NYU

NYU
DEPARTMENT OF
CHEMISTRY

# CHEMISTRY Notes

WINTER 2020 | ISSUE 5

ISSUE 5



## welcome

### LETTER FROM THE CHAIR

We hope that this letter finds you and your family healthy and secure during these turbulent times! I'm happy to report that the NYU Chemistry Community is doing well, with our community members rising admirably to the challenges that we have all faced recently. In fact, research in the Department never stopped throughout the pandemic, with some labs switching gears to focus on COVID-related chemistry and research. Most labs saw their members work remotely for a time, but as of this writing the majority of our researchers are back in the lab, albeit with PPE, social distancing, and other health practices. Much of this issue reports ongoing research activities in the Department.

You may know that instruction at NYU is currently "blended", which means that some students are remote but every student on campus has an opportunity for an in-person classroom or laboratory experience. Enrollment in Chemistry courses is remarkably robust—in fact our enrollment in first semester college chemistry this semester was the highest in our history! Our instructors and students have shown heroic commitment during this period, in which both teaching and learning take significant extra time and effort. A newly energized civil rights movement has engaged our community, leading to re-examination of many of our ongoing practices, and commitment to racial reconciliation and justice. The political season has also captured renewed attention and passion. In light of all this, we have committed to provide greater support and encouragement to our community members for their physical and emotional well being. Among several steps taken, Prof. Daniela Buccella has graciously agreed to serve as our first Director of Diversity, Equity, and Inclusion.

*Continued on the next page*

# DEPARTMENT NEWS

## Dirk Trauner is a 2021 Cope Scholar!

**Dirk Trauner**, NYU Chemistry's Janice A. Cutler Professor of Chemistry, is the recipient of a 2021 ACS Cope Scholar Award. With this award, the American Chemical Society recognizes and encourages outstanding excellence in organic chemistry.

Professor Trauner has established himself as a premier chemical biologist and synthetic organic chemist. The Cope Scholar Award recognizes his "elegantly crafted total syntheses and his pioneering contributions to Photopharmacology and Chemical Optogenetics." The hallmark of his synthetic approach is a deep understanding of how nature builds natural products. He devises insightful biomimetic routes and combines them with contemporary synthetic methodologies. Trauner co-founded the field of photopharmacology which aims to control biological function with light. He has developed a series of novel classes of switchable small molecules that can be triggered on or off as desired for a specific activity.

As one of ten scholars selected by the ACS for this honor, Dirk will deliver an address at the Arthur C. Cope Symposium at the American Chemical Society's National Meeting in August 2021. Dirk joins his NYU Chemistry colleagues David Schuster and Keith Woerpel on the illustrious list of Cope Scholars. **Congratulations to Dirk!.** ■

*Continued from the last page*

We welcome new faculty member Marvin Parasram who has set up lab in the newly renovated Brown 4 Chemical Biology Lab. Details on his background and research are included elsewhere in this letter. His energy and enthusiasm has already brought freshness to our activities! We are also very excited to welcome Stephanie Lee and Claudia Avalos to our faculty in the next several months.

Some of the impact of the pandemic on higher education institutions has involved budgets. Fortunately, we have managed to retain and support financially all of our faculty, students, and staff during this time. We welcomed a large and highly qualified group of graduate students this fall, and they represent the greatest diversity of any prior entering class. As we work hard to support our people, a couple of our ongoing projects are on pause. Nevertheless, the new offices in Waverly for Department staff, clinical faculty, and a new Learning Center are nearly finished and will become occupied by the time you read this letter. The next time you come to campus, look for us on the third floor of the Waverly building in a beautiful new space! In the meantime, we would love to hear from you! Please keep us updated at **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.

**James Canary**
*Professor of Chemistry and Department Chair*

## *NYU Chemistry*
# Welcomes New Faculty

**Marvin Parasram** joined the NYU Chemistry research program in chemical biology in August, 2020. Marvin earned his doctoral degree at the University of Illinois at Chicago under the direction of Vladimir Gevorgyan and comes to us from an NIH Postdoctoral Research Fellowship at Princeton University in the laboratory of Abigail Doyle. Research in the Parasram Lab will focus on developing novel synthetic methodologies for the difunctionalization of organic systems. Their approach will aim to provide innovative solutions to pressing challenges in synthetic chemistry.

**Stephanie Lee** will join us in January 2021 as Associate Professor of Chemistry in our Molecular Design Institute. Stephanie earned her doctoral degree at Princeton University under the direction of Yueh-Lin Loo and conducted her postdoctoral research right here at NYU in the lab of Mike Ward. She comes to us from Stevens Institute of Technology, where she was Associate Professor of Chemical Engineering and Materials Science with the Stevens Early Career Award for Research Excellence and an NSF CAREER Award under her belt. Research in the Lee Lab will be in the areas of: solution-processable materials for renewable energy applications, nanostructured materials, semiconducting polymers and small-molecules, metal-halide perovskites, and crystal engineering.

**Claudia Avalos** will join the NYU Chemistry research program in materials in Fall 2021. Claudia earned her doctoral degree at University of California at Berkeley under the direction of Alex Pines and did her postdoctoral research at L'Ecole Polytechnique Federale de Lausanne, in the laboratory of Lyndon Emsley.Research in the Avalos Lab will focus on developing and applying nitrogen-vacancy magnetometry and solid-state magnetic resonance methods to study structure-function relationships in photoactive and technologically relevant materials.

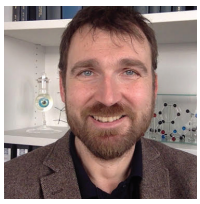
# Fall News

- The first ever virtual Chemistry Biology Symposium was held on August 7, 2020
- Professor Daniela Buccella was appointed the Department of Chemistry's first Director of Diversity, Equity and Inclusion (DEI).

- Professor Paramjit Arora received the 2020 CAS Golden Dozen Teaching Award.

- Assistant Professor Glen Hocky received a MIRA Award for Early Stage Investigators from the NIH.

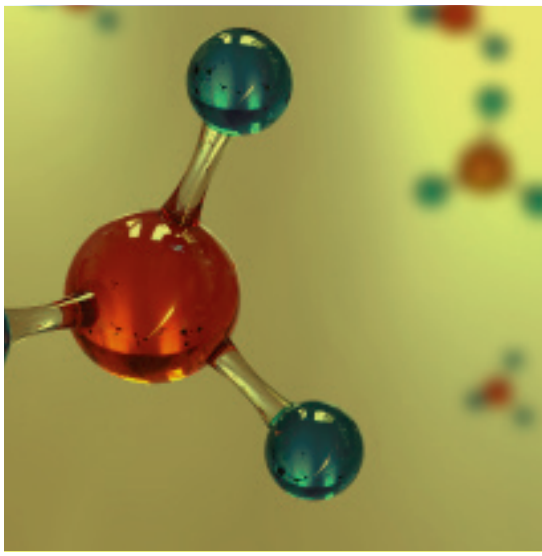
- Professor Dirk Trauner was the recipient of a 2020 McKnight Memory and Cognitive Disorders Award for his research on Parkinson's Disease.



## Heroic staff members:

Chin Lin, Keegan Garcia, Roger Fuertez, Abayomi Elesho, and Philip Morton. Without support by these staff members, COVID-related research could not have continued throughout the pandemic as it did. These staff members commuted to the department even during the most intense moments of the outbreak. Thanks also to our amazing teaching lab staff: John, Roldan, Noel, Tricia, Tarabeth, and Nerline!

# STUDENT & ALUMNI NEWS



## STUDENT NEWS

- **Johannes Morstein**, a doctoral student in the Trauner Group, won a Transition Award from the National Cancer Institute, which will support his research in lip-based cancer therapeutics over the course of his predoctoral and postdoctoral studies.

- **Qiao Lin**, a doctoral student in the Diao Group, won a WCC/Merck Research Award, including presentation of her work at the national meeting of the American Chemical Society in August.

- **Yuvraj Singh**, a doctoral student in the Hocky Group, received the 2020 Outstanding Teaching Award given by the NYU College of Arts and Science.

- The Chemistry Graduate Student Organization invested in a grand restructuring, including the creation of working groups, and encouraging inclusive representation. This was a group effort with unprecedented participation, but a big shout-out goes to **Elsy El Khoury** for much of the heavy lifting. Elections were held, and a horizontal structure was adopted. The fifteen elected members are part of one or more of the following five working groups (senior representatives named) **Diversity, Equity and Inclusion** (Amanda Ramdular), **Outreach** (Farhan Chowdhury), **Events** (Haley Merritt), **Seminar and Colloquium** (Yudong (Gary) Liu) and **Recruitment** (Amanda Ramdular). Ten members now serve on departmental committees and the Graduate Program Advisory Panel.

- Congrats to the Phi Lambda Upsilon Inductees of 2020, who created a virtual induction ceremony for these times! Special shout-out to Rhea-Donna Reyes, president of NYU's Alpha Lambda Chapter (and fresh alumna), who did a stellar job!

We look forward to rescheduling the NYU Chemistry Alumni Reception that was cancelled last April as soon as we can convene in person!

**@NYUChemistry**

## ALUMNI NEWS

- **Gertrude Elion was featured in National Geographic**
  Gertrude Elion (1918-1999) earned her masters degree in Chemistry from NYU in 1941. She had to study at night and on weekends, and was the only woman in her class. She went on to win the Nobel Prize in Chemistry in 1988. Her visionary research in antiviral drugs, and the direct path to potential treatments of the coronavirus, was highlighted in National Geographic.

  Click here to read the article: "Meet the woman who gave the world anti-viral drugs."

- **Tim Berkelbach received the 2021 ACS Fresenius Award NYU**

  Chemistry alumnus (2009) Timothy Berkelbach, currently Assistant Professor of Chemistry at Columbia University, is the recipient of the 2021 ACS National Fresenius Award, sponsored by the national chemistry honor society, Phi Lambda Upsilon. When Tim was earning his bachelor's degree at NYU, under the direction of Professor Mark Tuckerman, he was the president of NYU's own Alpha Lambda Chapter of PLU. Congrats to Tim!

**Our heroes: Young women alumni fighting COVID-19 in industry!**

**Brooke Bullock Lau** (Ph.D 2014 Arora Lab) is on the vaccine research team at Pfizer, where initial trials yield 95% effectiveness.

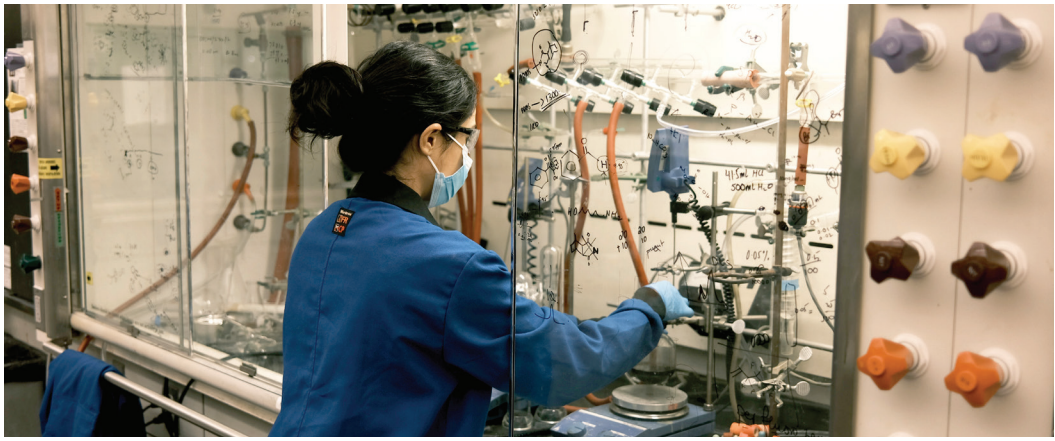
**Diane Lye** (Ph.D 2017 Weck Lab) and **Debra Rooker** (Ph.D 2017 Buccella Lab) were on the COVID response team at Gilead, each working on different aspects of the development of the drug Remdesivir, so important in the first months of virus treatment research.

## HISTORY

- **Mulliken paper selected by the ACS History of Chemistry Division's Citation for Chemical Breakthrough Award**
  Robert S. Mulliken's 1928 Physical Reviews paper on "The Assignment of Quantum Numbers for Electrons in Molecules. I" has been selected to receive a 2020 Citation for Chemical Breakthrough Award, from the American Chemical Society's Division of the History of Chemistry. Although the 1966 Nobel Laureate was not a member of our department, we are proud that Mulliken's seminal work was done at NYU, where he was on the Physics faculty early in his career, and take pleasure in seeing his name take its place in the ACS historical record.

## *Congrats*

to our freshest batch of alumni, who experienced the milestone as no class ever experienced it before. Take a look at our Class of 2020 Graduation Tribute Page honoring the students and their accomplishments.



# DEPARTMENT RESEARCH

**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!

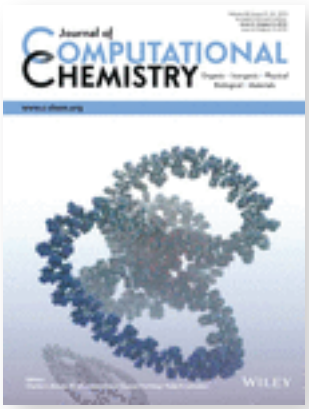
**NYU Chemistry** was strongly engaged in COVID-related research throughout the pandemic. The Department's Chemical Biology program was very well suited to shift efforts to support the nationwide effort to develop tools to combat this disease. **Nate Traaseth**, **Tania Lupoli**, **Paramjit Arora**, **Dirk Trauner** and **Yingkai Zhang** received an NYU Fast Grant to lead the Chemical Biology Initiative's multi-pronged approach to identifying drug candidates. **Kent Kirshenbaum**, together with Physics Professor David Grier, received an NSF RAPID award to develop technology that has the potential to form the basis for a highly accurate, easily administered, fast, and affordable test for SARS-CoV-2. **Tamar Schlick** received a similar award for exploring COVID-19 RNA viral genome targets by graph-theory based modeling. Efforts in the department have been very successful in making progress in this area. These and other labs continued research throughout the pandemic, supported by departmental staff who kept stockroom and instrumentation facilities operational.

**We are pleased to share some of the terrific research studies that hit the presses these past months. The research titles are linked to the articles, so please click away for details!**

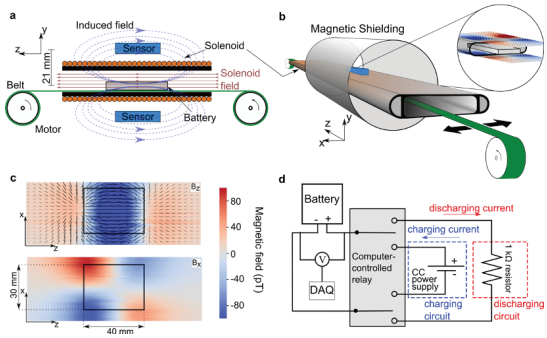
## 2 COVER STORIES

- Researchers in the laboratory of **Marcus Weck**, professor in the NYU Chemistry's Molecular Design Institute, published a study in *Nature Materials* called "Tunable Assembly of Hybrid Colloids Induced by Regioselective Depletion." Weck Group graduate students **Mingzhu Liu** (first author), **Veronica Grebe** and **Xiaolong Zheng** (alumnus) worked with colleague David Pine, of NYU Physics and Chair of NYU Tandon's Department of Chemical and Biomolecular Engineering.

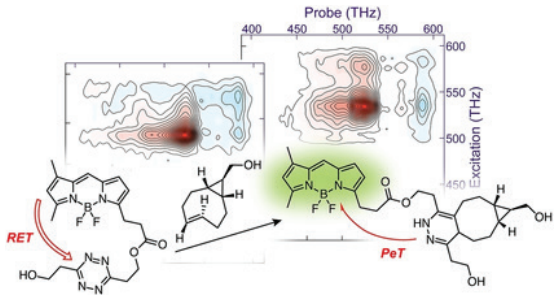

- NYU Chemistry Professor **Tamar Schlick** and LANL Colleagues made the cover of the Journal of *Computational Chemistry* with the first billion atom molecular dynamics simulation. As part of the Los Alamos National Laboratory group, Schlick used a GATA 4 gene model simulated with a chromatin mesoscale modeling program to build a billion atom molecular system. The article, entitled, "Scaling Molecular Dynamics Beyond 100,000 Processor Cones for Large-Scale Biophysical Simulations" was picked up widely by the press. The list of authors includes Schlick group postdoctoral fellow **Gavin Bascom**.



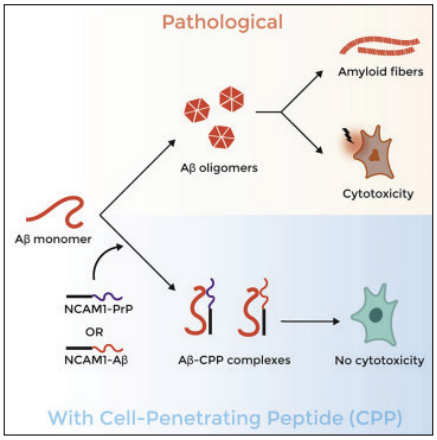
- NYU Chemistry Professor **Alexej Jerschow** and his group continue to delve into the sensitive world of rechageable batteries. The latest work is published in *Nature Scientific Reports*, titled, "Nuclear Magnetic Resonance Spectorscopy of Rechargeable Pouch Cell Batteries: Beating the Skin Depth by Excitation and Detection Via the Casing." Authors include postdoctoral fellow **Stefan Benders**, graduate student (fresh alumna) **Mona Mohammadi** and visiting professor Christopher Klug of the U.S. Naval Research Academy.




- First author, **Brismar Pinto-Pacheco** (Bucella Group) and NYU Chemistry colleagues have published a study in *Angewandte Chemie International Edition* entitled, "Fluorescence Quenching Effects of Tetrazines and Their Diel-Alder Products: Mechanistic Insight Toward Fluorogenic Efficiency." The study uncovers the influence of the dienophile on the fluorescence enhancement in reactions of tetrazine-decorated fluorophores, and reveals options for maximizing contrast in widely used biolabeling applications. Co-authors include **Will Carbery** (an alumnus currently a postdoc at City College's Center for Discovery and Innovation), **Sameer Khan** (CAS 2017), Daniel Turner and Professor **Daniela Buccella**.

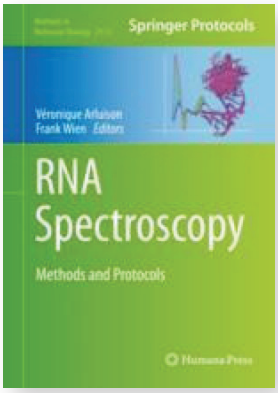



- NYU Chemistry Professor (and University President) **Andrew Hamilton** and postdoctoral fellow **Sunil Kumar** (currently Assistant Professor of Chemistry at the University of Denver) published research with colleagues from the University of Stockholm and from NYU Abu Dhabi in *Cell Reports, Physical Science*. The article, entitled, "Designed Cell-Penetrating Peptide Inhibitors of Amyloid-beta Aggregation and Cytotoxicity" was picked up by NYU Research Highlights, describing how protein-based therapeutics prevent protein aggregation associated with Alzheimer's and other neurodegenerative diseases.

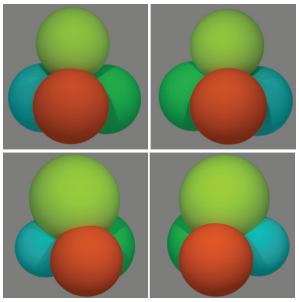



- NYU Chemistry Professor **Nate Traaseth** and colleagues published a study in *Nature Chemical Biology* called "Molecular basis for receptor tyrosine kinase A-loop tyrosine transphosphorylation." This work was possible through a close collaboration with Moosa Mohammadi's lab at the NYU School of Medicine and NYU Chemistry researchers **William Marsiglia** (co-first author and Traaseth Lab alumnus, currently a postdoc at Mount Sinai), **Joseph Katigbak** (Zhang lab alumnus, currently a data scientist at Prognos), and Professor **Yingkai Zhang**.

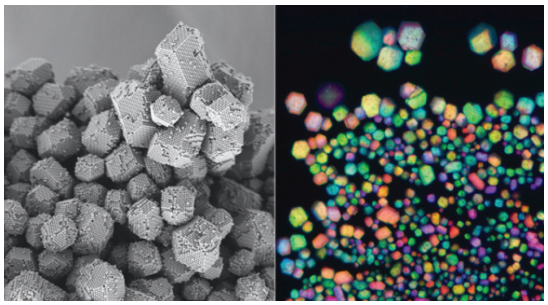
- NYU Chemistry Clinical Associate Professor **Somdeb Mitra** and Canadian colleague Borries Demeler published a study entitled, "Probing RNA-Protein Interactions and RNA Compaction by Sedimentation Velocity Analytical Ultracentrifugation" in *RNA Spectroscopy*. This publication is part of the Methods in Molecular Biology series.



- Researchers in the NYU Department of Chemistry's Molecular Design Institute have developed a synthetic strategy to construct colloidal molecules with specific features and capabilities. "Customized Chiral Colloids" was published in **JACS**, where the work has been spotlighted in "Colloidal Clusters Made to Order." Authors include doctoral students **Mingzhu Liu**, **Fangyuan Dong** and **Nicolle Jackson**, as well as professors **Mike Ward** and **Marcus Weck**.

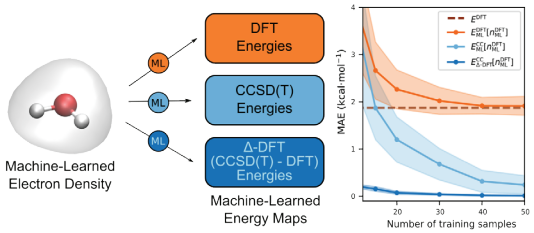


- NYU Chemistry Professor **Stefano Sacanna** led a study using electrostatic charge to assemble particles into materials mimicking gemstones and salt crystals. The process offers a simple and scalable approach to particle self-assembly. Researchers include first author **Ted Hueckel** (alumnus, currently a postdoc, in the Sacanna Lab), NYU Assistant Professor **Glen Hocky** and UCSD colleague Jeremie Palacci. The *Nature* article is entitled, "Ionic Solids from Common Colloids."

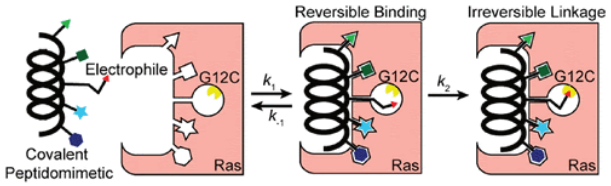


- The Arora and Zhang Groups describe the design of a protein tertiary structure mimic to target Kaposi's sarcoma herpesviral oncoprotein. The study was performed in collaboration with researchers at Weill Cornell Medical College and describes a compound that suppresses NF-kB signaling and delays tumor growth in a PEL xenograft model. NYU Chemistry contributors include first author **Michael Wuo** (Arora lab alumnus, currently a postdoc at MIT), **David Rooklin** (Zhang lab alumnus, currently CEO of Redesign Science), **Seong Ho "Johnny" Hong**, and professors **Paramjit Arora** and **Yingkai Zhang**. The article appeared in in *Nature Communications*: Modulation of virus-induced NF-kB signaling by NEMO coiled coil mimics.

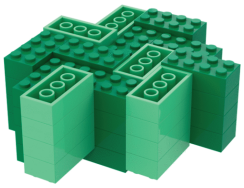
- NYU Professor of Chemistry and Mathematics **Mark Tuckerman** and postdoctoral fellow **Leslie Vogt-Maranto** published a collaborative study in *Nature Communications*, entitled, "Quantum Chemical Accuracy from Density Functional Approximations via Machine Learning." Using machine learning, a map from the external potential of a system to its electron density was trained, which allows explicit solution of the electronic Schroedinger equation to be bypassed. Using this map, a second machine learning model can be trained to obtain the total energy at quantum chemical accuracy with no requirement of self-consistency.




- NYU Chemistry graduate student **Dan Yoo,** in the **Arora Lab**, describes compounds that covalently target oncogenic Ras—a key driver of many cancers. Dan collaborated with the Bar-Sagi Lab, at the NYU School of Medicine, to show the potential of the designs to modulate Ras signaling in cancer cells. This work builds on the earlier efforts by alumnus **Steve Joy** (currently a postdoc at the University of Michigan). Read the article in *ACS Chemical Biology*: "Covalent Targeting of Ras G12C by Rationally Designed Peptidomimetics."

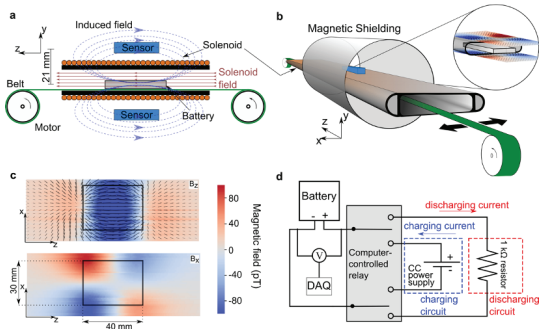



- First author **Noalle Fellah** and collaborators from the groups of professors **Mike Ward**, **Bart Kahr** and **Mark Tuckerman** published a study entitled, "Disorderly Conduct of Benzamide IV: Crystallographic and Computational Analysis of High Entropy Polymorphs of Small Molecules" in *Crystal Growth & Design*. The authors list, consisting of mostly NYU Chemistry members, includes **Alexander Shtukenberg**, **Eric Chan**, **Leslie Vogt-Maranto** and **Chao Li**.



- NYU Chemistry Professor **Marcus Weck**, doctoral candidate **Cicely Shillingford** and undergraduate researcher **Brandon Kim** (currently at Temple School of Med) expand the synthetic toolbox for topdown, scalable, hierarchically engineered materials. The study entitled, "Capillary Assembly of Liquid Particles" was published in the Wiley online journal, *small*.

- Batteries are notoriously difficult to analyze. NYU Chemistry Professor **Alexej Jerschow** and colleagues in Germany developed a technique that could help in designing next-generation battery cells. The research was published in *PNAS*: "Sensitive magnetometry reveals inhomogeneities in charge storage and weak transient internal currents in Li-ion cells" and was picked up by *Scientific American*: "Ultrasensitive Fuel Gages Could Improve Electric Vehicle Batteries." NYU Chemistry authors include graduate student **Mohaddese Mohammadi** (fresh alumna!) and postdoctoral fellow **Emilia Silletta**.




- Researchers in the NYU Department of Chemistry's Molecular Design Institute use a simple, inexpensive technique to develop a new fast-acting form of deltamethrin that may help with growing insecticide resistance. NYU researchers include postdoctoral fellow **Jinxiang Yang** (first author), grad student **Bryan Erriah**, x-ray crystallographer **Chunhua (Tony) Hu**, REU researcher **Ethan Reiter** and grad student **Xiaolong Zhu**, as well as Professors **Bart Kahr** and **Michael D. Ward**. The MDI scientists teamed up with colleagues Vilmalí López-Mejías and Isis Paola Carmona- Sepúlveda at the University of Puerto Rico. Read the article in *PNAS*: "A Deltamethrin Crystal Polymorph for More Effective Malaria Control." or get the layman's take: "Chemists Create a New Crystal Form of Insecticide, Boosting its Ability to Fight Mosquitos and Malarial."