

NYU  
DEPARTMENT OF  
CHEMISTRY

# CHEMISTRY Notes

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### LETTER FROM THE CHAIR

The Department of Chemistry at NYU is at a hub of intellectual and cultural activity at Washington Square in New York City. The Department continues on a steep upward trajectory, following major faculty hiring and renovation. There is so much going on in the department these days, and it is my pleasure to share some highlights with you here in this newsletter. We would love to hear from you! Please keep us updated at [chemistry@nyu.edu](mailto:chemistry@nyu.edu). We welcome your news and, of course, your support. To find ways that you can support NYU Chemistry, please visit the following web site: [as.nyu.edu/chemistry/alumni/giving-opportunities](http://as.nyu.edu/chemistry/alumni/giving-opportunities).



**James Canary**

*Professor of Chemistry and Department Chair*

## Chemical Biology Initiative

**NYU announces an initiative to advance scientific research and education at the interface of chemistry, biology, and medicine.** The Chemical Biology Initiative will allow renovation of over 68,000 square feet in the Silver Complex and allow recruitment of six faculty members in this area to the Department of Chemistry.

The stated aim of the interdisciplinary field of chemical biology is to develop molecular solutions to challenges in biology and medicine. As the fundamental understanding of biological mechanisms deepens, the solutions often require intricate chemical approaches.

### Chemical Biology Events at the New York Academy of Sciences:

- On February 20, 2019, the one-day symposium Phase Separation in Biology and Disease brought together scientists from academia and industry to dissect the latest advances in the field of biological phase separation and discuss the implications for human disease. It featured presentations from Cliff Brangwynne (Princeton) and other leaders in the field.
- On May 22nd, 2019, the annual Chemical Biology Discussion Group Year-End Symposium will take place. This year, the program includes distinguished keynote speakers Emma Parmee, (Merck) and David Spiegel (Yale), in addition to short, cutting-edge talks in chemical biology.

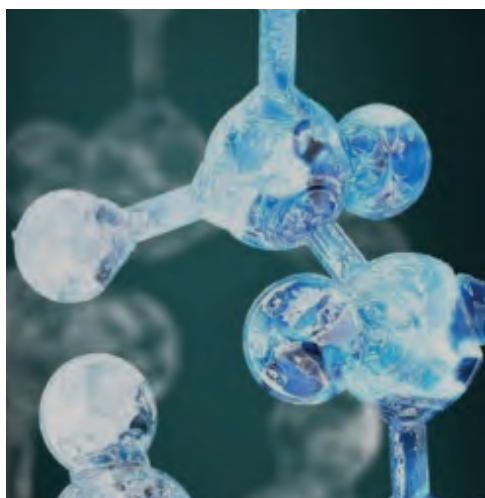
These integrate a range of synthetic and analytical techniques to elucidate and manipulate biological systems and provide therapeutic solutions for pathological states.

Chemical Biology will play an integral role in further enhancing NYU's reputation in the sciences by providing a platform for interdisciplinary studies between NYU's Faculty of Arts and Science Departments, the NYU School of Medicine, and the NYU Tandon School of Engineering. The Initiative will develop expertise in four core areas: Cancer Chemical Biology, Chemical Immunology, Chemical Neuroscience, and Molecular Spectroscopy and Imaging. These core areas will build on existing expertise while adding new dimensions and creating specific areas of collaborations with different NYU units.

NYU occupies a central location in Manhattan, a world-class hub for biomedicine. Further enhancement of chemical biology infrastructure will offer a platform for collaborative studies at NYU.

The Chemical Biology initiative builds on existing strengths in the NYU Chemistry Department. One area that has long been emphasized in the Department is macromolecular biophysics, where the labs of Geacintov, Seeman, and Traaseth continue to have a strong presence today. Another prominent area is in the design and application of biomimetic molecules to disrupt protein-protein interactions, where the labs of Arora, Kirshenbaum, Hamilton, and Zhang have a strong presence. The synthesis of bioactive small molecules is also key to Chemical Biology, where the Diao, Trauner, and Woerpel labs provide significant strength. Other notable labs in this area include Buccella, Hocky, Lupoli, and Schlick.

In connection with this initiative, the Department has ordered approximately \$4 million in research instrumentation, including an ultra-high field (800 MHz) nuclear magnetic resonance (NMR) spectrometer which is key to the characterization of biomolecules, a top-of-the-line electron paramagnetic resonance (EPR) instrument, and an update to an existing 500 MHz NMR spectrometer. After installation, the department will boast an amazing suite of NMR instruments, including cryoprobes operating at 400, 500, 600 and 800 MHz. ■







◀ Neil Garg and Marc Walters at the Distinguished Alumni Awards Ceremony

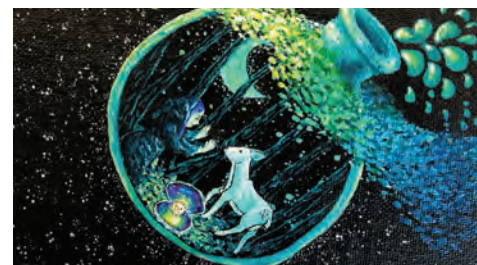
## Faculty News

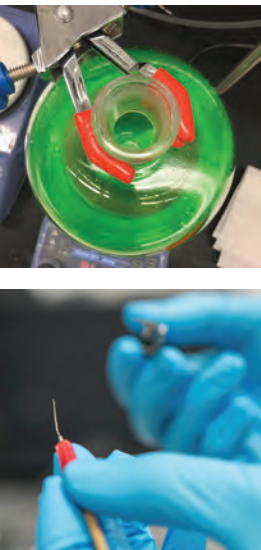
- **Daniela Buccella** was named a Scialog Fellow by the Research Corporation for Science Advancement and the Gordon and Betty Moore Foundation. The Scialog Program ([rescorp.org/scialog](http://rescorp.org/scialog)) selects “highly promising early to mid career scientists that work on the chemistry or biology of the cell or a related research area” to participate in a program to identify and address scientific challenges of global significance.
- **Tianning Diao** and **Nate Traaseth** received funding from the National Science Foundation (NSF) to acquire an Electron Paramagnetic Resonance (EPR) spectrometer. This instrument will support and enhance research in groups in the Chemistry and Chemical Engineering Department at NYU, as well as institutes in the tri-state area, across fields of organic, inorganic, chemical biology, and materials. The spectrometer will allow hands-on EPR measurements to be included in the curriculum of undergraduate and graduate education, and improve science education in New York City and surrounding areas. As mentioned above this addition is part of the Chemical Biology Initiative.
- **Tianning Diao** was selected as a Camille Dreyfus Teacher-Scholar. This award, given by the Camille and Henry Dreyfus Foundation, supports the research and teaching careers of talented young faculty in the chemical sciences. Criteria for selection include an independent body of scholarship attained in the early years of their appointment, and a demonstrated commitment to education, signaling the promise of continuing outstanding contributions to both research and teaching.

## Alumni News

- **Neil Garg** is the recipient of a 2019 NYU Distinguished Alumni Award! Neil is the Kenneth N. Trueblood Endowed Chair in Chemistry and Biochemistry at UCLA but once upon a time he was an undergraduate chemistry major at NYU, conducting his research in the laboratory of Professor Marc Walters. Since receiving his bachelor's degree from College of Arts & Science in 2000, Neil has achieved great success in his academic career, including a Ph.D. from CalTech, a postdoc at UC/Irvine and mounting honors and awards. It is a thrill to see him honored by NYU this year. [Read more about Neil and the other five honorees here.](#)
- **Danielle Nalband** is the administrator for the Chemical Biology Program and an alumna of the Department of Chemistry, having earned her Ph.D in the Kirshenbaum Lab in 2018. However, Danielle is also a self-taught painter, and she is featured in the Fall 2018 issue of NYU Arts Digest! Danielle's beautiful, often miniature, paintings present a magical dreamworld, with their subjects suspended in a luxurious blue sea of sky or water. Wondrously, she creates a sort of intimate eternity, combining the effects of a microscopic and telescopic view simultaneously. She is truly a scientist/artist! [Danielle's art can be seen here.](#)

Nalband recently displayed her art publicly for the first time at the NYU Administrators' Art Exhibit at the Kimmel Center for the University Life





We love to hear from alumni!

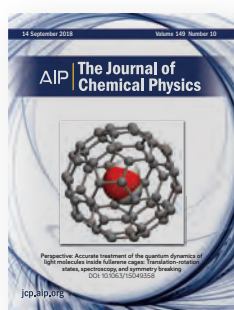
Please send us your news!  
If nothing is new, tell us what's old! Write to:

chemistry@nyu.edu

# Hello!

- Are pentameric rings dominant transient structures in liquid water? In her *Journal of Molecular Structure* article “From the trimer, through the pentamer, to liquid water,” Clinical Professor (and alumna) **Margaret Mandziuk** provides arguments strengthening this hypothesis. Her model, developed initially for the water trimer, and now applied to liquid water, accounts surprisingly well for the 2-D vibrational spectra of the liquid, observed by the Tokmakoff group. The model assumes a quantum mechanical, wave-like nature for protons delocalized between oxygen neighbors in a hydrogen bond. Mandziuk also demonstrates that the thermally excited states of a pentamer, or its isomers, contribute to the changing properties of the liquid at higher temperatures.

## Featured Publications

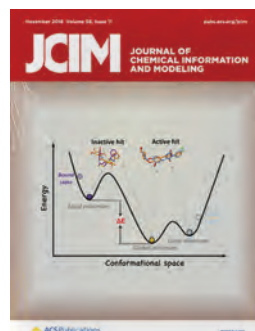


- Zlatko Bacic's** perspective article is featured on the cover of the *Journal of Chemical Physics* 149, 100901, (2018). Graduate student Joseph Cedagorta is credited with preparing the figure that graces the cover of the American Institute of Physics journal.



- Marcus Weck's** study on “Multicompartment Polymeric Nanoreactors for Non-Orthogonal Cascade Catalysis” was a featured article in *Molecular Rapid Communications*. The authors are postdoctoral fellow C. Tyler Womble and graduate student Michael Kuepfert.

- Professors **Alexej Jerschow** and **Mark Tuckerman** collaborated on a study yielding experimental proof of the asymmetry in ion transport mechanisms in water that was previously only hypothesized theoretically. The publication in *Physical Review Letters*, called “Unusual Proton Transfer Kinetics in Water at the Temperature of Maximum Density,” credits first author postdoctoral fellow Emilia Silletta. The work was picked up by NYU Research Highlights in an article called, “The Behavior of Water: Scientists Find New Properties of H<sub>2</sub>O.”

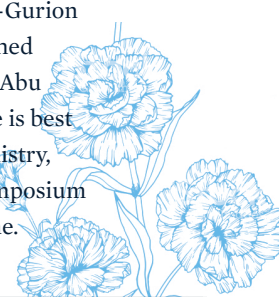


- Yingkai Zhang's** group and collaborators at Shandong University have published a study entitled, “Computational Strategy for Bound State Structure Prediction in Structure- Based Virtual Screening: A Case Study of Protein Tyrosine Phosphatase Receptor Type O Inhibitors,”

which is featured on the cover of the *Journal of Chemical Information and Modelling*. First author credit goes to Xuben Hou, and other NYU Chemistry authors include David Rooklin, Jianing Lu and Cheng Wang.

## IN MEMORIAM

We mourn the loss of **Joel Bernstein**, former Barry and Carol Kaye Professor of Applied Science at Ben-Gurion University and more recently Global Distinguished Professor of Chemistry at New York University Abu Dhabi, who passed away on January 2, 2019. He is best known for his work on organic solid-state chemistry, and his life will be celebrated at a Memorial Symposium linked to the ICCOSS conference at NYU in June.





# DEPARTMENT EVENTS

## NYU Chemistry Around the World

- This June NYU Chemistry will serve as the host site for the 24th International Congress on the Chemistry of the Organic Solid State (ICCOSS XXIV). Since its inception in 1968, ICCOSS has become the premier forum for discussing groundbreaking research on the chemistry and physics of organic materials. Although it was born in New York (Brookhaven, to be exact), this is the first year this conference will take place at NYU, having made its last stop in South Africa. Co-organizers are NYU Chemistry Professors **Mike Ward** and **Bart Kahr**.
- NYU Chemistry Professor **Zlatko Bacic** and NYU Shanghai Assistant Professor **William Glover** co-organized The International Symposium on Quantum Effects in Chemistry and Biology, to take place at NYU Shanghai June 1-3.
- NYU Chemistry Professor **Tamar Schlick** was on the organizing committee of The Biophysical Society's interdisciplinary meeting, "Multiscale Modeling of Chromatin: Bridging Experiment with Theory," which took place in Les Houches, France on March 31-April 5.

## NYU Chemistry in NYC

- The 2019 McNelis Distinguished Lecture, entitled, "Molecular Cloaks and Daggers: Expanding the Pharmacopeia" was presented by Ronald Raines (MIT) on April 26th.
- Sir John Meurig Thomas (Cambridge) presented a historical lecture entitled "Bragg, Perutz, Kendrew, and Hodgkin: Architects of Structural Biology" on April 19th.



- ◀ The McNelis Lecturer Ronald Raines with the McNelis Lecture Plaque, presented by Jim Canary
- ✓ Ron Raines with graduate students Peter Reuhmann, Belinda Hetzler, Ashley Modell and Haley Merritt.



- The Novartis Lecture in the Chemical Sciences at NYU had its debut on March 29, 2019. This symposium featured speakers Christian Hackenberger (FMP Berlin & Humboldt), Howard Hang (Rockefeller), Andy Patterson (Novartis) and Tom Muir (Princeton). The afternoon was hosted by NYU Chemistry faculty: veteran **Dirk Trauner** and newbie **Tania Lupoli**.

## Local Outreach

- New York University Chemistry undergraduate student continued their tradition of participation in the annual ACS STEM outreach event **CHEMISTRY DAY**. The New York Section of the American Chemical Society celebrated National Chemistry Week at the New York Hall of Science in October. Each year, this event showcases chemistry principles using demonstrations performed by local college students and volunteers from local industries for children of all ages. The NYU group was coordinated by Draper Chemical Society's Olivia Maffei. Olivia and volunteers Daisy Zheng and Sumaita Mahmood engaged kids and their parents with the following demos including acid and base chemistry with cranberry juice, and marker chromatography.



ACS Chemistry Day at the New York Hall of Science.



- NYU Chemistry continued the tradition of hosting the American Chemical Society's Olympiad Exam, administered nationally to high school students. The exam was proctored by graduate student Michael Brady, who is in his 4th year of research in the laboratory of Daniela Buccella and of service to the department and the community.
- Other continuing outreach traditions for NYU Chemistry students and faculty are participation in the March for Science NYC and the World Science Festival, both annual events championing science education and research in America and the world. This year, the March

for Science takes place on May 4 and the ACS Student Chapter begins the day with breakfast at NYU and proceeds to Foley Square, where the citywide march begins. The World Science Festival runs from May 22 to June 2. This year, Professors Lara Mahal and Kent Kirshenbaum are among the great variety of scientific minds contributing to the event. For instance, Mahal Group graduate student Thu Chu will lead lab tours for girls interested in science. Fun fact attesting to the richness of this event: Listed alphabetically, the first participant in the WSF is basketball legend Kareem Abdul-Jabbar! ■



## Applications to the **FALL 2020 DOCTORAL PROGRAM**

The deadline for applications to the **doctoral program in Chemistry** at NYU is **December 12, 2019**. For full consideration, get your application in by the deadline date, when we will begin our review! The application is available on the department website and also on the Graduate School of Arts and Science Admissions Resource Page: [gsas.nyu.edu/page/grad.admissionsapplication](https://gsas.nyu.edu/page/grad.admissionsapplication)



Photo by Dirk Trauner