In Conjunction with the American Chemical Society
Student Affiliates at the University of Pittsburgh

CHEM MAJOR NEWS

Volume 32, Issue 5 February 2, 2024

REGISTRATION TIME!

Dates:

February 1	**Students can start to apply for 2024 August graduation.**
February 12	**Summer Term (2247) registration begins for all students.**
March 11–15	**Spring Break!**
March 25	**Fall Term (2251) registration begins for all students.**

IMPORTANT: WHEN SHOULD YOU SEE YOUR ADVISOR?

Students who already have a permanent advisor should make a registration appointment with their advisor starting on February 12th.

If you don't have a permanent advisor, you will be asked via email to select your permanent advisor starting on February 5th.

New chemistry major students can sign up for your first-time advising appointment on Feb. 12th for the 2024 Summer Term (2247) and March 18th for the 2024 Fall Term (2251) in Chevron 107.

2023–2024 ACS-SA Officers and Staff

Ahssan Sekandari – *Co-President*
Dhruthi Gunduaro – *Co-President*
Rebecca Babendreier – *Co-Vice President*
Shane Osborne – *Co-Vice President*
Christina Raad – *Secretary*
Dennis Skiba – *Co-Treasurer*
Donny Truong – *Co-Treasurer*

Holly Krug – *Technology Wizard*
Anna Welser – *Outreach Coordinator*
Joe Storey – *Outreach Coordinator*
Rebecca Hotton – *Feature Writer/Editor*
Victoria Zerbach – *Newsletter Editor*
Piper Read – *Green Chem Contributor*
Jimmy Rekowski – *Pharm Contributor*

Visit us at http://www.chem.pitt.edu/acs-sa/

A Nan♡particle Heart F♡r Valentine's Day

By Victoria Zerbach, *Co-Newsletter Editor*

Valentine's Day. It's not just a day for couples. It's an excuse to share joyful and heartfelt moments with everyone that you love, friends and family included. It's a day that encourages wearing your heart on your sleeve.

Giving and receiving love, care, and affection can make our hearts ache, skip a beat, or feel as light as a balloon full of helium. And while our hearts have little role in controlling our emotions, the heart has been a symbol of love for much longer than humanity can remember. The heart symbol serves as a way of expressing our love to those we care about. And with Valentine's Day right around the corner, hearts have been popping up everywhere. From the supermarket to social media, you can't escape hearts on Valentine's Day. It seems, you sometimes can't even escape them in the lab.

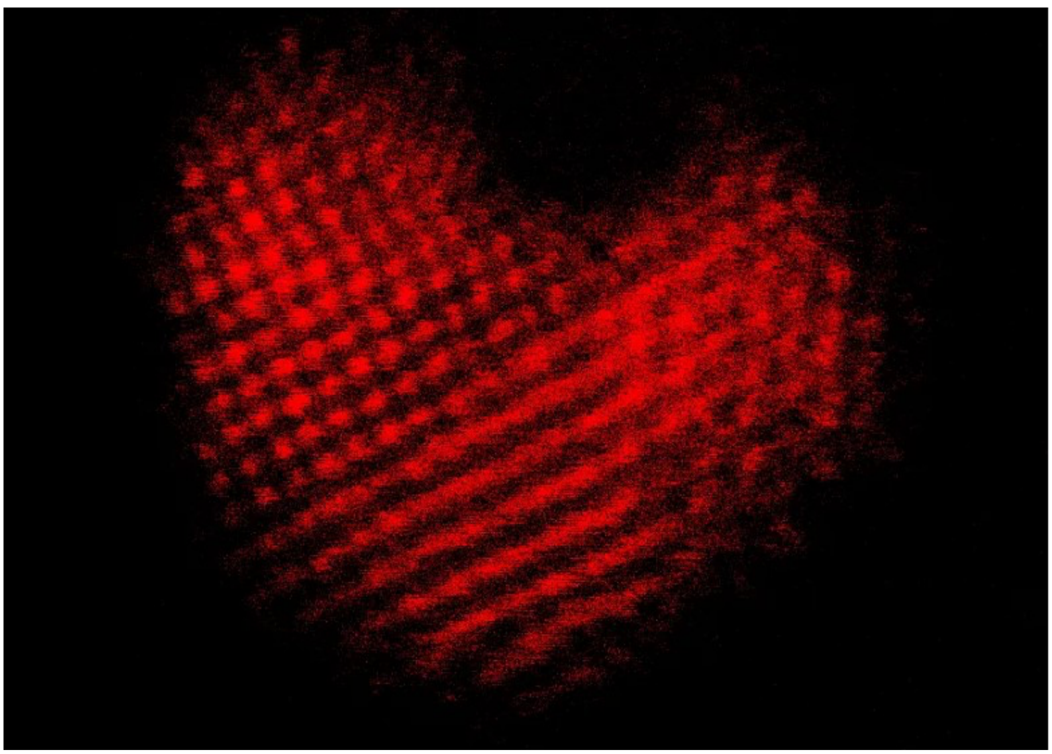


Image by Dong Su (Brookhaven National Lab)

The heart shaped nanoparticle arrangement shown above solves an interesting problem for chemists working under the U.S. Department of Energy (DOE) at Brookhaven National Laboratory (BNL). For the past decade a few groups of scientists at BNL have been investigating how to make clean-energy fuel cells less expensive. Chemists at BNL have been developing innovative fuel cells with platinum, iridium, and tin alloy nanoparticles, like the ones shown above.

Fuel cells are versatile power sources with applications in transportation, residential/industrial/commercial electricity, and even long-term energy storage in reversible grid systems. Fuel cells also boast several benefits over the conventional combustion-based technology used in most power plants and vehicles. Fuel cells operate at higher efficiencies, have lower or zero emissions compared to combustion engines, create no smog-causing air pollutants, and fuel cells are quiet during operation. Additionally, fuel cells that run on hydrogen emit only water–meaning no carbon dioxide emissions–and thus are an enticing eco-friendly technology.

However, there are still some issues with hydrogen fuel cells. Firstly, most hydrogen is produced via natural gas reforming, which is a process that combines natural gas and steam to produce hydrogen and carbon dioxide. Then the hydrogen needs to be stored and shipped, producing emissions before the hydrogen ever gets to your car or power generator. There are some cleaner hydrogen manufacturing methods available, like sun-powered electrolysis or hydrogen-producing algae, but these are still too expensive for most companies to willingly adopt. Secondly, hydrogen fuel cells are still quite expensive to produce. This second issue is where chemists at BNL have been focusing their work. But, to understand why fuel cells are expensive, we first need to understand how they work.

A fuel cell has an anode and a cathode, sandwiching an electrolyte center. Hydrogen is fed to the anode and oxygen is fed to the cathode. A catalyst at the anode causes hydrogen molecules to separate into protons and electrons, which travel to the cathode via different paths. The protons travel through the electrolyte to the cathode, while the electrons go through an external circuit, creating a flow of electricity. When the electrons and protons unite with oxygen at the cathode water and heat are produced.

As of 2016, most fuel-cell-powered vehicles contained platinum-based catalysts, which are the best at catalyzing hydrogen separation. However, platinum is expensive. BNL chemists have some great ideas for how to reduce cost while retaining catalytic activity. In their initial designs they replaced the solid platinum catalysts with nanoparticles of cheaper metals coated in platinum. This core-shell design reduced costs, improved catalytic activity, and decreased the risk of corrosion from the highly acidic environment of the fuel cell. In succeeding evolutions of this design, cores of different nitride metals and alloys were introduced. Cores made of platinum, iridium, and tin alloys, like the nanoparticle heart shown above, provide interesting benefits to the fuel cells. For example, the addition of tin can make the reaction go ten to thirty times faster.

Dong Su, a scientist at BNL, used an electron microscope to reveal the interesting heart-shaped nanoparticle structure seen above. In the image, which has been digitally colored red, each dot is a singular atom. The heart shape wasn't intentional, but the team of scientists at BNL believe that this unusual shape may expose more active sites for catalytic reactions.

Introducing nanoparticles into catalyst design have made fuel cells cheaper, more stable, and have increased catalytic activity. More efficient, cleaner vehicles may be right around the corner with the help of scientists at BNL. And this certainly warms my heart.

Wishing you all a heart-filled, lovely Valentine's Day from my nanoparticle heart to yours!

Are No Two Snowflakes Really Alike?

How Chemistry Controls Snowflake Structure

By: Rebecca Hotton, *Feature Writer*

It looks (and certainly feels) like winter is in full force here in Pittsburgh! This is the time of the spring semester where, unfortunately, we are all forced to trudge through treacherous streets and icy sidewalks to get to our favorite building—Chevron Science Center—on the daily. Although some of us may hate the snow and wish for warmer, drier times that are soon to come in May, I think it's worth taking a closer look at the way we can apply some general chemical and physical concepts to the appearance and structure of the snow that we will encounter this semester! I'm sure we've all heard through one way or another that no two snowflakes are exactly alike—and for any two snowflakes, being exactly alike would be statistically impossible. This is a very peculiar phenomenon, as we don't see this extreme type of structural anisotropy in many other naturally occurring materials or substances. How, scientifically, is this possible? Additionally, how do we define "uniqueness" is snowflake structure? The answer to this lies in the lens you take when examining snowflake shape and composition.

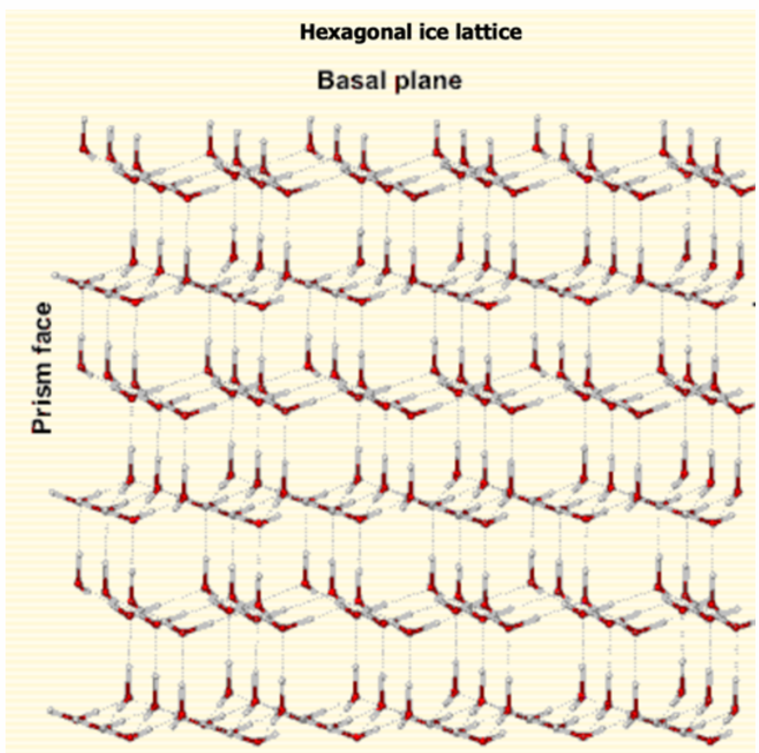
First, we can examine the microscopic chemical and structural composition of the smallest structural units of snowflakes. Snow, as we all know, is composed of solid phase H_2O molecules. In a snowflake, the water molecules are hexagonally packed, meaning that 6 bent H_2O molecules will arrange in the shape of a hexagon, with the oxygen atoms of one water molecule facing the hydrogen atoms of other water molecules to optimize hydrogen bonding interactions in the snow crystal. These hexagonal repeating units are uniform and periodic, meaning the core structure of snow is crystalline. This indicates that, on a microscopic structural scale, all snowflakes are alike, and no snowflake is unique.

However, snowflakes are very dissimilar and unique from each other in both their macroscopic structure, but also potentially in their isotopic composition. The dissimilarity in their macroscopic structure is due to the nucleation process that occurs in the atmosphere to create macroscopic snowflakes. The nucleation process involves the interaction between ice crystals as they fall through clouds and the supercooled droplets contained within the clouds that will freeze onto the existing crystal. Branching then occurs to create the macroscopic snow "flake" and these flakes are very different in shape, as the shape of this branching onto existing snow crystals is dependent on the temperature, humidity, and general atmospheric conditions like wind speed and altitude. This being said, the unique shapes and pattens are a result of the unique path that every supercooled droplet and original snow crystal will take to form a flake.

It is also worth noting that every snowflake formed in the atmosphere has a uniqueness related to its isotopic chemistry. In the first general chemistry course offered at Pitt, we are introduced to the ideas of isotope abundance, and their difference in masses (due to a difference in the number of neutrons in the nucleus). This applies to all elements and is certainly true of water molecules. There are approximately four naturally occurring isotopes of oxygen (^{15}O, ^{16}O, ^{17}O, and ^{18}O) and three naturally occurring isotopes of hydrogen (^{1}H, ^{2}H, and ^{3}H). This leads to much more variation (even if slight) in the isotopic composition of snowflakes, making them even more unique from each other!

All in all, even if the chemical concepts behind the chemistry of snowflakes seems more elementary, I think the argument of the individuality of snowflake structure and composition brings up an important nuance of science: the lens of examination. There are many ways to group and define chemical or macroscopic structures and categorize them as similar or dissimilar, and this all depends on the lens and size regime considered. This is a common and essential aspect of scientific research and writing: delineation and operationally defining your target property of interest. We can consider both how snow crystals are exactly similar to each other, if we only consider their microscopic crystal structure, but also how they are entirely different when considering their isotopic variation or macroscopic pattern. Therefore, if we wanted to arrive at a conclusion on the unique properties of snowflakes, we, as scientists, would first need to come to a consensus on the size regime and perspective we are examining! This can be a common theme in science and can be the root of scientific debates and disagreements when it comes to more subjective data interpretation.

I hope, through reading this short article on the chemistry of snowflakes, you've developed some sense of understanding on the subjectivity that can be present in science. So, next time you're asked a more elementary question like "are two snowflakes alike?" or "is water actually wet?", I encourage you to challenge yourself and consider both routes of chemical (or physical) reasoning for how both positions could be correct, and the evidence present for them!



February Drug of the Month: *Paxlovid*

By: Jimmy Rekowski, *Pharm Writer*

With the onset of the COVID-19 pandemic in 2020, the pharmaceutical industry was forced to come up with novel ways of treating Coronaviruses that could be used on many different populations in a safe, effective manner. This means that the drugs and treatments would need to be created by trusted producers and be able to be stored in a wide variety of conditions. This led to the production of many mRNA-based vaccines by large pharmaceutical companies such as Pfizer, Moderna, and AstraZeneca. However, these vaccines are not perfect in completely preventing any individual from contracting the disease. Instead, Paxlovid is advertised to reduce the symptoms and make a recovery much easier for those effected. For older and immunocompromised populations, despite the vaccine, recovery can still be difficult. This need for a drug more effective in reducing the symptoms and side effects of COVID-19 led to the creation of another novel treatment called *Paxlovid*, which includes *Ritonavir* and *Nirmatrelvir*. This medication is prescribed for the treatment of mild-to-moderate COVID-19 in adults who are at high risk for the progression of severe COVID-19, which could result in hospitalization or death.

Paxlovid is the brand name for *Ritonavir/Nirmatrelvir* tablets created by Pfizer. *Nirmatrelvir* is a peptidomimetic inhibitor of the SARS-CoV-2 main protease. This protease, termed (M^{pro}) is primarily responsible for processing two important viral polyproteins that are directly involved in the replication of COVID-19. These two proteins are termed ppla and pplab. Therefore, by inhibiting this protease, the drug can attempt to prevent viral replication altogether. Furthermore, experimentally, *Nirmatrelvir* was found to directly bind to the active site of SARS-CoV2, making it a competitive inhibitor. A peptidomimetic inhibitor is a small protein-like chain that is designed to mimic another peptide. Essentially, a peptidomimetic inhibitor functions as a synthetic tool to mimic the functionality of other, natural peptides. *Paxlovid* is to be administered as soon as possible after diagnosis of COVID-19, preferably within 5 days of symptom onset. The drugs are to be taken together twice daily for 5 days. By co-packaging the two tablets together, this means that they must be administered directly together. The simultaneous administration of the two drugs is done so that the drug can remain active in the body for longer periods. The low-dose *Ritonavir* is used to slow down the breakdown of the *Nirmatrelvir* providing more time to make an impact.

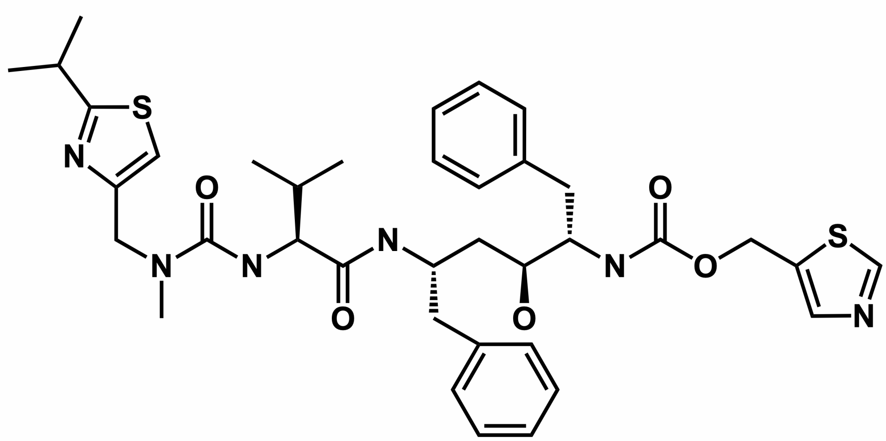


Figure 1. Chemical structure of *Ritonavir*.

With the continued development of viruses and diseases that effect millions of people worldwide, such as COVID-19, pharmaceutical companies are continuously required to come up with innovative ways to combat such ailments. *Paxlovid* has helped many vulnerable populations around the world since its introduction to the market in May 2023. When considering the impact of drugs, it is important to consider not only the health benefits but also the economic and ethical impacts of the drugs. I encourage you to consider what some of these impacts may be! Feel free to email me to chat about it more at jar309@pitt.edu!

Update on the September Drug of the month, *Leqembi*:

I wanted to give a quick follow-up to my drug of the month article in September on *Leqembi* (Lecanemab), a new FDA approved drug that can help the breakup of brain plaque that contributes to the progression of Alzheimer's Disease. Last week, CBS News' 60 Minutes spoke about a new, revolutionary treatment for the disease that works in tandem with *Leqembi* and other drugs. Dr. Ali Rezai, a neurosurgeon at West Virginia University School of Medicine, has used technology that has been around for 70 years in ultrasound to penetrate the skull, and easily focus like a magnifying glass on the blood brain barrier. The ultrasound uses high-frequency sound waves from a transucer to reflect on different tissue types such as the blood brain barrier. This allows drugs such as *Leqembi* to pass the blood brain barrier easier easier and, ultimately, be more effective. This also makes the administration of the drug easier on both the health care professional and patient, as this increased efficiency means that individuals will not need to be given an IV treatment, which was the standard protocol for *Leqembi*.

Painting a Picture of Greener Future

By: Piper Read, *Green Chemistry Writer*

In recent years, the global community has witnessed a surge in environmental consciousness, propelling industries to explore advanced sustainable practices. Within this context, the field of coatings and polymers (for those who attended our industry talks by scientists at Sherwin Williams and PPG, this should sound familiar!) has been at the forefront of adopting the principles of Green Chemistry, showcasing substantial advancements towards an eco-friendlier future.

One notable example of industry innovation comes from Procter & Gamble and Cook Composites and Polymers, who collaborated to create a replacement for the fossil-fuel-derived paint resins and solvents that were prominently used in the industry. Their solution, a mixture of soya oil and sugar, has effectively cut hazardous volatiles produced in product production by 50%. The resulting innovation served to replace petroleum-based solvents, contributing to the creation of safer paints that produce less toxic waste.

Similarly, Sherwin Williams has made significant strides in developing sustainable paint solutions. Their water-based acrylic alkyd paints boast low Volatile Organic Compound (VOC) levels and can be crafted from recycled soda bottle plastic called polyethylene terephthalate (PET), acrylics, and soybean oil. This approach combines the performance benefits of alkyds with the low VOC content of acrylics. In 2010 alone, Sherwin Williams manufactured enough of these innovative paints to eliminate over 800,000 lb, or 362,874 kg, of VOCs, marking a substantial contribution to reducing environmental impact.

These industry examples exemplify how companies are integrating Green Chemistry principles into formulations, pushing the boundaries of sustainability. The utilization of biobased oils and recycled materials not only reduces dependence on fossil fuels but also addresses concerns related to hazardous substances and waste generation. Such innovations align with the overarching goal of Green Chemistry—creating products and processes that are environmentally responsible without compromising performance.

The application of Green Chemistry, coupled with industry innovations from companies like Procter & Gamble, Cook Composites and Polymers, and Sherwin-Williams, is revolutionizing the coatings and polymers industry. As research and design teams embrace low-VOC formulations, renewable resources, and cutting-edge technologies, we hope for a swift transition into a future where the chemical industry aligns seamlessly with the principles of sustainability.

ACS-SA February Schedule

February

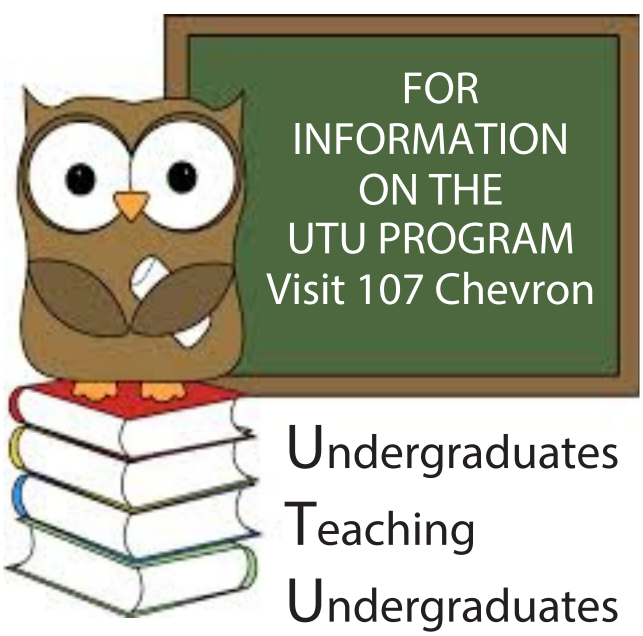
02 *Medical and Dental School Round Table*

09 *Meet Our New Faculty – Professor Jessica Anna*

16 *Graduate School Round Table*

23 *Spring Term Pasta Lunch from the Pleasure Bar and Restaurant – Reservations Required*

Ever wonder what it is like on the other side of the podium? Becoming a UTU is great way to find out. As a UTU, you get the chance to teach General, Organic or Analytical Chemistry. This is a great experience, no matter what your career path is!



The Kenneth P. Detrich School of Arts & Sciences

Summer Undergraduate Research Awards (SURA)

The Summer Undergraduate Research Awards (SURA) provide a $4,000 stipend to conduct independent research over the summer. Titles of recent SURA topics range from "Queer Cinema and the Spectator/Voyeur Narrative: Performance and Performativity" to "Migrant Health and Human Rights". SURA recipients also enroll in a 12-week summer SURA course to learn how to communicate their research findings to a general audience.

Eligible Dietrich School undergraduates who

- are interested in joining a community of scholars
- are interested in conducting self-directed research
- can secure a faculty mentor within the disciplinary area of the research topic

Application:
https://www.asundergrad.pitt.edu/research

Deadline: March 4, 2024