Vol 111, No. 2 February 2024

THE CHEMICAL BULLETIN

Chicago Section of the American Chemical Society Newsletter

February Virtual Monthly Meeting

Friday, February 16, 2024 7:00 - 8:30 PM CST

Integrating Molecular Machinery in Smart Materials: From Adhesives to Tattoos

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ABSTRACT

Much of the excitement surrounding artificial molecular machines (AMMs) is tied to an intuition that they have an important role to play in the nanotechnologies we anticipate will revolutionize our future by making materials "smart", as biology does. Biological tissues have remarkable self-regulating, self-healing, stimulus-responsive and adaptive properties because they are made of smart building blocks (cells) that exhibit these features themselves. Cell behavior is driven by countless biological molecular machines (enzymes and other proteins) which have evolved to perform tasks at the expense of ATP, the body's chemical fuel. AMMs still lag far behind their biological counterparts in sophistication – this fact often motivates research to build ever more complex molecular contraptions. We take the opposite approach in the Emergent Nanomaterials Lab, asking how sophisticated functions might emerge in nanomaterials constrained to only simple and highly accessible AMMs. We believe that AMMs can compensate for low complexity with high diversity, since they can be designed with numerous structural motifs to run on virtually any type of fuel. Furthermore, the expansion of AMMs from fundamental chemistry to applied science and engineering demands an interdisciplinary approach among chemists, other scientists, and engineers; "simple" chemistry can lower the barrier to these collaborations. This talk will discuss examples of sophisticated nanomaterial functions emerging from relatively simple molecular machines embedded in polymer systems, including "slide-ring" adhesives and smart intradermal tattoos for augmenting human capability.

MEETING PROGRAM

7:00–7:10 PM	Introductory remarks
7:10–8:00 PM	Main lecture
8:00–8:15 PM	Q&A, closing remarks

REGISTRATION

By phone (847-391-9091), email (chicagoacs@ameritech.net), or online:

REGISTER HERE

MEET THE SPEAKER

A creator of color-changing tattoo inks and shape-shifting molecular machines, chemist and artist **Carson Bruns** uses nanoscience to invent new materials and technologies. He is currently an Assistant Professor of Mechanical Engineering with the ATLAS Institute at the University of Colorado Boulder, where he directs the Emergent Nanomaterials Lab. He has co-authored more than 50 peer-reviewed scientific publications and received the National Science Foundation's CAREER Award in 2023. Dr. Bruns earned a Bachelor of Arts degree at Luther College in Iowa, where he majored in Chemistry and Religion, before completing a Ph.D. in the area of supramolecular chemistry under the mentorship of Professor Fraser Stoddart at Northwestern University. He completed his training at the University of California, Berkeley where he took part in the prestigious Miller Research Fellowship program. Dr. Bruns is illustrator and co-author with Sir Fraser on the book titled, *The Nature of the Mechanical Bond* (2016).

FROM THE EDITOR'S DESK

Celebrating Black History in Chemistry

The arrival of Black History Month presents an opportunity to reflect on the many contributions to the field made by Black chemists and chemical engineers, such as James Andrew Harris. Harris grew up in California and Texas, attending Huston-Tillotson College in Austin where he earned his bachelor's degree in 1953.

Harris (left) and team lead Al Ghiorso inspect one of Harris's superheavy element targets (1970).

He had a difficult time finding a job as a chemist due to discrimination, but did eventually find work in California at a radiotracer lab, where he worked for five years. Following that period, Harris joined a team of five scientists at the Lawrence Radiation Laboratory at the University of California, Berkeley (now Lawrence Berkeley National Laboratory) where he would do the work for which he is best known, discovering elements 104 and 105 in 1969 and 1970, known since 1997 as the rutherfordium and dubnium.

Harris's specific contributions to that work, typically summarized as "creating heavy element targets" for the group's linear accelerator experiments, sells short the full extent of his efforts. He performed over 20 painstaking purification steps on a 60-microgram sample of californium before electroplating a pure californium-249 target. The target, initially designed for the element 104 experiments, was pure enough to be used in the discovery of element 105, as well.

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FROM THE EDITOR'S DESK

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A less widely known chapter of Harris's career began six years after those experiments, when he left the laboratory to take on an administrative position in Berkeley's nascent Office of Equal Opportunity. There he sought to clear a path for a new generation of underrepresented students and scientists. Similar efforts are ongoing today, but more must be done. The percentage of Black ACS members has roughly tripled since 1985, but still sits at just under 3%. The chemical community must continue the work of removing discriminatory barriers to educational and professional attainment within our field.

Thanks to those who offered their contributions to this issue of *The Chemical Bulletin* : Fadwa Al-Taher, Paul Brandt, Gowri Kuda-Singappulige, Josh Kurutz, Raelynn Miller, and Margaret Schott.

MATT VAN DUZOR

PROJECT SEED

Project SEED Summer Internships

Project SEED is a highly successful ACS program that matches enthusiastic high school students interested in chemistry with mentors from academia and industry. Students can apply for either virtual or in-person summer internships. Student eligibility includes low-income background with at least one high school chemistry class completed. Project SEED students work on their projects for eight weeks, 40 hours/week, over the summer, and are eligible for up to two summers of support. **Student applications open on February 13th.**

Mentors are key to the success of the Project SEED Program. The **deadline for project proposals is fast approaching: Thursday, February 8th. Please reach out to Raelynn.Miller@Honeywell.com if you are interested.**

We are looking for mentors that have an internal fire for service and a desire to promote STEM careers. In your department or company, a group of mentors can create a community of mentorship by sharing your passion for science with local high school interns. Graduate students can leverage this teaching opportunity for leadership and professional development. Taking on a Project SEED intern will give your grant proposal that extra boost with "Broader Impact." Mentors are scientists from academia, industry, nonprofit or government organizations.

Please visit the program website at www.acs.org/projectseed or contact chicagoacsprojectseed@gmail.com for more details.

RAELYNN MILLER

RECENT RESEARCH

Cost Impact of Decarbonization Methods for Iron and Steel Furnaces Quantified

It can be difficult for industry to assess the value of different carbon-reduction technologies and many assessments compare only a few variables. Recently, researchers at Argonne have published a robust assessment of combinations of carbon reduction technologies in both blast furnaces and electric-arc furnaces for iron and steel. Materials, fuel extraction and transportation, electricity generation and transmission, materials pretreatment, iron-making and steel-making steps were all included. The assessment used harmonized assumptions for representative energy- and mass-conversion data across the US steel industry, steady-state operating conditions, and average historical fuel costs to provide an assessment that is not region or plant specific. (Plant-construction costs were not included.) The highest amounts of CO_2 emission reduction were achieved by combining carbon capture with energy-source switching from fossil fuels to renewables. The paper has details around potential decarbonization options including cost impact of those options. The work is expected to help reduce investment risks and accelerate low-carbon manufacture technology deployment.

The link for the paper is here: https://doi.org/10.1016/j.ijggc.2023.103958.

Machine Learning Methodology Offers Improved Predictability of Complex Industrial Systems

Some industrial processes are difficult to sample or have sparse data, a scenario which generally results in low-confidence surrogate models making return on investment decision-making difficult. With hydrogen-blend combustion in microturbines as the example, researchers at Argonne have developed and validated a novel machine-learning-based methodology to generate a high-confidence surrogate model from relatively sparse data points; the high-confidence model should result in lower risk of implementation for new processes or technologies.

As expected, high-fidelity sparse experimental data coupled with an active-learning approach improves the predictability of the model by smarter sampling of the system's operating space. Further improvement in predictability comes from the use of sparse data and qualitatively correct low-fidelity computational fluid dynamics (CFD) data. The researchers built an in-house Gaussian process (GP) modelling tool using PyTorch to accomplish this multi-input, multi-output multi-fidelity methodology. Through comparison of predicted emissions versus actual emissions from the microturbine, the researchers showed that incorporation of low-fidelity CFD data into the multi-fidelity learner model improves surrogate-model predictability with lower error scores using fewer high-fidelity data points. The improved methodology can reduce the need for extensive / expensive experimentation before investment decisions in decarbonization technologies are made.

The link for the paper is here: https://doi.org/10.1115/GT2023-103229

SAFETY FIRST

Hazards of Bisphenol A in Food Packaging

Chemicals from food packaging may come into contact with food and cause serious health concerns. Bisphenol A (BPA) is a chemical used in polycarbonate plastics to manufacture hard food and beverage containers. BPA is also used to manufacture epoxy resins found in the protective coatings and linings of some metal cans, where it prevents corrosion of the can and the migration of metal into food. BPA has been used since the 1960s to make polycarbonate plastics, epoxy resins, metal can coatings, and other materials that contact food.

BPA may migrate into foods and beverages through the packaging material. A person becomes exposed to low levels of BPA when eating food stored in food containers or drinking water in water bottles that contain BPA. The extent to which BPA may leach from polycarbonate bottles into liquids depends more on the temperature of the liquid or bottle than on the age of the bottle.

In 2012 and 2013, the FDA changed its regulations to prohibit the use of BPA-based polycarbonate resins in baby bottles, sippy cups, and infant formula packaging. BPA triggers children's immune systems, in a process that primarily involves allergic lung inflammation and autoimmune disorders. BPA can cause harm to organs after entering the body through respiration, dermal contact, and through the gastrointestinal tract. Exposure to BPA has been linked to cancers, endocrine disruption, immunosuppression, and reproductive defects. In 2022, environmental and public health groups urged the FDA to limit all food packaging that contains BPA a level of more than 0.5 ng/kg food.

Infants and children are the most vulnerable to the effects of BPA. Here are steps to reduce exposure to BPA:

- Don't place polycarbonate food containers in microwave ovens as they may degrade at high temperatures.
- Buy fresh, frozen, or dried foods instead of canned foods.
- Replace polycarbonate and metal cans with glass, porcelain, or stainless-steel containers
- BPA may be present in various metal jars, lids, aerosol cans, and aluminum beverage cans.
- Many polycarbonate plastic containers marked with recycle code 7 are made with BPA.
- Some large water-cooler bottles and food-storage containers may contain reusable polycarbonate plastics.
- Use baby bottles that are manufactured without the use of BPA.

References

Wilhelm, Erika. News Release. June 2, 2022. FDA agrees to reconsider safety of BPA in food packaging: Americans are exposed to BPA at levels 5,000 times above safe levels.

U.S. FDA. 2023. Bisphenol A (BPA): Use in food contact application. https://www.fda.gov/food/food-packaging-other-substances-come-contact-food-information-consumers/bisphenol-bpa-use-food-contact-application

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FADWA AL-TAHER

CHEMSHORTS FOR KIDS

Elephant Toothpaste

Many have heard of this experiment or seen it on videos but here is how you can do it in on your own without the highly caustic 30% hydrogen peroxide.

Materials:

- Empty water bottle
- 3% hydrogen peroxide (1/2 cup)
- Dish soap (approximately 1 Tablespoon)
- Dry yeast (1 packet – 2 teaspoons)
- Warm water (6 Tablespoons – 1/3 cup)
- Glass to mix yeast solution
- Spoon to stir yeast solution
- Measuring cups
- Tablespoon
- Teaspoon
- Tray or container for water bottle to sit in
- Food coloring (optional)

Caution: Hydrogen peroxide (even 3%) can be dangerous. Adult supervision is necessary. The foam that forms is not toothpaste and should not be used for that purpose. The resulting solution is safe to touch if you use yeast as the catalyst (however the food coloring may stain you, your clothes, table, etc.). Often potassium iodide gets used for this reaction and if that catalyst is used, the resulting foam will stain your skin.

Experiment:

Pour the warm water from the faucet into the glass and add the dry yeast. Stir the solution with the spoon. This solution should set for about 5 minutes while you add the hydrogen peroxide to the water bottle along with the dish soap. Add food coloring at this point if desired. Swirl the bottle to mix the ingredients. Once the yeast solution has sat for 5 minutes, pour the yeast into the water bottle and watch what happens.

What's happening?

Hydrogen peroxide has the chemical formula H_2O_2. This is very similar to the much more stable water molecule, H_2O. The hydrogen peroxide has an extra oxygen atom that makes it fairly unstable. The warm water will activate the yeast which has an enzyme in it called catalase that catalyzes (speeds up) the decomposition of H_2O_2 into H_2O and O_2. The oxygen molecule that is released is a gas and the gas gets caught up in the soap and causes bubbles to form. The faster the reaction, the faster the bubbles will form and the greater the foaming of the "toothpaste". You may have noticed some steam being released. This is due to the heat that is generated when the hydrogen peroxide decomposes.

Extension:

Normally when you see this demonstration done it is performed with much higher concentrations of hydrogen peroxide (30%). This is highly caustic and will burn your skin if you get it on you. You can dilute your 3% peroxide to see how this would affect the reaction. You can add more or less yeast as well. The size of the opening on the container will affect how high the bubbles shoot out. If you go with a smaller opening you will want to do this experiment outside so that the soap won't spray (and stain) your ceiling (see https://www.youtube.com/watch?v=Kou7ur5xt_4)

References

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https://www.thoughtco.com/kid-friendly-elephant-toothpaste-demo-604164

https://www.youtube.com/watch?v=j2m7odcvqMA

To view all past "ChemShorts for Kids", go to: https://chicagoacs.org/ChemShorts

PAUL BRANDT

AMERICAN CHEMICAL SOCIETY
Chicago Local Section

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Have fun working with others!

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for more information or to volunteer

UPCOMING EVENTS

Feb. 8	Chicago Board of Directors Meeting
Feb. 10	Articles due for the March 2024 Bulletin issue
Feb. 16	February Virtual Meeting
Feb. 27	IUPAC Global Women's Breakfast 2024

The Chemical Bulletin
February 2024, Vol. 111, No. 2
Published by the
Chicago Section of the American Chemical Society

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