CHEM NEWS

Fall 2021



COLUMBIA CHEMISTRY

GREETINGS FROM THE CHAIR, PROFESSOR TOMISLAV ROVIS

Dear Friends,

Greetings from Morningside Heights! We are in the middle of summer, with fine sunny days on a campus slowed partly by COVID and partly by the vagaries of academic calendars. As we anticipate a full return to campus, and a welcome to a new incoming graduate class as well as a new crop of freshmen, it is time to take stock of where we are and to update you, our alumni, colleagues and friends of the department, on life in and around Havemeyer, Chandler and the Northwest Corner buildings.

This past year has been a challenge to many institutions, individuals and families, and Columbia is not immune. The worldwide epidemic has changed the way we work, travel and interact with our family, friends and colleagues. The University transitioned to largely remote instruction last Fall and has gradually changed back with the intent to return to full in-person instruction this coming Fall. Likewise, after the initial shutdown in Spring 2020, research also returned to campus at the beginning of last summer and we gradually raised occupancy in labs from an initial 33%, with (nearly) all restrictions to be lifted by the Fall. The campus is heavily vaccinated and life is almost back to normal.

Research took a brief hiatus but never stopped and we continue to innovate in our science and teaching. With that comes the arrival of new faces. The past few years have seen us successfully recruit several young faculty. In this issue, we profile one such arrival, Professor Tim Berkelbach. Of course, it is inherent to the nature of any thriving department that as young colleagues arrive, so too must we



occasionally see our older distinguished colleagues as they retire to pursue other things. Professor Bruce Berne, known to all of you, officially retired this year. We profile him and his exceptional career in the pages of this newsletter.

As you all know, we have always had amazing students at both the graduate and undergraduate level. We recognize their achievements in science and scholarship with departmental Fellowships and Awards. This year's awards were, unfortunately, delivered virtually, so a group picture would have to be a zoom screenshot. Nevertheless, we have highlighted the accomplishments of our various spectacular undergraduates and the Pegram and Hammett graduate award winners. It is not hyperbole to say that these are the faces that will prove as impactful in the future as our previous award winners have been and continue to be.

The life of the department is made richer and more fulfilling by many individuals. For graduate students in every class, one individual that plays an important role is their class rep. This tradition goes way back (and if someone knows exactly how far, please let me know). To update all of you, we have also included photos and brief bios of our current class reps to tell you about the type of individuals that have been chosen (and have agreed to) give selflessly of their time so that their colleagues' Columbia experience can be richer.

Science continues to evolve with new directions, new opportunities bringing new challenges and new rewards. Columbia Chemistry continues to be at the forefront with a vibrant intellectual environment coupled with a supportive and inclusive culture. We strive to recruit, mentor and support the very best students, regardless of background, and then watch their careers blossom upon graduation, the way we have been from well before Gilbert and Ron were young faculty here. I hope to continue these updates and welcome each of you to contact us, to reach out to myself or any of my colleagues. Tell us how you are doing and what exciting accomplishments you have to share. If you find yourself in the NYC area, stop by and say hi.

Warmest regards,

Tom

INTERVIEW WITH PROFESSOR TIMOTHY BERKELBACH



The Chemistry Department welcomed Dr. Timothy Berkelbach as one of our newest faculty members in 2019. Assistant Professor Berkelbach has a joint appointment with the Flatiron Institute, where he is a Research Scientist in the Center for Computational Quantum Physics.

Professor Berkelbach came to New York City for the first time as an undergraduate student to study chemistry and physics at New York University. He then moved uptown to Morningside Heights to pursue his PhD in the Chemistry Department at Columbia. After a postdoctoral position at Princeton University and an assistant professorship with University of Chicago, Professor Berkelbach returned to New York City, now dividing his time between Morningside Heights and Flatiron.

At Columbia, Professor Berkelbach's research group focuses on theoretical and computational chemistry. Explaining why he chose to locate his research here, he says, "Columbia is one of the best universities in that research area. That was part of what drew me to Columbia as a graduate student. Obviously, to be back and on the faculty to contribute to that is great. The other side of the research part that's been great is the collaborative work. All of the faculty know each other and work together."

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GRADUATE STUDENT AWARDS

The Department of Chemistry celebrated the winners of its 2021 Graduate Student Awards at the 34th Annual Student Awards ceremony on Tuesday, April 27. The winners received certificates and monetary awards for their contributions to research and teaching.

The Hammett Award is the department's most prestigious award for academic excellence. It is awarded annually to a student in the final year of the program in recognition of outstanding fundamental studies in chemical research. This year, the department honored Suman Gunasekaran with this award. Of Suman's work, his research advisor, Professor Latha Venkataraman, writes,

"Suman Gunasekaran earned his bachelor's degree from Harvard University and joined Columbia University as a PhD student in the Chemical Physics graduate program in



Suman Gunasekaran

2016. He joined the group of Prof. Latha Venkataraman for his doctoral studies where he completed his dissertation titled 'Investigating Electron Transfer Across Single-Molecule Junctions.' His graduate research focused on understanding how electrons flow across singlemolecules, focusing on how quantum interference, photoconduction and redox processes could tune current in these nanoscale devices. Suman has co-authored nine publications in top interdisciplinary journals such as Nature Nanotechnology, Nano Letters and the Journal of the American Chemical Society, including four where he is first-author. Suman will continue his research at Cornell University starting in August of



this year, where he will be the Kavli Institute Post-doctoral fellow. He plans to work in the lab of Prof. Andrew Musser on ultrafast spectroscopy to expand his understanding of chemical physics, transitioning from studying the ultra-small, as a Ph.D. student to studying the ultra-fast as a post-doctoral researcher."

The Pegram Awards honor meritorious achievements by students in their final year of the program. This year's winners included Carla Bezjian, Matthew Carbone, Isra Hassan, Benedikt Kloss, Sumin Lee, Jake Russell, Yeongsu

INTERVIEW WITH PROFESSOR BRUCE BERNE



A native New Yorker who grew up in Brooklyn and attended the legendary Erasmus Hall High School, Higgins Professor Emeritus Bruce J. Berne made Columbia University his research and teaching home for 55 years before retiring this summer.

Professor Berne received his BS in Chemistry from Brooklyn College, CUNY in 1961 and his PhD in Chemical Physics from the University of Chicago in 1964. After a postdoctoral fellowship in Bruxelles, Professor Berne joined the Columbia University faculty in 1966. "Columbia Chemistry was one of the best chemistry departments in the world at that time," as it still is, he says.

Professor Berne was among the small band of chemists to recognize the significance of computers to the field of liquid state chemistry. He was an assistant professor when a graduate student asked him if he had a problem that could be solved using the university's cutting-edge computer, which at the time was available to only a few researchers at a time. He came up with a problem to take advantage of the new technology. With his first graduate student, George Harp, he developed the methodology for and performed the first molecular dynamics simulation ever done on a molecular liquid. He was granted free use of the university mainframe for the eight-hour evening shift-- but George Harp had to join a union to operate the computer at that time because there would be no other operator on duty.

In more than 350 publications and four books since then, Professor Berne has written about time-correlation and memory function theory, the theory of light scattering, new methodologies in both classical and quantum Monte Carlo and molecular dynamics, reaction rate theory, the theory of quantum liquids, the small and large scale hydrophobic effect, the design of polarizable force fields for water and complex molecules, the biophysics of proteins, and proteinligand binding. He developed many methods used in molecular dynamics and Monte Carlo simulations.

Professor Berne credits his students. "Obviously, without my students, we would have done much less," he says. "I regard them as very important. I've always acted toward my students as collaborators, not as in any way inferior, and I am still very friendly with many of them. It's like having an extended family all around the world."

Professor Berne has been an Alfred P. Sloan Foundation Fellow (1967-70), and John Simon Guggenheim Founda-

INTERVIEW WITH PROFESSOR BRUCE BERNE

(Continued from page 4)

tion Fellow (1972). He received the Alexander von Humbold-Stiftung Senior Scientist Award (1992); the ACS National Award in Theoretical Chemistry (1995); the Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids of the American Chemical Society (2002); the Joseph O. Hirschfelder Prize in Theoretical Chemistry from the University of Wisconsin (2001): IBM Research Achievement Awards (2005) and 2007); the Mulliken Medal from the U. Chicago (2009); The Peter Debye Award in Physical Chemistry of the American Chemical Society (2017). He is also a Fellow of the American Physical Society and the American Association for the Advancement of Sciences. He was elected fellow of the American Academy of Arts and Sciences (1995) and was elected member of the National Academy of Science (1998). Although he now lives in the suburbs, Professor Berne remains a New Yorker at heart. "New York to me is always changing and incredibly exciting," he says. Among his post-retirement accomplishments, Professor Berne, his wife and two sons will celebrate his 60th wedding anniversary this summer. He will continue as a Special Research Scientist at Columbia and is currently writing a manuscript on statistical mechanics and pursuing some research ideas.

INTRODUCING THE CLASS REPRESENTATIVES

Hello, Chemistry Department Alumni! With this first edition of the newsletter, we wanted to take a moment to introduce ourselves, the Student Representatives. You may likely know us as the students who host admitted applicants during Visit Weekends, organize social events during the STAT orientations for incoming graduate students, and put together Winter Shows (or in 2021, the Summer Show). In addition to these events, we also advocate for the students among the faculty and staff. We are....

Felisa: Alumni of Columbia, of Chemistry, my Brothers. I am the 5th year class representative (who could be a Dr. by the time you're reading this) in the Zhu Group. I would expand on the research I did here, but I just wrote a whole thesis on it, so if you really want to know more, feel free to read it. I am originally from Virginia, where I got my BS in Chemistry at George Mason University. Fun fact, my ultimate goal is to run a cat cafe wine bar. So, do with that what you will.

Alex: Hello, I am a member of the Roy Group, and the 4th year class rep-



From left to right: Felisa Conrad-Burton, Jesse Gray, Han Yang, Xiao Zhang, Inki Lee, Alex Aydt, Allyson Li

resentative. My research is focused on developing extended structures using superatoms to hopefully create novel, interesting magnetic materials. I grew up in Edwardsville, Illinois before moving to Tucson, Arizona for my undergraduate studies at the University of Arizona. Here in New York, you might find me running in Central Park or exploring the city. **Xiao:** Hello! I am the international class representative, and I'm a 4th year in the Rovis Group. My hometown is Shanghai, China, and I've also spent some years of my childhood in Osaka, Japan. I did my undergraduate study in Shanghai Jiao Tong University, and also spent several semesters at Yale, UC Berkeley and Cambridge University. My current research focuses on

INTRODUCING THE CLASS REPRESENTATIVES

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photoredox catalysis and organometallics. Other than running auto-column, my favorite things in New York are running in Central Park and Riverside Park, dancing, exploring museums, and trying to find the best piano on campus.

Allyson: Hi! I am the 3rd year class representative from the Shah Lab. I grew up in Queens, New York and I went to Grinnell College for my undergraduate studies. In the lab, I study signaling proteins. Outside of the lab, I enjoy discovering new restaurants and binge-watching RuPaul's drag race!

Jesse: Hello world, my name is Jesse. I am the 2nd year class representative and member of the Nuckolls group. I hail from rural Lebanon, CT, but now I'm a city boy. I graduated from Andrews University with a double major in Biochemistry and Viola performance. In the lab I make batteries out of organic polymers, but in the kitchen I make pies with bourbon. On the weekends you can find me in the climbing gym, biking through New Jersey, or playing music for hours while trapped in my apartment.

Inki: Hi everyone! I am the first year class rep from the Delor group. My research involves using ultrafast spectroscopy and microscopy to study energy transport in solid state and plasmonic materials. I grew up in Denton, TX, and I got my undergraduate degree in chemistry at the University of Texas in Austin. You can talk to me about anything sports related! I love to watch basketball, football, and hockey.

Han: Hi! I am Han. I am the international class rep and from the Kaufman group. I am from the south of China and I went to USTC for my undergraduate studies. In the lab I do single molecule imaging, so basically I am taking movies of the 'stars' and sometimes I can see constellations. One of my goals is to try all the best food in New York. If you have any questions on New York restaurants, I might be the person you would turn to.

That's us! Aside from all of this, we want to let you know about some of the great things we've accomplished recently for the department.

- We established a subsection of the Faculty Hiring Committee made up of graduate students to provide input in the hiring process;
- We collaborated with the Committee on Inclusion, Equity, and Diversity to facilitate more conversations and provide more resources on topics concerning equity and inclusion in science, specifically with a series of

forums and panels in 2020 and the formation of the Columbia Chemistry Outreach group;

- We advocated to restructure the lab joining process, to accommodate all students and facilitate student-PI relations from the start;
- We established a Peer Mentorship Program to aid in the transition to grad student life, the city, and the department for incoming students;
- We helped the department move to an online format for its virtual Visit Weekends during the COVID pandemic.

Some of our future projects that we are currently working on and planning on working on include:

- We are debuting the first (and, hopefully, only) Summer Show 2021!;
- We are piloting a new structured annual review system between students and their advisors, to improve communication about research progress and future prospects;
- We are working towards rebuilding the social events in order to strengthen and reignite the sense of community in the department;
- We want to improve the International Student experience;
- We want to continue to promote diversity and work toward a more equitable department;
- We want to continue to improve relationships between students, their advisors, and the department.

Thanks for your interest in our work! We have enjoyed being able to advocate for the people in this department. We'll be back next year! (Some of us. Not Felisa.)



Summer Show 2021, in 309 Havemeyer Hall

UNDERGRADUATE STUDENT AWARDS



Vanessa Dippon

Michael Van Duinen Chemistry Department Honors and Chandler Society Award

Hometown: Zeeland, MI

Hobbies: In my free time, I run, I play video games, and I read.

Research area: I have worked in the Venkataraman lab with single-molecule conductance since September 2018, starting by working with silver in the STM break junction technique and moving to computationally modeling quantum interference since the pandemic started.

Favorite memory about Columbia: I will most miss my walks and runs at Riverside Park, my quiet mornings working for the library, and the group walks the Chandler Society would take together every night

gy PhD at Harvard University

What's next? I will be at the University of Chicago for my PhD in Chemistry.

Kaitlyn Otte

after our weekly meetings.

Bent Undergraduate Teaching Award Hometown: Spring City, PA *Hobbies:* Drawing and walking in Central Park

Research Area: Inorganic Chemistry

Favorite Memory about Columbia: Getting my first SCXRD structure *What's next:* Georgia Tech!



Michael Van Duinen

Kaitlyn Otte

Yi Cheng Kang Thomas J. Katz Prize *Hometown:* Singapore

Hobbies: Cycling, reading, cooking, eating spicy food

Favorite thing about Columbia: Access to all the sights and sounds of the city.

Rachael Mow

Chemistry Department Honors *Hometown:* San Diego, CA

Hobbies: Baking, photography, calligraphy

Research area: Organic synthesis for materials science applications

Project titles: Tuning the Properties of Dimer and Trimer Helicene Nanoribbons through Synthesis

Favorite memory about Columbia: Going out in the middle of the night my freshman year to see the first snow



Rachael Mow

What's next? I'm going on to Stanford to pursue my PhD in chemistry!



Salvador Moncayo von Hase Bent Undergraduate Teaching Award Hometown: Buenos Aires, Argentina

Hobbies: I really enjoy baking, exploring places to eat out at (I'm a huge foodie) and exploring East Asian culture through art, architecture and forms of entertainment like literature and film, but also philosophy and hopefully one day also travel.

Research area: Pharmacology for the brain. I design novel chemicals in the ibogaine and aleph class, in the hopes of treating pain and depression much more effectively.

Salvador Moncayo-von Hase

Wheat's next? In the future I am pursuing a M.S. degree in tissue engineering at Columbia for another year and look forward to applying to PhD programs at the end of this year!

Jenny Jin Richard Bersohn Prize Hometown: Elk Grove, CA

Hobbies: I love reading, playing the violin and piano, and exploring the city to find hidden gems and good food!

Research area: I've worked in Dr. Brent Stockwell's lab on various projects around a cell death process known as ferroptosis, which is characterized by the irondependent accumulation of phospholipid peroxides. It has been very exciting to explore the biochemical mechanisms behind a relatively recently-discovered phenomenon such as ferroptosis, especially in the context of disease.



Jenny Jin

What's next? I will be moving on to pursue my MD-PhD dual degree at Columbia as well! I am very thankful to my family, friends, classmates, and faculty in the Chemistry department and beyond who have supported me, and am excited to embark on my journey to become a physician-scientist!

Yi Cheng Kang

GRADUATE STUDENT AWARDS (Continued from page 3)

Cho, Alexander Devanny, Matthew Hammond, Brandon McMurtry, and Ilana Stone.

Brandon McMurtry: 'Brandon is a fifthyear PhD student in the Owen group studying the nucleation and growth kinetics of colloidal nanocrystal formation. Leveraging a mechanistic understanding of how nanocrystals form, he is working toward developing new synthetic routes to incorporate quantum dots into light emitting diodes. After graduation, Brandon will begin a AAAS Congressional Science and Technology Fellowship funded by OSA and SPIE. Prior to arriving at Columbia, he earned a degree in chemistry from the University of Hawai'i at Mānoa in Honolulu, HI where he was born and raised."

Matthew James Hammond: I am in the Parkin group and my research primarily focuses on the synthesis and reactivity of Group XII metal hydride complexes, as well as the synthesis of novel transition metal and Group XIII atrane compounds. I am passionate about education and my Catholic faith. Next year, I will be a chemistry/physics teacher at Bishop Eustace Preparatory School in Pennsauken, NJ.

Matthew Carbone: In terms of research, I have a split focus between methods development in condensed matter, especially in electron-phonon polaron models, and in machine learning for chem-informatics and computational spectroscopy applications. Next year (or rather, in June), I'm going to be starting as an assistant computational scientist at Brookhaven National Lab.

Jake Russell: Jake recently defended his PhD under the direction of Prof. Xavier Roy. He studied the electrical transport properties of cluster-based materials, including superconductivity, as well as energy storage in organic networks in collaboration with the Nuckolls lab. Jake is now a Fellow at the Advanced Research Projects Agency-Energy (ARPA-E) with the US Department of Energy, where he



From top, left to right: Brandon McMurtry, Carla Bezjian, Suman Gunasekaran, Alex Devanny, Matthew Hammond, Matthew Carbone, Isra Hassan, Sumin Lee

supports the development of moonshot energy technologies.

Isra Hassan: I am a fifth year graduate student in the lab of Professor Tomislav Rovis. I just defended and graduated. I am working on monomeric streptavidin artificial metalloenzymes. I am starting a job this summer as a Chemical Biologist at Novartis Institutes for Biomedical Research.

Yeongsu Cho: I work on developing semiempirical GW-BSE to study electronic and optical properties of nanomaterials. I will start a postdoctoral position in Heather Kulik's group at MIT next year.

Carla Bezjian: In Brent Stockwell's lab, I have worked over the past few years to determine a genetic fingerprint in cancer cell lines that can sensitize cells to ferroptosis inducers. The goal for this research is to create personalized medicine. Most recently, I have focused on unique phospholipids and how they can regulate cell death in cancer cells. I hope that in the next year I can work in science communication, teaching and writing science to make it accessible to all audiences. While at Columbia I have participated in WISC, IDEaS, and women's water polo. Before coming to Columbia, I received my BS in biochemistry at Cal State LA.

Ilana Stone: Before joining the chemistry department, Ilana was a Wall Street trader, journalist and professional poker player. Her research incorporates her organic synthetic chemistry background into the inorganic materials lab that surrounds her. Next year she will start her VMD at Penn Vet.

Benedikt Kloss: I will be starting a Postdoc position at the Center for Computational Quantum Physics at the Flatiron Institute, NYC, in the fall. I am working on non-equilibrium dynamics in quantum lattice systems. **The Arun Guthikonda Fellowship** is given to an outstanding dissertationlevel student in organic chemistry or the biological-chemical sciences. This year's award was given to Sean Treacy, a rising the year in the Rovis group.

The Kathy Chen Fellowship covers all expenses for one year for a rising 5th-year student in any subfield. This year's Chen Fellow is Rachel Avard. Rachel attended Assumption College for undergrad, where she actively studied both chemistry and biology. While at Assumption she partook in research on axonal patterning in C. elegans under the direction of Dr. Michele Lemons, and she also worked on biomimetic synthesis of biaryl

macrocycles under the guidance of Dr. Elizabeth Colby Davie. She was also a member on the track & field and cross

PROFESSOR TIMOTHY BERKELBACH (Continued from page 3)

Professor Berkelbach explains what makes his research unique. "Properties can be simulated on the computer pretty accurately. Molecules are small. For problems that have to do with materials - for example materials that might be used for energy harvesting or energy storage - simulating their properties on the computer is much more challenging. A pretty big part of the research going on in my group is to try to take the tools that have been developed for molecular quantum chemistry and bring them to solid state or condensed matter."

His research at the Flatiron Institute compliments his research at Columbia, as Flatiron is an institute that is exclusively dedicated to computational science. Professor Berkelbach works in computational quantum physics as part of a small but growing group of researchers, including recent Columbia Chemistry graduates. country teams, as well as a lead tutor at the on campus center. While at Columbia, Rachel works with Dr. Laura Kaufman on investigating migration modes and requirements of breast cancer in 3D model systems to help increase the understanding of how cancer becomes metastatic in vivo. Rachel has a passion for teaching and spends her free time volunteering at local schools as a tutor and mentor. Rachel hopes to become a college professor when she finishes her degree at Columbia.

Excellence in teaching is also recognized by the department through its **Jack Miller Awards**. This year's Miller Award recipients include David Cabanero, Julia Dorsheimer, Jesse Gray, Daniel Malinowski, Angela Paoletta, Claudia Prindle, Davida Rios, Daniel Shlian, and Jack Weber.

Of course, teaching is also a large part of Professor Berkelbach's work at Columbia. So far, he has been teaching both undergraduate and graduate courses in chemistry. "I like teaching so much because the gratification is so instant. Research is a long haul. There are long periods of time where things aren't working. Big successes are few and far between. But with the teaching, it's immediate. That's a good motivator for me."

Professor Berkelbach has been named as a recipient of the AFOSR Young Investigator Award, the Alfred P. Sloan Research Fellowship, the NSF CAREER Award, the Hermann Kuemmel Early Achievement Award in Many-Body Physics, and the Presidential Early Career Award for Scientists and Engineers (PECASE). At Columbia, he is a co-chair of the Committee for Equity, Diversity and Inclusion.

GRADUATE STUDENT AWARDS RECIPIENTS 2020-2021

Hammett Award

Awarded to the most outstanding PhD student in his or her final year in our graduate program in recognition of his or her excellent fundamental studies in chemical research.

• Suman Gunasekaran (Venkataraman)

Pegram Award

Awarded for meritorious achievements by graduate students in their final year in our graduate program.

- Carla Bezjian (Stockwell)
- Matthew Carbone (Reichman)
- Isra Hassan (Rovis)
- Benedikt Kloss (Reichman)
- Sumin Lee (Rovis)
- Jake Russell (Roy)
- Yeongsu Cho (Berkelbach)
- Alexander Devanny (Kaufman)
- Matthew Hammond (Parkin)
- Brandon McMurtry (Owen)
- Ilana Stone (Roy)

Kathy Chen Fellowship

Awarded to a rising 5th year graduate student in the Chemistry Department in any sub-field. This fellowship pays for the cost of a single student for the 9 month academic year.

• Rachel Avard (Kaufman)

Arun Guthikonda Fellowship

Awarded to a dissertation-level student in organic chemistry or biologically related science in recognition of that student's distinguished achievements and potential.

• Sean Treacy (Rovis)

Jack Miller Teaching Award

Recognize excellence in teaching by graduate students. Only graduate students with secondyear or higher standing are generally considered for the awards.

- David Cabanero (Rovis)
- Julia Dorsheimer (Rovis)
- Jesse Gray (Nuckolls)
- Daniel Malinowski (Campos)
- Angela Paoletta (Venkataraman)
- Claudia Prindle (Nuckolls/Venkataraman)
- Davida Rios (Cornish)
- Daniel Shlian (Parkin)
- Jack Weber (Reichman)

LIFE IN THE CHEMISTRY DEPARTMENT, SUMMER 2021



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STAY IN TOUCH!

To share important updates and experiences in your career and life after Columbia, email your stories and photos to our Graduate Program Manager, Sheila Skaff at <u>sms2281@columbia.edu</u>

We'd love to hear from you!

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