probe Microscopy" will be supported with an unrestricted research grant of $100,000.

The award winners are selected from faculty who are within the first five years of their academic careers, have created an outstanding independent body of scholarship, and are deeply committed to education. According to the Foundation's website, their purpose is to advance the science of chemistry, chemical engineering, and related sciences as a means of improving human relations and circumstances throughout the world.

The Xu Lab research focus is to develop methods and instruments for spectroscopic study of nanostructured polymers and energy-related material measurement and imaging at the nanoscale with < 10 nm spatial resolution. As described in the *Lehigh News*, "They employ two infrared nanoscale imaging methods invented by Xu: peak force scattering-type near-field optical microscopy (PF-SNOM) and peak force infrared (PFIR) microscopy. . . His group also recently invented the pulsed force Kelvin probe force microscopy, a new type of imaging tool that allows for ~10 nm spatial resolution for measurement of surface potential under ambient conditions." (Read more)

In addition to probing new frontiers in microscopy, Xu also designed a research-related simulation for his students to enhance their remote learning during the virtual instruction days of the COVID-19 transition--further reinforcing the unique learning opportunities that arise from an outstanding, dedicated, and creative researcher- educator.

IM AWARDED 2021 LIBSCH RESEARCH AWARD

On September 15, 2021, Lehigh University announced its prestigious Lehigh University Awards--among which was the 2021 Libsch Research Award honoree: Wonpil Im.

Dr. Im has joint appointments in Biological Sciences, Bioengineering, and Chemistry at Lehigh University. He obtained his Bachelor's and Master's in chemistry from Hanyang University (Seoul, Korea). In 1997, he started his Ph.D. studies in chemistry at the University of Montreal under the guidance of professor Benoît Roux and followed him to the Weill Medical College of Cornell University where he received his Ph.D. in 2002. After a post-doctoral appointment at the Scripps Research Institute, he joined the faculty of the University of Kansas in the Center for Computational Biology in 2005, working on membrane (protein) simulations, publishing extensively, and receiving numerous scholarly recognitions. In 2016, he joined Lehigh University where he has been named the Presidential Endowed Chair in Health - Science and Engineering and received the Friedrich Wilhelm Bessel Research Award from Humboldt foundation (2017) as well as the CAS Dean's Research Award (2019)

His research interests include protein/peptide interactions with/in biological membranes; transmembrane-induced signaling and regulation; NMR structure calculation & refinement; modeling and simulation of glycoconjugates; bacterial outer membranes and interactions with proteins; and protein-ligand and protein-protein interactions (Read more)

When asked his thoughts on receiving this honor, Im stated that he was humbly thrilled and honored to hear that he had received this prestigious award. He feels thankful to the selection committee for favorably considering his research activities thus far--and fortunate for the opportunities he has received at Lehigh which have allowed him to continue to build on his almost 20 years of research. He is also thankful to have great undergraduates, graduates, and postdocs in his lab. since their creative, hard work has made so many research accomplishments possible.

Mark Chen

Despite research challenges, the Chen Lab managed to maintain productivity through the pandemic by advancing their science, and importantly, being awarded two new research grants in Fall 2020: one from the National Science Foundation (NSF), and one from the American Chemical Society Petroleum Research Fund (ACS-PRF). Prof. Chen was a recipient of a prestigious National Science Foundation CAREER award for the group's work in developing new optoelectronic organic materials through the exploitation of air-stable, open-shell molecules. The group was also awarded an ACS-PRF New Directions grant for their proposal to study conjugated molecules as materials for singlet oxygen sensitization, binding, and release. Preliminary work in this project by graduate student Muhammad Imran has already resulted in a manuscript that is currently under peer-review. Caleb Wehrmann's final paper in the group, with support from Prof. Fredin, is soon to be submitted and describes new organic materials that can generate amorphous, transparent, conductive films. In collaboration with Prof. Young and Prof. Fredin of Chemistry, and Prof. Biaggio of Physics, the Chen Lab was also awarded a Lehigh Accelerator Grant for their proposal to look at molecular materials for photonics and optoelectronics.

In the absence of in-person conferences, Caleb and Imran each presented a virtual talk at the Spring 2021 ACS National Meeting. The Chen Lab has grown in the past year with new member additions of Fatema Amin (graduate) and Nick Bowers (undergraduate). Nick joined the group in February, 2021 and won a CAS Undergraduate Research Grant Award that funded his summer research efforts. This past summer is also when 2nd year graduate student Gisselle Rojas passed her general exam to enter Ph.D. candidacy. Imran's papers have gained him recognition--and he was selected as a finalist in the 2021 Merck Research Award for Underrepresented Chemists of Color and as a student speaker at the Graduate Research Symposium hosted by the ACS Organic Division held at the University of New Mexico in November 2021. Finally, this past academic year marked a milestone for the group as the first Chen Lab graduate student, Caleb Wehrmann, defended and graduated (Dec. 2020). Caleb earned a rare distinction upon graduating as he won the CAS Dean's Dissertation Award. Though we are sad to see him go, we are excited for the science Caleb will do (but may never have the appropriate security clearance to hear about) since he started this fall as a research engineer at the U.S. National Reconnaissance Office (NRO).

Greg Ferguson

In comings and goings since our last newsletter, Tarannuma Ferdous Manny joined the research group, and Kiran Khadka successfully defended his dissertation. Tarannuma is currently working on a novel synthetic route to porous metal films, and Kiran is enjoying his job at Versum Materials. We are delighted that Zahed Ghelichkhah's pandemic research project was published this year in the *Journal of Electrochemical Society* (see reference below), and Kiran's paper describing the angle of inclination required for liquid droplets to roll off of a surface should be the next one to appear. Professor Ferguson gave a seminar this year at the University of British Columbia (by Zoom!) on the group's work on the formation and decomposition of gold oxide.

Ghelichkhah, Z.; Ferguson, G.S.; Macdonald, D.D. and Sharifi-As, S. "Point Defect Model Description of the Formation of Anodic Gold Oxide in H2SO4 Solution" *J. Electrochem. Soc.* **2021**, *168*, 041506.

Oriana Fisher

During the past year, the Fisher lab has continued its studies of bacterial copper homeostasis and enzymes implicated in the bacterial stress response. Last fall, the group welcomed two new members who are pursuing this work: Chemistry graduate student Aarshi Singh and undergraduate Biochemistry major Jing Guo. Jing participated in Lehigh's STEM-Summer Institute which culminated with a poster presentation on her research. In May, Prof. Fisher gave an invited seminar (virtual) at the University of Maryland—Baltimore County. In more recent news, the group published their findings in September:

Damle, M.S.; Singh, A.N., Peters, S.C.; Szalai, V.A. and Fisher, O.S. "The Ycnl Protein from *Bacillus subtilis* Contains a Copper-Binding Doman" *Journal of Biological Chemistry* **2021**, 297, DOI: https://doi.org/10.1016/j.jbc.2021.101078.

Lisa Fredin

The Fredin Group kept busy this year working on large scale computational problems at the intersection of photochemistry and material disorder. In particular, projects looking at inherent disorder (packing defects or molecular vibration) and induced disorder (dopants) have allowed the group to solve important problems in light-driven faceted-metal nanoparticle catalysis, vibrational effects on conduction in organic materials, the photoexicited state dynamics of metal-centered and open-shell organic molecules, and manganese dopants and vacancies in perovskite oxides.

Prof. Fredin, along with Prof. Young, received funding from the Pittsburgh Foundation to establish PURE (Photochemistry Undergraduate Research Experience), which combines computational and experimental physical chemistry research, in an innovative experience for Lehigh undergraduates. Four Lehigh undergraduate students completed their immersive in-person summer research experience. Building off the skills they learned during the summer, each student will work for the 2021-2022 academic year in order to complete their research projects on novel azo-dye photophysics. In addition, Prof. Fredin, along with PIs in Engineering and at Lehigh Research Computing, oversaw the installation and launch of Lehigh's new high-performance computational cluster, Hawk, that includes both CPU and GPU compute technology, funded by *NSF CC* Compute.* This new supercomputer system will triple the computing hours available to Lehigh faculty for research and teaching.

Additionally, in Summer 2021, Prof. Fredin Co-Chaired the **Photochemistry Spotlight** virtual symposium, where 12 speakers and four discussion leaders had discussions around some of the big questions in photochemistry. Over 500 unique users joined from 35 countries making it one of the largest photochemistry meetings ever! In addition, Prof. Fredin gave an invited virtual talk for the Lehigh I-DISC Faculty Member Forum and the American Chemical Society (ACS) Division of Inorganic Chemistry (DIC) Periodic Table Talks this year.

Publications:

Repa, G.; Fredin, L. A.* "Parameter Space Exploration Reveals Interesting Mn-doped SrTiO3 Structures" *PhysChemChemPhys*, **2021**, *23*, 23486-23500

Martin, S. M.; Oldacre, A. N.; Pointer, C. A.; Huang, T.; Repa, G.; Fredin, L. A.; Young, E. R.* "Proton-controlled Non-exponential Photoluminescence in a Pyridyl-Amidine-substituted Re(I) Complex" *Dalton Transactions* **2021**, *50*, 7265 – 7276.

Wehrmann, C. M.; Imran, M.; Pointer, C. A.; Fredin, L. A.*; Young, E. R.*; Chen, M. S.* "Spin Multiplicity Effects in Doublet versus Singlet Emission: The Photophysical Consequences of a Single Electron" *Chem. Sci.* **2020**, *11*, 10212-10219.

Jebrell Glover

The Glover Lab received an NIH R15 award entitled "Biophysical Studies of Caveolin" (See Page 5 for additional details). In addition, they welcomed graduate student Katrina Brandmier as part of the research lab. Dr. Glover also gave an invited talk at Kalamazoo College entitled, "Biophysical Insights into Caveolin-1 Structure." The Glover group also submitted a paper that was published in Spring, 2021: Julien, J.A.; Pellett, A.L.; Shah, S.S.; Wittenberg, N.J. and Glover, K.J. "Preparation and Characterization of Neutrally-buoyant Oleosin-rich Synthetic Lipid Droplets." *Biochimica et Biophysica Acta - Biomembranes*, **2021**, *1863*, 183624.

Wonpil Im

During the previous academic year, Dr. Im conducted the following professional endeavors:

Grants:

NIH R01 (Co-Investigator: 2021-2026; PI: Frank Zhang) Mechanical regulation of von Willebrand Factor. NSF MCB (PI: 2021-2024) Molecular Modeling and Simulation of the Mycobacteria Cell Envelope

NIH R21 (Multi-PI with Frank Zhang: 2021-2023) Biophysical characterization of SARS-CoV-2 spike protein - receptor interactions

NIH R15 (Co-Investigator: 2021-2024; PI: Jebrell K. Glover) Envelope Biophysical Studies of Caveolin

Wonpil Im (Continued)

Publications :

Zhang, H.; Kim, S.; Giese, T.J.; Lee, T-S; Lee, J.; D.M. York, D.M. and Im, W. "CHARMM-GUI Free Energy Calculator for Practical Ligand Binding Free Energy Simulations with AMBER" *J. Chem. Inf. Model.* **2021**, *61*, 4145−4151.

Cao, Y.; Choi, Y.K.; Frank, M.; Woo, H.; Park, S-J ; Yeom, M.S.; Seok, C. and Im, W. "Dynamic Interactions of Fully-glycosylated SARS-CoV-2 Spike Protein with Various Antibodies" *J. Chem. Theory Comput.* **2021**, *17*, 6559−6569.

Guterres, H.; Park, S-J; Zhang, H. and Im, W. "CHARMM-GUI LBS Finder and Refiner for Ligand-Binding-Site Prediction and Refinement" *J. Chem. Inf. Model.* **2021**, *61*, 3744−3751.

Aleshin, A.E.; Yao, Y.; Iftikhar, A.; Bobkov, A.A.; Yu, J.; Cadwell, G.; Klein, M.G.; Dong, C.; Bankston, L.A.; Liddington, R.C.; Im, W.; Powis, G.; Marassi, F.M. "Structural Basis for the Association of PLEKHA7 with Membrane-embedded Phosphatidylinositol Lipids" *Structure,* **2021**, *29*, 1029-1039.e3.

Aiman, S.; Kim, S.; Bae, H.E.; Wang, H.; Nygaard, A.; Uegaki, Y.; Du, Y.; Munk, C.F.; Katsube, S.; Bae, J.; Choi, C.W.; Choi, H-J; Byrne, B.; Gellman, S.H.; Guan, L.; Loland, C.J.; Kobilka, B.K.; Im, W. and Chae, P.S. "Conformationally Flexible Core-bearing Detergents with a Hydrophobic or Hydrophilic Pendant: Effect of Pendant Polarity on Detergent Conformation and Membrane Protein Stability" *Acta Biomater.*, **2021**, *128*,393-407.

Croitoru, A.; Park, S-J.; Kumar, A.; Lee, J.; Im, W.; MacKerell, Jr., A.D. and Aleksandrov, A. "Additive CHARMM36 Force Field for Nonstandard Amino Acids" *J. Chem. Theory Comput.* **2021,** *17*, 3554-3570.

Dong, C.; Choi, Y.K.; Lee, J.; Zhang, X.F.; Honerkamp-Smith, A.; Widmalm, G.; Lowe-Krentz, L.J. and Im, W. "Structure, Dynamics, and Interactions of GPI-Anchored Human Glypican-1 with Heparan Sulfates in a Membrane" *Glycobiology* **2021** *31*, 593-602.

Garst, E.; Lee, H.; Das, T.; Bhattacharya, S.; Percher, A.; Wiewiora, R.; Witte, I.; Li, Y.; Peng, T.; Im, W. and Hang, H.C. "Site-specific Lipidation Enhances IFITM3 Membrane Interactions and Antiviral Activity" *ACS Chem. Biol.* **2021**, *16*, 844−856.

Feng, S.; Wang, R.; Pastor, R.W.; Klauda, J.B. and Im, W. "Location and Conformational Ensemble of Menaquinone and Menaquinol, and Protein-Lipid Modulations in Archaeal Membranes" *J. Phys. Chem. B.* **2021**, *125*, 4714−4725.

Zhou, C.; Shi, H.; Zhang, M.; Zhou, L.; Xiao, L.; Feng, S.; Im, W.; Zhou, M.; Zhang, X, and Huang, Y. "Structural Insight into Phospholipid Transport by the MlaFEBD Complex from P. aeruginosa" *J. Mol. Biol.* **2021**, *433*, 166986.

Choi, Y.K.; Park, S-J; Park, S.; Kim, S.; Kern, N.R.; Lee, J. and Im, W. "CHARMM-GUI Polymer Builder for Modeling and Simulation of Synthetic Polymers" *J. Chem. Theory Comput.* **2021**, *17*, 2431-2443.

Choi, Y.K.; Cao, Y.; Frank, M.; Woo, H.; Park, S-J; Yeom, M.S.; Croll, T.I.; Seok, C. and Im, W. "Structure, Dynamics, Receptor Binding, and Antibody Binding of Fully-glycosylated Full-length SARS-CoV-2 Spike Protein in a Viral Membrane" *J. Chem. Theory Comput.* **2021**, *17*, 2479-2487.

Cao, W.; Dong, C.; Kim, S.; Hou, D.; Du, L.; Im, W. and Zhang, X.F. "Biomechanical Characterization of SARS-CoV-2 Spike RBD and human ACE2 Protein-Protein Interaction" *Biophys. J.* **2021,** *120*, 1011-1019.

Luna, E.; Kim, S.; Gao, Y.; Widmalm, G. and Im, W. "Influences of Vibrio cholerae Lipid A Types on LPS Bilayer Properties" *J. Phys. Chem. B.* **2021,** *125*, 2105-2112.

Wonpil Im (Continued)

Y. Gao, Y.; J. Lee, J.; I.P.S. Smith, I.P.S.; H. Lee, H.; S. Kim, S.; Y. Qi, Y.; J.B. Klauda, J.B.; G. Widmalm, G.; S. Khalid,S. and W. Im, W. "CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides" *J. Chem. Inf. Model.* **2021,** *61,* 831-839.

Cao, Y.; Park, S-J and W. Im, W. "A Systematic Analysis of Protein-Carbohydrate Interactions in the Protein Data Bank" *Glycobiology* **2021,** *31,* 126-136.

Kanhaiya, K.; Kim, S.; Im, W. and Heinz, H. "Accurate Simulation of Surfaces and Interfaces of Ten FCC Metals and Steel Using Lennard-Jones Potentials" *Npj Comput. Mater* **2021**, 7, 17

Guterres, H.; Park, S-J; Jiang, W. and Im, W. "Ligand-Binding-Site Refinement to Generate Reliable Holo Protein Structure Conformations from Apo Structures" *J. Chem. Inf. Model.* **2021**, *61*, 535-546.

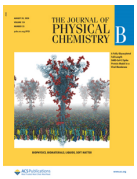
Ramesh, S.; Park, S.; Call, M.J.; Im, W. and Call, M.E. "Experimentally Guided Computational Methods Yield Highly Accurate Insights into Transmembrane Interactions within the T Cell Receptor Complex" *J. Phys. Chem. B.* **2020**, *124*, 10303-10310.

Kim, S.; Oshima, H.; Zhang, H.; Kern, N.R.; Re, S.; Lee, J.; Roux, B.; Sugita, Y.; Jiang, W. and Im, W. "CHARMM-GUI Free Energy Calculator for Absolute and Relative Ligand Solvation and Binding Free Energy Simulations" *J. Chem. Theory Comput.* **2020,** *16*, 7207-7218.

Shin, K.; Kent, J.E.; Singh, C.; Fujimoto, L.M.; Tian, Y.; Im, W. and Marassi, F.M. "Calcium and Hydroxyapatite Binding Properties of Human Vitronectin Provide New Insights for Abnormal Deposit Formation" *Proc. Natl. Acad. Sci. USA* **2020,** *117*, 18504-18510.

Ryzhov, P.; Tian, Y.; Yao, Y.; Bobkov, A.A.; Im, W. and Marassi, F.M. "Conformational States of the Cytoprotective Protein Bcl-xL" *Biophys. J.* **2020**, *119*, 1324-1334.

Lee, J.; Hitzenberger, M.; Rieger, M.; Kern, N.R.; Zacharias, M. and Im, W. "CHARMM-GUI Supports the Amber Force Fields" *J. Chem. Phys.* **2020**, *153*, 035103.



Woo, H.; Park, S-J; Choi, Y.K.; Park, T.; Tanveer, M.; Cao, Y.; Kern, N.R.; Lee, J.; Yeom, M.S.; Croll, T.L.; Seok, C. and Im, W. "Developing a Fully-glycosylated Full-length SARS-CoV-2 Spike Protein Model in a Viral Membrane" *J. Phys. Chem. B.* **2020**,*124*, 7128−7137 . [cover]

Gao, Y.; Lee, J.; Widmalm, G. and Im, W. "Modeling and Simulation of Bacterial Outer Membranes with Lipopolysaccharides and Enterobacterial Common Antigen" *J. Phys. Chem. B.* **2020**, *124*, 5948-5956.

Kai Landskron

During the past year, Muhammad Bilal Zarafullah joined Professor Landskron's research group as a graduate student. He is working in the lab on improving porous carbon materials for supercapacitive swing adsorption for carbon capture. Graduate student Jiajie Li continued her research studying the influence of carbon dioxide partial pressure on supercapacitive swing adsorption for carbon capture. Graduate student Jacob Dooley continued to construct his lab for ammonothermal cubic boron nitride crystal growth (collaboration with Siddha Pimputkar). Research Fellow Dr. David Roberts worked on crystalline, covalent ferrocenic, frameworks (collaboration with Lisa Fredin and Liz Young). Research Fellow Dr. Guido Pez constructed a fuel cell system for the electrocatalytic dehydrogenation of perhydrodibenzyltoluene. Professor Landskron wrote a textbook "Inorganic Coordination Chemistry" published on the Libretext platform. It is available for free to Lehigh students, and students worldwide. He co-founded Energy 18H, a benefit LLC that aims at the development and commercialization of direct fuel cells that dehydrogenate perhydrodibenzyltoluene for safe, CO_2 emission-free power generation.

Steve Regen

One of the most important and also one of the most controversial hypotheses that has emerged in the biomembrane area in recent years is the lipid raft hypothesis. In essence, cholesterol is presumed to combine with sphingolipids to form transient domains that are vital for cellular function; e.g., signal transduction and protein trafficking. However, the size, lifetimes and even the very existence of lipid rafts has remained uncertain. In a recent Perspective that I published in *Biochemistry*, I have summarized key studies that have been carried out in my laboratories using our nearest-neighbor recognition method. These studies provide a basis for understanding why lipid rafts must exist: Regen, S. L. "The Origin of Lipid Rafts" *Biochemistry*, **2020**, *59*, 4617-4621.

The need for new classes of drugs is apparent by the recent emergence of SARS-CoV-2, the virus that has led to the COVID-19 pandemic. While not at the same level of urgency as SARS-CoV-2, the need for creating new classes of antibacterial and antifungal agents has also become urgent due to the evolution of drug-resistant forms of bacteria and fungi. In a recent Perspective, I have highlighted the lack of attention that has been paid to the aggregation state of membrane-disrupting molecules as therapeutic agents in general, and how aggregation can affect the selectivity of such agents: Regen, S. L. "Membrane-disrupting Molecules as Therapeutic Agents: A Cautionary Note. *JACS* Au, **2021**, *1*, 3-7.

We have introduced novel approaches for improving the cellular selectivity of membrane-disrupting antimicrobial agents by monomer control and "taming". In a recent Perspective, I have highlighted each of these novel approaches: Regen, S. L. "Improving the Cellular Selectivity of a Membrane-disrupting Antimicrobial Agent by Monomer Control and by Taming" *Molecules*, **2021**, *26*, 374.

In an effort to create hyperthin membranes that could be used for the separation of CO2 and N2 from flue gas, we have recently shown that defects that are present in polyelectrolyte bilayers can be repaired by simple ion exchange using a common surfactant; i.e., sodium dodecyl sulfate: Pramanik, N.B.; Shaligram, S.; Regen, S.L. "Defect Repair of Polyelectrolyte Bilayers Using SDS: The Action of Micelles Versus Monomers" *Langmuir*, **2021**, *37*, 5306-5310.

David Vicic

Since the last newsletter, David Vicic has been preparing for his role as the Vice-Chair of the ACS Winter Fluorine Conference (WFC) that will be held in Clearwater, FL in January 2022. The WFC is the flagship meeting of the ACS Division of Fluorine Chemistry. David will serve as Chair of the meeting in 2023. David also gave a keynote lecture at the Science Forum Chemistry virtual meeting: WiFo (Wissenschaftsforum Chemie) organized by the German Chemical Society (GDCh) in August of 2021.

The published scientific contributions from the group include:

Shreiber, S. T. and Vicic, D. A "Synthesis and Characterization of the Dinuclear Cobalt(III) Complex: [(C2F5)3Co(mu-F)]22- " *J. Organomet. Chem.* **2021**, *949*, 121974.

Shreiber, S. T. and Vicic, D. A. "Solvated Nickel Complexes as Stoichiometric and Catalytic Perfluoroalkylation Agents" *Angew. Chem. Int. Ed.* **2021**, *60*, 2-8.

Vogt, N.; Sandleben, A.; Kletsch, L.; Schäfer, S; Chin, M. T.; Vicic, D. A.; Hörner, G.; Klein "On the Role of the X Colilgands in Cyclometalated [Ni(Phbpy)X] Complexes (HPhbpy = 6-phenyl-2,2'-bipyridine)" *A. Organometallics* **2021**, *40*, 1776-1785.

Xue, T. and Vicic, D.A. "Routes to Acetonitrile-Supported Trifluoromethyl and Perfluorometallacyclopentane Complexes of Cobalt" *A. Organometallics* **2020**, *39*, 3175-3720. **This work was listed as one of the "most-read" articles of the journal during the month of October.**

Shreiber, S. T. and Vicic, D. A. "Synthesis and Oxidative Stability of an Anionic Perfluoroethyl Cobalt(III) Complex" *Helv. Chim. Acta* **2020**, *103*, e2000149. (Special issue dedicated to Antonio Togni).

Nate Wittenberg

In 2021, Prof. Wittenberg received an NSF CAREER Award for a project entitled, "CAREER: Investigating the Molecular Factors that Underlie Myelin-Associated Glycoprotein Binding." (read more) This $665,000 grant will fund research activities in the Wittenberg lab for the next five years. In the past year, Nate presented the group's research at virtual versions of the ACS National Meeting, PittCon, and the Eastern Analytical Symposium. The Wittenberg lab welcomed Alexandria Pellett, a junior biochemistry major at Lehigh, for Summer 2021 undergraduate research.

In 2021, the Wittenberg lab published the following articles:

Cawley, J.L.; Blauch, M.E.; Collins, S.M.; Nice, J.B.; Xie, Q.; Jordan, L.R.; Brown, A.C. and Wittenberg, N.J. "Nanoarrays of Individual Liposomes and Bacterial Outer Membrane Vesicles by Liftoff Nanocontact Printing" *Small*, **2021**, doi: 10.1002/smll.202103338.

Cawley, J.L.; Jordan, L.R. and Wittenberg, N.J. "Detection and Characterization of Vesicular Gangliosides Binding to Myelin-Associated Glycoprotein Binding on Supported Lipid Bilayers" *Analytical Chemistry*, **2021**, *93*, 1185-1192.

Baxter, A.M.; Jordan, L.R.; Kullappan, M. and Wittenberg, N.J. "Tubulation of Supported Lipid Bilayer Membranes Induced by Photosensitized Lipid Oxidation" *Langmuir*, **2021**, *37*, 5753-5762.

Julien, J.A.; Pellett, A.L.; Shah, S.S.; Wittenberg, N.J. and Glover, K.J. "Preparation and Characterization of Neutrally-Buoyant Oleosin-Rich Synthetic Lipid Droplets" *Biochim Biophys Acta*, **2021**, *1863*, 183624.

Xiaoji Xu

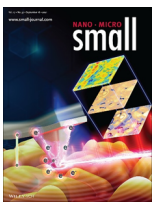
Dr. Xu has been named a Camille Dreyfus Teacher-Scholar by the Camille and Henry Dreyfus Foundation (see Page 6 to read more.) Haomin Wang and Devon Jakob have successfully defended their doctoral dissertations and they have started their post-doctoral research at Caltech and NIST, respectively.

Dr. Xu has given several invited presentations at conference and universities:
1. Invited presentation , Advanced Chemical Microscopy for Life Science and Translational Medicine, SPIE Photonics West Conference, San Francisco, CA, USA. Feb. 1-6, 2020.
2. Invited presentation, Microscopy and Microanalysis Meeting 2020, Milwaukee, WI, USA, Aug.2-6, (online)
3. Invited seminar, Department of Chemistry, University of Washington, Seattle, WA. Feb. 5 of 6 8, 2021 (online)
4. Invited seminar, Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY, USA, Apr. 2. 2021 (online)
5. Invited colloquium, Department of Chemistry, University of British Columbia, Okanagan, British Columbia, Canada. Apr. 6, 2021. (online)
6. Invited presentation, Material Research Society 2021 MRS Spring Meeting and Exhibit, Seattle, Washington, Apr. 18-23 2021. (online)
7. Invited presentation , Enhanced Spectroscopies and Nanoimaging 2021, SPIE Optical + Photonics Meeting, San Diego, CA, USA. Aug. 1-5, 2021 (online)

His lab has contributed to the following publications:

Li, N.; Niu, X; Li, L.; Wang, H.; Huang, Z.; Zhang, Y.; Chen, Y.; Zhang, X.; Zhu, C.; Zai, H.; Bai, Y.; Ma, S; Liu, H.; Liu, X.; Guo, Z.; Liu, G.; Fan, R.; Chen, H.; Wang, J.; Lun, Y.; Wang, X.; Hong, J.; Xie, H.; Jakob, D.S.; Xu, X.G.; Chen, Q. and Zhou,, H. "Liquid Medium Annealing for Fabricating Durable Perovskite Solar Cells with Improved Reproducibility" *Science*, **2021**, *373*, 561-567.

Jakob, D.S.; Li, N.; Zhou, H. and Xu, X.G. "Integrated Tapping Mode Kelvin Probe Force Microscopy with Photo-induced Force Microscopy for Correlative Chemical and Surface Potential Mapping" *Small*, **2021**, doi.org/10.1002/smll.202102495 (Featured as a back cover)



Xiaoji Xu (Continued)

Wang, H.; Xie, Q.; Zhang, Y. and Xu, X.G. "Photothermally Probing Vibrational Excited-State Absorption with Nanoscale Spatial Resolution through Frequency Domain Pump-Probe Peak Force Infrared Microscopy" *The Journal of Physical Chemistry C* **2021**, *125*, 8333-8338.

Wang, H.; González-Fialkowski, J.M.; Li, W.; Xie, Q. Yu, Y. and Xu, X.G. "Liquid-Phase Peak Force Infrared Microscopy for Chemical Nano-imaging and Spectroscopy" *Analytical Chemistry* **2021**, *93*, 7, 3567-3575.

Zhang, Y.; Yurdakul, C.; Devaux, A.J.; Wang, L.; Xu, X.G.; Connor, J.H.; Ünlü, M. S. and Cheng, J-X. "Vibrational Spectroscopic Detection of a Single Virus by Mid-Infrared Photothermal Microscopy" *Analytical Chemistry* **2021**, *93*, 8, 4100-4107.

Wang, H.; Wang, L.; Janzen, E.; Edgar, J.H. and Xu, X.G. "Total Internal Reflection Peak Force Infrared Microscopy" *Analytical Chemistry* **2021**, *93*, 2, 731–736.

Li, M.; Wang, H.; Li, W.; Xu, X.G. and Yu, Y. "Macrophage Activation on "Phagocytic Synapse" Arrays: Spacing of Nanoclustered Ligands Directs TLR1/2 Signaling with an Intrinsic Limit" *Science Advances* **2020**, *6*, DOI: 10.1126/sciadv.abc8482.

Gusenbauer, C.; Nypelö, T.; Jakob, D.S.; Xu, X.G.; Vezenov, D.V; Asaadi, S.; Sixta, H. and Konnerth, J. "Differences in Surface Chemistry of Regenerated Lignocellulose Fibers Determined by Chemically Sensitive Scanning Probe Microscopy" *International Journal of Biological Macromolecules* **2020**, *165*, 2520-2527.

Liz Young

The Young Lab kept busy in the lab this past year carrying out synthesis and time-resolved spectroscopy experiments to understand the photochemistry of several systems ranging from photosensitizers for photodynamic therapy, to excited-state proton-coupled electron transfer, to antimony-sulfide based photovoltaics. Professor Young gave virtual seminars at Philadelphia University of the Sciences, SUNY Binghamton, Arizona State University, and Youngstown State University. She also gave a talk in the Lehigh University I-FMD (Institute for Functional Materials and Devices) Grand Rounds series.

Professor Young, along with Professor Fredin, received funding from the Pittsburgh Foundation to create impactful research experiences for Lehigh undergraduates. In doing so, Young and Fredin established the PURE program (Photochemistry Undergraduate Research Experience), which combines computational and experimental physical chemistry research. Four Lehigh undergraduate students completed their first summer of work and they are now continuing their research projects during the 2021-2022 academic year.

Professor Young published several articles over the past year on her work with proton-coupled electron transfer, the photophysics of several interesting donor-acceptor systems, and on the photophysics of antimony sulfide as a light absorbing material for next generation solar cells. Recent publications include:

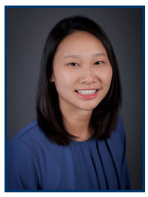
Pointer, C.; Buettner, P.; Scheler, F.; Döhler, D.; Mínguez-Bacho, I.; Bachmann, J.; Young, E.R. "Elucidating Mechanistic Details of Photo-Induced Charge Transfer in Antimony Sulfide-Based pin Junctions." *J. Phys Chem. C.* **2021**, *125*, 18429–18437.

Martin, S.M.; Oldacre,A.N.; Pointer, C.; Huang, T.; Repa, G.M.; Fredin, L.A.; Young, E.R.* "Proton-controlled Non-exponential Photoluminescence in a Pyridylamidine-substituted Re(I) Complex." *Dalton Transactions*, **2021**, *50*, 7265-7276.

Büttner, P.; Scheler, F.; Pointer, C.; Döhler, D; Yokosawa, T.; Spiecker, E.; Boix, P.P.; Young, E.R.*; Mínguez-Bacho, I.*, Bachmann, J.* "ZnS Ultrathin Interfacial Layers for Optimizing Carrier Management in Sb2S3-based Photovoltaics." *ACS Appl. Interfaces.*, **2021**, *13*, 11861–11868.

Wehrmann, C.M.; Imran, M.; Pointer, C.A.; Fredin, L.A.*; Young, E.R.*; Chen, M.S.*, Spin Multiplicity Effects in Doublet versus Singlet Emission: The Photophysical Consequences of a Single Electron. *Chem. Sci.*, **2020**, *11*, 10212-10219.

WELCOME NEW FACULTY



Crystal Chu

Dr. Crystal Chu attended the University of California, Berkeley, where she earned a B.S. in Chemistry. At Berkeley, she performed undergraduate research in organic materials and gained an appreciation for multidisciplinary research, particularly at the intersection of organic chemistry, materials, and medicine. In 2012, Dr. Chu moved to southern California to pursue her doctorate in chemistry at the California Institute of Technology. She studied novel reactivity and selectivity in transition metal-catalyzed reactions, including cross couplings, oxidations, and olefin metathesis, and earned her Ph.D. in 2017 with Nobel Laureate, Professor Robert H. Grubbs.

Before joining Lehigh as an Assistant Professor of Chemistry, Dr. Chu was an NIH NRSA postdoctoral fellow with Professor Robert Langer and Professor Daniel Anderson in the Koch Institute for Integrative Cancer Research at the Massachusetts Institute of Technology. Her postdoctoral research focused on structure-property relationships that enable the molecular design of biomaterials, including bioinspired fibers and glucose-responsive hydrogels for drug delivery.

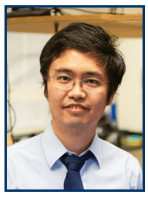
Dr. Chu's research interests lie at the intersection of chemistry, engineering, and materials science. The overarching goal of her research group at Lehigh is to decipher molecular mechanisms to tune the mechanical properties and functions of soft materials synthesized for biomedical applications.

Hannah Cronk

Joining Lehigh University in January, 2020, (and quickly adapting her course design to provide virtual instruction during the early days of the COVID-19 transition to remote learning) Visiting Professor Hannah L. Cronk obtained her Ph.D. in Materials Chemistry from the Department of Chemistry at Binghamton University SUNY where her research was in alloy nanoparticle synthesis.

Before joining Lehigh University, she taught at a range of institutes where she focused on general chemistry education. Hannah found that many students fear failing chemistry but do not know how to succeed--so she shifted her teaching style to include study tips, memorization tricks, and test anxiety resources. She also enjoys STEAM community outreach, sewing, needle felting, and reading. Hannah is enjoying being a part of the Department of Chemistry.

ANNOUNCING THE PROMOTION AND TENURE OF DR. XIAOJI XU



Dr. Xiaoji Xu has been promoted to the rank of Associate Professor and granted tenure effective October, 2020. He came to Lehigh University in the Fall of 2014 as an Assistant Professor from a Postdoctoral Research Associate position under Gilbert C. Walker at the University of Toronto where his research focused on the study of biological and condensed phase matter material with near-field and far-field techniques.

He received his BSc in Analytical Chemistry from Peking University and his PhD in Physical Chemistry from the University of British Columbia in 2009, studying ultrafast spectroscopy, nonlinear optics, and photonics under John W. Hepburn.

His research at Lehigh University has been focused on the organization and interaction of molecules, materials, and structures with spatial heterogeneity, particularly in regard to nanoscale characterizations of polymers, aerosols, polaritonic materials, and biological samples.

In response to challenges of optical microscopy and the diffraction limit of light (nano-materials often have features smaller than the diffraction limit that is not resolvable by traditional optical microscopy) Xu's lab has developed two types of super-resolution infrared microscopies that combine atomic force microscopy with laser radiations: 1.) Peak force infrared (PFIR) microscopy and multipulse PFIR microscopy in both air phase and liquid phase, and 2.) Scattering-type scanning near-field optical microscopy (s-SNOM)--and more specifically, Peak force scattering-type near-field optical microscopy (PF-SNOM) that can collect 3D near-field response cube.

In addition, they have also developed and refined other modalities of atomic force microscopy through instrumentation. For example, the Pulsed force Kelvin probe force microscopy (PF-KPFM) to map the surface potentials with < 10 nm spatial resolution under ambient conditions.

His lab's focus is on materials that may be nanoscale heterogeneous, such as block copolymers, blends, protein aggregates, polaritonic nanostructures, oil shale, urban aerosols, cellular structures, and photovoltaics.

Xu has been named a 2018 Beckman Young Investigator, a 2020 Sloan Research Fellow and (as spotlighted on Page 6 of this newsletter) a 2021 Camille Dreyfus Teacher-Scholar!

Dmitri Vezenov

January 21, 1967 - October 29, 2021

Arriving at Lehigh University in January of 2006, Dmitri Vezenov brought a wealth of physical chemistry knowledge from both his educational and research background--as well as his real-world experiences. He demonstrated every day his caring commitment to educating students on the intricacies of physical and surface chemistry, microscopy, and nanomechanics--within a field of science that he relished so deeply .

Born and raised in Ryazan (a city in the Russian Federation southwest of Moscow), he earned a B.S. (cum laude) in chemistry from Moscow State University in 1991. He then travelled to the United States to expand upon this knowledge through a master's program at Case Western Reserve University--earning his M.S. in 1994. He received his Ph.D. from Harvard University in 1999. Gathering experience in the industry, Vezenov then worked for several years as a senior engineer and science advisor for a corporation focused on nanoscale optical technology. Returning to Harvard in 2003 as a postdoctoral fellow in chemistry, he worked with the eminent and highly-respected Dr. George M. Whitesides on light sources and optical waveguiding for microfluidic applications.

It was while completing his work at Harvard that he applied for the position of assistant professor at Lehigh University and was happy to receive an offer to come to the Lehigh Valley to begin this new role. A skilled professor, he taught courses in general chemistry and physical chemistry, including a course in statistical mechanics and thermodynamics. His research interests included physical and surface chemistry; chemical force microscopy; nanomechanics and analytical microdevices. He received a grant from the National Human Genome Research Institute in 2006 for a project that applied force spectroscopy to DNA. In 2011, he was awarded a patent for a quicker, more efficient method of sequencing DNA.

Within his lab, his research interests included intermolecular interactions in soft matter; chemical force microscopy; bio-nano-photonics; analytical microdevices; controlled synthesis and assembly of materials at mesoscale. He described his research as interdisciplinary, where approaches of chemistry, physics and engineering converge. Vezenov's doctoral student, Bil Leon, appreciated this broad research methodology, stating, "Dmitri was a wonderful mentor . . . who shared a love of science, unending curiosity in the research lab . . . and [who] was always supportive of his students' work and would strive to get the best out of them, working constantly to ensure their success."

In addition to his expertise in teaching and research protocols, Vezenov also contributed to a multitude of administrative functions including serving on department committees and serving as faculty search committee chair for several key faculty hires. He served in these roles as he served in his professorial role --greeting each challenge with a smile and a calm response to address concerns and steer the conversation and processes to a positive outcome.

Department of Chemistry Chair Greg Ferguson, who worked with Vezenov throughout his tenure at the university, spoke for the entire department when he stated for the Lehigh News, "Dmitri was a kind and generous friend and collegue who never hesitated to help others, whether it was contributing to the preparation of a departmental proposal or sharing his thoughtful insights on research or teaching. We are poorer for his loss, but richer for having had him with us at Lehigh for the past 15 years."

Vezenov is survived by his parents; his wife, Marina Busuek, and their three children, Maxim, who holds a BS in Chemical Engineering and Computer Science from Lehigh University and is currently a Lehigh graduate student, Elizabeth, and Zoe; as well as his brother Roman and extended family in Russia.

Dmitri spent 15 dedicated years investing in passing along his knowledge and outstanding research skills to the next generation of young scientists. The measure of a man can be seen in what he has done with his life. Through his influence on generations of scientists, the loving family he built with his wife, and the memories he leaves within the department, Dmitri was a giant whose infinite measure will still be felt for succeeding generations to come.

EMERITUS PROFESSOR KAMIL KLIER

And now you know . . . . . the rest of the story

Through the years, few Lehigh University professors have stood firm and risen above life's challenges more profoundly than Emeritus Professor Kamil Klier. Born in 1932, Klier grew up in the city of Prague, Czechoslovakia (at the time, a democratic republic sovereign state) enjoying a happy family life and participating in normal childhood activities, such as soccer and ice hockey.

The advent of World War II changed everything about Klier's native land—from government to education and even including the name and borders of his country when the beautiful city of Prague became a part of a German-occupied Protectorate of Bohemia and Moravia. Prague was bombed numerous times during World War II at the cost of approximately 1,200 lives. At the conclusion of the war, this area was reunified with Slovakia as part of the 1948 Ninth of May Constitution enforced by the Soviet Union, becoming a part of the Eastern Bloc.

As a young man in 1950, Klier matriculated to Prague's renowned Charles University where he earned his Diploma in Chemistry in 1954. Interested in gaining more knowledge in his chosen field, he pursued graduate studies at the Czechoslovak Academy of Sciences in Prague (and ultimately at the Institute of Physical Chemistry working under Dr. Rudolf Brdička) from 1954 to 1959. He then spent a year in the UK working with Dr. T. I. Barry as a Fellow at the Wantage Research Laboratories in Oxfordshire--a part of the UK Atomic Energy Research Establishment (AERE)--which was the main center for atomic energy research and development in the United Kingdom at that time.

He returned to Prague to obtain his Ph.D. in Physical Sciences in 1961 from what is now the Academy of Sciences of the Czech Republic. As noted in the Academy's historical publication, *Sixty Years of the J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague (1953-2013)*, "Conditions for research and contact with foreign scientific institutions were rather modest in the fifties. Instrument purchases from abroad was [sic] all but impossible; all necessary mechanical, vacuum, and electronic equipment had to be made in-house. The supply of journals to the library was limited. Foreign travel and conference participation was restricted. Meetings with foreign scientists were largely limited to international conferences held in Czechoslovakia."

Even under the difficult conditions described, Klier became known for his contributions to strengthening research into heterogeneous catalysis at the Institute. From 1961 to 1968 he was a Senior Research Scientist at the Institute and was part of a group of young scientists whose significant discoveries were disseminated to the world during a relatively stable time in the country's governance. Although under the Communist regime of the USSR, some changes in governance brought an easing of tensions that resulted in permission for some scientists at the Academy to visit western universities and international conferences. Despite these changes, however, many travel applications were still routinely rejected by state authorities.

Klier's work during those years concentrated on chemisorption on metal oxides and the factors that directed oxygen exchange reactions on transition metal oxide catalysts, as well as on the exchange and chemisorption properties of transition metal cations in zeolites. His research demonstrated the utility of diffuse reflectance UV/Vis/NIR spectroscopy in providing quantitative information about the state of reactive surface centers. This work opened doors for him to attend an international conference in 1967 where he met Dr. Frederick Fowkes, then the Director of Research at the Sprague Electric Company's Research Center in North Adams, Massachusetts (and who was also serving as the chairman of the division of colloid and surface chemistry of the American Chemical Society [ACS]). Fowkes would join Lehigh University in the summer of 1968 as the chair of the Department of Chemistry, at which point he invited Klier to come to the university as a Visiting Professor. Klier and his wife Jana and their two small sons, John and Peter, arrived in Bethlehem, Pennsylvania in that summer of 1968.

In Czechoslovakia, the year 1968 also saw the beginnings of a liberalization period known as the *Prague Spring* when the reformer Alexander Dubček was elected as the First Secretary of the Czechoslovak Communist Party on January 5, 1968. Dubček lead a political movement that sought to grant additional rights (including access to media, freedom of speech, and the ability to travel abroad) to the citizens of

Czechoslovakia through a partial decentralization of the economy and also through democratization (sometimes referred to as "Communism with a heart"). At first the Soviets were amenable to these changes, but the reforms, especially the decentralization of administrative authority, were ultimately rejected by Moscow. The Prague Spring ended abruptly after failed negotiations with the Soviets resulted in half a million Warsaw Pact troops and tanks forcefully occupying the country on August 20-21, 1968.

Klier and his family had just recently arrived in the United States at the time of the military occupation. He correctly interpreted what a restrictive regime would mean for the scientific community in his native land and sought political asylum for himself and his family. His request was granted, thereby opening the door for his continued employment at Lehigh University.

A well-respected researcher with an already voluminous body of work, Klier was successful in applying for funding to support and expand his research endeavors at Lehigh. He was promoted to the rank of associate professor--and in 1973 he was promoted to a full professor.

In 1978 he was appointed the Associate Director of the Center for Surface & Coatings Research. During this time, he contributed to the filing of two patents: one related to catalysis and a method for the production of methylamines, and a second for a process for selective production of di- and tri-alkylamines. He ultimately received five US patents for his work in catalysis.

Named the Chair of the Department of Chemistry in 1992, he served in this role until 1996, while simultaneously continuing a long-time collaboration with Dr. Rick Herman (Executive Director and Principal Research Scientist of the Lehigh University Zettlemoyer Center for Surface Studies) and with Department of Chemistry Professor Gary W. Simmons on spectroscopic characterization of active surfaces. Klier led the effort in obtaining the world-class X-Ray Photoelectron Spectrometer (XPS) instrument, which was the only high resolution instrument of its kind in the United States. He also established a leading research laboratory for the design, characterization, and testing of catalysts for the synthesis of methanol, higher alcohols, and other chemicals from H2/CO synthesis gas at elevated pressures and temperatures

Throughout his tenure at Lehigh, Klier taught classes ranging from introductory chemistry to advanced undergraduate and graduate-level courses in solid state chemistry, physical inorganic chemistry, quantum mechanics, and surface spectroscopy. In 2010, Klier embarked upon a new path as an emeritus faculty member, continuing his research throughout much of the decade.

Both an outstanding researcher and an excellent teacher, Klier received many accolades from the University and also from the broader chemical community. Recognition included an Outstanding Educator of America Award in 1973, a University Distinguished Professorship in 1982, and the Libsch Distinguished Research Award in 1984.

Accolades received from the industrial sector include the Union Carbide Award for Innovative Chemistry-1981-1986, , the Excellence in Research Award from the New York Catalysis Society in 1983, the Langmuir Lectureship from the American Chemical Society in 1987, the Burwell Lectureship in Catalysis from the North American Catalysis Society in 1991, and the Heyrovsky Medal of the Czech Academy of Science in 1997. He has chaired numerous symposia at research society meetings all across the country and was the organizer and chairman of a symposium at the International Chemical Congress of Pacific Basin Societies in Hawaii in 1989. Of particular note is his establishment of a leading laboratory in catalytic alcohol synthesis (at the time, one of the only academic research laboratories that could carry out long-term catalyst testing under real industrial process conditions.) He is renowned as a research leader in high resolution XPS (ESCA) characterization of active sites and surface interactions of a wide range of materials including catalysts.

Additionally he has been a prolific lecturer, presenting more than 200 seminars at diverse venues including Gordon Research Conferences, the U.S.-China-Japan Symposium on Catalysis in Osaka, Japan, and the Symposium on Environmental Catalysis at the Fifth North American Chemical Congress in Cancun, Mexico. He has served on the editorial boards of numerous catalysis journals, was co-editor of Catalysis Reviews—Science and Technology throughout the 1990's. During his career he authored and contributed to over 250 research papers.

A long-term resident of Bethlehem, Dr. Klier is well-known in his community and is regarded with high esteem for his willingness to share his knowledge at home and abroad.

The man who struggled under a repressive regime to conduct experiments in his youth rose above the political unrest in his homeland and seized the opportunity to participate in the education of hundreds of undergraduate and graduate students, postdoctoral research associates, and visiting scientists in his adopted country. He willingly and openly shared his vast knowledge in myriad ways and, in doing so, built a solid framework upon which current and future scientists will continue to solve the problems of the world while probing the secrets of nature.

2021 UNDERGRADUATE STUDENT AWARDS

AMERICAN CHEMICAL SOCIETY AWARD	ACS INORGANIC CHEMISTRY AWARD	AMERICAN INSTITUTE OF CHEMIST'S AWARD	BIOCHEMISTRY AWARD
Presented to the outstanding senior majoring in Chemistry	Granted to the outstanding senior majoring in Inorganic Chemistry	For an outstanding senior majoring in Chemistry or Biochemistry	Granted to the highest-ranking junior or senior Biochemistry major
GAO LONGHUI	NICOLE KARPOWICZ	LINNAN FANG	DAVID KHAYATA

ACS ORGANIC CHEMISTRY AWARD (Organic Division)	ACS ORGANIC CHEMISTRY AWARD (Physical Division)	HARRY M. ULLMANN CHEMISTRY PRIZE	ALPHA A. DIFENDERFER AWARD (ACS Analytical Chemistry Award)
Recognizes a senior student who displays a significant aptitude for Organic Chemistry and encourages further interest in the field	Presented to the outstanding senior majoring in Physical-Organic Chemistry	In honor of Lehigh University Professor and Department Chair (1914-38) Harry M. Ullman--this award goes to the highest-ranked senior in Chemistry	In honor of Lehigh University President and Department Chair Alpha Diefenderfer--and sponsored by the ACS Division of Analytical Chemstry, this award is presented to the highest-ranking junior in Analytical Chemistry
LAUREN FURST	KIERA ENGLEHART	LINNAN FANG	DAVID KHAYATA

Established in 1920 by Mrs. Chandler, the prize is in honor of her husband, William H. Chandler, Professor of Chemistry at Lehigh University from 1871 to 1905--and twice an acting Lehigh President

WILLIAM H. CHANDLER SOPHOMORE PRIZE	WILLIAM H. CHANDLER JUNIOR PRIZE	WILLIAM H. CHANDLER SENIOR PRIZE
Presented to the highest-ranking sophomore in the Department of Chemistry	Presented to the highest-ranking junior in the Department of Chemistry	Presented to the highest-ranking senior in the Department of Chemistry
JUEUN HAN	THOMAS DRESSLER	LINNAN FANG

2020-2021 GRADUATES

Bachelor's Degrees

NAME	MAJOR	HONORS NOTATION
Meriam Deeb	Biochemistry	Summa Cum Laude-Phi Beta Kappa
Kathryn Dunn	Pharmaceutical Chemistry	Cum Laude
Linnan Fang	Chemistry	Summa Cum Laude
Lauren Furst	Pharmaceutical Chemistry	Summa Cum Laude
Longhui Gao	Biochemistry	Summa Cum Laude
Timothy Hartnagel	Biochemistry	
Gioorgos Hiotis	Biochemistry	Summa Cum Laude-Phi Beta Kappa
Nicole Karpowicz	Chemistry	Cum Laude
Sarah Ko	Biochemistry	
Elizabeth Kolaski	Biochemistry	Summa Cum Laude
Rachel Kulakofsky	Biochemistry	Magna Cum Laude
Emanuel Luna	Biochemistry	
Poorva Patel	Pharmaceutical Chemistry	
Alana Rosen	Chemical Engineering	
Joseph E. Saba, Jr.	Biochemistry	Magna Cum Laude
Alexis Shanley	Biochemistry	Magna Cum Laude
Xiomin Shi	Pharmaceutical Chemistry	Cum Laude
Tess Van Buskirk	Biochemistry	
Ivy Yu	Biochemistry	Cum Laude

Doctoral Degree

George Ongwae - "Leveraging Nature's Bacterial Surface Homing Molecules to Combat Pathogens" (January 20, 2021)

WELCOME NEW GRADUATE STUDENTS

NAME	MATRICULATING FROM	LOCATION
Alysson Bermudez	SUNY Buffalo	Buffalo, NY
Joseph Conlin	Colgate University	Hamilton, NY
Jesika DeDonato	Moravian College	Bethlehem, PA
Andrea Dorsa	Bowdoin College	Brunswick, ME
Ruth Ebubechukwu	Federal University of Agriculture	Abeokuta, Nigeria
Walter Espinoza Pax	East Stroudsburg University	East Stroudsburg, PA
Dominica Fertel	Columbus State University	Columbus, GA
Christian Guzman	East Stroudsburg University	East Stroudsburg, PA
Ryann Kemmerling	University of Scranton	Scranton, PA
Leah Knepper	Geneva College	Beaver Falls, PA
Jessica Mickno	Moravian College	Bethlehem, PA
Adeyemi Odudimu	University of Ibadan	Ibadan, Nigeria
Amanda Prascsak	Monmouth University	West Long Branch, NJ
Dane Santa	East Stroudsburg University	East Stroudsburg, PA
Korina Vida Sinad	University of the Phillipines Los Banos	Los Banos, Phillipines
Termeh Teymoorian	Amirkabir University of Technology	Tehran, Iran
Lydia Yorks	Lycoming College	Williamsport, PA

Graduate Student Fellowships: 2021-2022

HORNOR FELLOWSHIP: Scott Shreiber

FULBRIGHT SCHOLARSHIP: Muhammad Imran (Pakistan)

SUMMER 2021 CAS FELLOWSHIP: Jeff Julien

FALL 2021 CAS FELLOWSHIP: Ashley Baxter

Ashley Baxter

2020-2021 Teaching Assistants of the Year

Jeff Julien

This award was created to recognize those individuals who, through their dedication to academic rigor and student success, have distinguished themselves as outstanding teaching assistants.

It documents the high regard with which these two TA's are held by both the teaching faculty and the students they have supported in their learning endeavors throughout the year

STAFF NEWS

Welcome New General Chemistry Lab Manager Dan Prendergast

Daniel Prendergast

Daniel Prendergast (ABD) became our new Manager of General Chemistry Labs in January of 2021, arriving upon completion of his PhD coursework at the Massachusetts Institute of Technology.

Prendergast, who is a native of Old Saybrook, Connecticut, received his B.S. in Chemical Engineering from Brown University and an M.S. in Civil and Environmental Engineering from MIT. His Masters research was done in a collaboration with Italy's national oil Company, Eni, to develop and understand novel, lab-scale oil cleanup devices incorporating hydrophobic surfaces, and their efficiency in scaled wave experiments. His PhD research focused on analytical chemistry techniques and hydrodynamic modeling to study the fate, transport, and sources of anthropogenic organic contaminants in natural waters and sediment. Working with Dr. Philip Gschwend in the Parsons Laboratory at MIT, he focused on developing new passive samplers and devising ways to identify the source(s) of contaminants in complex environments so that organizations such as the Environmental Protection Agency (EPA) and other entities could effectively detect and mitigate toxic chemicals.

In 2019, he joined Harvard University's Active Learning Labs as an Environmental Engineer where he was responsible for their chemical teaching laboratory management, safety and instrument maintenance. In this role, he trained and supervised lab teaching assistants who assisted him in conducting laboratory exercises for multiple courses, as well as developing demonstrations of chemical and fluid phenomena for lecture-based courses and video demonstrations for distance and asynchronous learning.

With the advent of COVID-19 and its impact to on-campus classroom learning, Daniel utilized his training in distance learning to assume the role of Chemistry Specialist at the University of Califonia, Davis where he provided remote instruction in weekly workshops for general chemistry and also designed supplementary curriculum to address the new demands of virtual learning.

We welcome Dan to the Lehigh University Department of Chemistry!

ALUMNI NEWS

'68 James Frazee reports he is "VERY happily retired after 39 years as a synthetic organic chemist for GlaxoSmithKline. I loved the job, loved the folks I worked with, but love the retirement!" For the last 12 years, Jim has been working part time for Stags Leap Ranch and the Biebel Farms Association doing estimates of total population and diversity of wildlife found in and around selected private ponds in New Jersey. The information is provided to land owners to give them guidance for stress factors affecting their ponds. This data can lead to the owners placing private restrictions on the taking of the various wildlife from those aquatic areas.

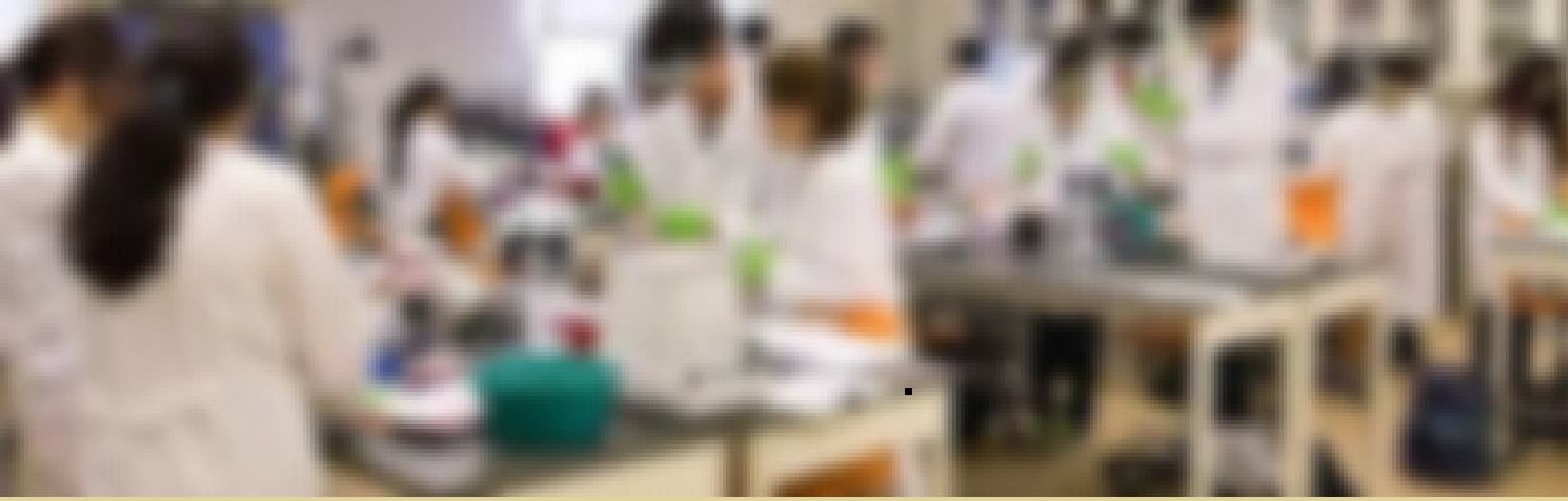
'89 George Marchesini has been promoted to the Senior Director, Commercial Regulatory Affairs, Hematology & Cell Therapy, Bristol Myers Squibb, Bridgewater, New Jersey.

'04 Peter DeMatteo has completed three years with a research-for-hire and scale-up kilo lab facility (Adesis) located in the former Dupont Experimental Station. Adesis is growing rapidly (> 350 employees) and Peter is part of that growth.

Their recent news release on businesswire.com describes the organization as "a contract research organization (CRO) supporting the pharma, biotech, catalysis and a number of other industries. The CRO specializes in organic and organometallic synthesis, in milligrams to multi-kilogram quantities. Adesis has a business model of providing clients with organic chemistry services in three areas: early stage research, scale up and development, and specialty manufacturing. They are a wholly-owned subsidiary of the Universal Display Corporation. This expansion will provide new state-of-the-art laboratory growth to support Adesis' growing research and development pipeline. Situated in Wilmington, Delaware, this expanded lab space approximately triples Adesis' footprint in the DuPont Experimental Station.

'15 Mengzhao (Lucy) Xue completed her PhD in Biochemistry at Yale University and joined the research staff at Rockefeller University in New York City as a Postdoctoral Research Associate.

'16 Gabrielle Haddad-Weiser is in her third year of service as Senior Engineer in the Environmental Toxicology Laboratory of the Veterinary Sciences College of the Norwegian University of the Life Sciences located in As, Norway.



Your donations can fund student research and travel, expanding the Lehigh University reputation across the nation and around the globe.

Donations also represent an important part of our continuing efforts to create a "state-of-the-art" environment for teaching and research at Lehigh.

If you are at a point in your life where you can "Pay It Forward" please consider a donation to support those students following in your footsteps.

Donations can be made fast and easy in either of two ways:

- By contacting Dept. Chair Greg Ferguson (gf03@lehigh.edu) to discuss specifica projects
- By contacting Lehigh's Advancement Office at (800) 533-9656

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