



## **Inaugural 3-Minute Thesis Presentation 2025**

**Jointly organised by**

**Australian Chapter of American Chemical Society**

**and**

**Royal Australian Chemical Institute**

**National Finale, 2 pm AEDST, 2 December 2025**

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### **Presentation Abstracts**

Participating states/territory: ACT, NSW, QLD, SA, VIC

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## **Super-Reducing Photoenzymes: Advancing Photobiocatalysis for Sustainable Asymmetric Synthesis**

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Imagine two keys that look almost the same, but only one turns the lock properly. Drugs can be like that too: molecules that seem identical at first glance, yet a tiny twist in their shape can decide whether they heal or harm.

To craft the perfect “keys” for our bodies, chemists design catalysts, tools that guide and accelerate molecular transformations. However, nature’s own catalysts, enzymes, remain unmatched. They are precise, sustainable, and work gracefully in the mildest of conditions, just in water.

This research gives these biological tools new capabilities by shining light on them. By attaching blue light-absorbing dyes to enzymes, we create super-reducing photoenzymes that can activate stubborn chemical bonds and build complex, three-dimensional molecules with precision. This approach merges nature’s craftsmanship with renewable light energy, paving the way for sustainable, efficient methods to create the life-saving medicines of tomorrow.

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## **Zooming in on Batteries for a Better Future**

**Tanika Duivenvoorden**  
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My thesis is on designing and investigating new safe and sustainable materials for batteries. The motivation for my work is to support the transition from fossil fuels to renewable energy, which is variable and requires sustainable energy storage. The electrolyte material is crucial to optimising battery performance, and must allow the fast transport of ions across the cell. I use molecular dynamics simulations to study the atomic structure of different electrolyte materials and predict how well they will transport ions. These simulations give detailed information which help us to systematically design better electrolyte materials.

## **Molecular Staplers: Latching Peptides for Smarter Medicine**

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Peptide stapling is a powerful strategy for stabilising natural shapes of peptides to boost their bioactivity, especially for targeting protein–protein interactions. We work with stapled peptides by locking them into stable ring-like structures through covalent linking two specific points along their chain. This approach works under physiological conditions and produces stable, functional structures without the need for unnatural building blocks. The resulting stapled peptides show remarkable improvements in stability, binding affinity and inhibitory potency compared to their linear counterparts. For example, peptides designed to bind streptavidin displayed over 100-fold higher affinity and inhibitors targeting Zika virus protease achieved nanomolar potency with 20-fold greater resistance to degradation. This strategy is versatile, compatible with genetic systems and opens new opportunities for developing peptide-based therapeutics.

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## **An In-Built Depolymerisation Solution for Polyethylene Waste**

**Carolyn Bapp**  
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Plastic waste remains a major environmental challenge, particularly with the widespread use of single use plastics, most of which are composed of polyethylene (PE). My research aims to enable the controlled biodegradation of PE through the incorporation of an enzyme directly into the polymer matrix. Specifically, I investigate the use of manganese peroxidase (MnP), a promising candidate for PE degradation. The key challenge lies in preserving enzymatic activity. To address this, I design polymers to enable the encapsulation of MnP and ultimately stabilisation of the enzyme, maintaining its functionality while being embedded in PE. These enzyme-polymer nanoconjugates stay inert during use but activate selectively under defined degradation conditions such as elevated temperature.

This approach integrates a solution for plastic waste management into the material, offering a strategy for on-demand, enzyme-driven decomposition of conventional plastics.

## **Fertiliser to Fuel: Unlocking Hydrogen from Ammonia**

**Pallavi Saini**

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Hydrogen is central to a carbon-neutral energy future, but most production methods still depend on fossil fuels. Ammonia is a compound already produced at scale for fertilisers and offers a practical alternative. It is carbon-free, energy-dense, and easily transported, making it an ideal hydrogen carrier. My research focuses on designing advanced catalysts to efficiently “crack” ammonia into hydrogen at lower temperatures, reducing energy demand and emissions. This approach leverages existing infrastructure to deliver clean hydrogen without the challenges of storage and distribution that limit other methods. By transforming an agricultural staple into a renewable fuel source, we can accelerate the transition to a sustainable hydrogen economy by bridging the gap between today’s fertiliser and tomorrow’s fuel.

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## **Breaking Through the Biofilm Matrix**

**Lily Kenchington-Evans**

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Antimicrobial resistance poses a significant threat to health and is worsened by the propensity for bacteria to form biofilms. There is an urgent need for new antimicrobials, ones that overcome resistance mechanisms and target bacterial biofilms. This project utilises in-house azide-derivatised antibiotics and alkyne-bearing antibiofilm moieties to generate antibiotic-antibiofilm conjugates using copper(I) catalysed azide-alkyne cycloaddition ‘click’ chemistry. This approach led to the discovery of ROX-PCM5, a conjugate with enhanced activity against planktonic and biofilm populations of bacteria including multidrug resistant species.

## Using Computers and Analytical Chemistry to Kill Superbugs

**Gerardo Urbina**  
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Antibiotic resistance is becoming one of the world's most urgent health problems. Bacteria known as superbugs are evolving faster than we can develop new drugs, leaving many infections harder to treat. My research focuses on designing artificial DNA-like molecules that can bind to bacterial DNA and stop it from functioning. Traditionally, finding effective molecules involves extensive trial and error in the lab, wasting time and resources. In my PhD, I am developing a faster approach that uses computer simulations to predict which molecules are most likely to bind DNA before they are made. To do this reliably, I have first compared and validated different experimental techniques used to measure DNA binding in the laboratory. By combining experimental and computational results, my goal is to create a predictive model that helps design better antibacterial molecules, potentially accelerating the discovery of new treatments to combat antibiotic-resistant infections.

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## From Water to Sustainable Hydrogen Fuel: The Atomic Blueprint for a Decarbonised World

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Hydrogen generation through photocatalytic water splitting offers a sustainable pathway toward a carbon-free future. Among visible-light photocatalysts, graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) stands out as a remarkable candidate. However, progress has been limited by an incomplete understanding of how its atomic structure governs photocatalytic performance. Most previous theoretical studies have modelled g-C<sub>3</sub>N<sub>4</sub> as a perfectly flat, graphene-like structure. This long-standing assumption leaves a critical gap in explaining inconsistencies in stability and light-absorption performance. My research employs density functional theory (DFT) to systematically explore the atomic configurations of g-C<sub>3</sub>N<sub>4</sub>. I found that the flat model is only metastable, whereas a buckled configuration emerges as the true ground state. This buckling enhances both thermodynamic stability and optical absorption, providing a structural foundation for improved photocatalytic efficiency. By addressing this fundamental gap, my work extends our understanding of g-C<sub>3</sub>N<sub>4</sub> and informs the design of next-generation solar photocatalysts for clean hydrogen production.

## **Addressing Sewer Corrosion: Enhancing sewer pipe durability and sustainability through mine waste utilisation**

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The construction industry faces sustainability challenges, as cement and concrete production contribute nearly 8% of global CO<sub>2</sub> emissions. Concrete pipes made with Ordinary Portland Cement (OPC) are also susceptible to microbiologically induced corrosion. This PhD research investigates the use of mining waste to partially replace clinker and aggregates, aiming to reduce CO<sub>2</sub> emissions and minimise mining waste.

Laboratory tests analysed the properties of mine tailings compared to traditional sand and OPC. Standard leaching tests confirmed that the cement samples met environmental standards for the release of harmful substances. Three novel cement formulations replacing 20%, 25%, and 30% of OPC were developed without compromising strength or durability, with two blends showing improved performance in acidic sewer conditions. This research promotes carbon reduction, enhances sewer infrastructure, and supports Australia's net-zero 2050 targets.

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## **Taking the “Forever” out of Forever Chemicals**

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Per- or polyfluoroalkyl substances (PFAS) are a class of chemicals featuring strong C-F bonds which are used in a wide range of industries for their durability and heat, water, and oil resistant properties. It is these properties that also make PFAS impervious to environmental breakdown, earning them their nickname, “forever chemicals”. They pose a risk to the environment and human health.

My research addresses this challenge by developing a light-initiated degradation (photocatalytic) approach using carefully designed nanoparticles (zinc sulfide, ZnS). These nanoparticles can breakdown PFAS into benign products (F<sup>-</sup> and CO<sub>2</sub>) when activated by UV-A (365 nm) light.

A custom photocatalytic flow reactor was used to degrade PFAS and treat contaminated water samples.

The results are promising, showing nearly 90% of PFOS mineralised within 24 h of illumination. This research demonstrates a viable method of PFAS degradation, contributing to the development of sustainable technologies for environmental remediation.