

# Bulletin Board

## Contents

SEP. 06, 2024

(click on page numbers for links)

### REGULATORY UPDATE

#### ASIA PACIFIC

Version 3 of the AICIS Categorisation Guidelines will be published on 24 September 2024.....4

OCEAN ENERGY EVENT IS COMING DOWN UNDER.....5

Community invited to have their say on new thresholds for PFAS in regulated waste .....5

#### AMERICA

State sets new limits for toxic chemicals in water .....6

EPA's Final Formaldehyde IRIS Assessment Ignores Peer Reviews and Best Available Science .....7

#### EUROPE

Degraded ecosystems to be restored across Europe as Nature Restoration Law enters into force.....8

Is a blanket ban on plastic packaging really viable? Why automation can help reduce the environmental impact of packaging.....9

#### INTERNATIONAL

Researchers show that pesticide contamination is more than apple-skin deep .....10

Medical Product Alert N°3/2024: Falsified (contaminated) Oxymorphone Hydrochloride 40mg.....11

Why Denmark is ramping up its support for UNEP and building resilience.....12

### REACH UPDATE

Nine intentions have been submitted.....13

### JANET'S CORNER

Air Conditioning .....14

### HAZARD ALERT

Zinc Phosphide .....15

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## Bulletin Board

## Contents

SEP. 06, 2024

## GOSSIP

|   |    |
|---|----|
| Can supercapacitors be the next energy superheroes? .....   | 20 |
| Chemists create industrially important alkyl amines from dinitrogen and alkenes.....                | 21 |
| Hotter Than Lava: The Surprising Science of Molten Uranium .....                                    | 22 |
| Simple technique removes over 98% of nanoplastic particles from water                               | 25 |
| New process vaporizes plastic bags and bottles, yielding gases to make new, recycled plastics ..... | 26 |
| New filter removes chemical contaminants from water even at very low concentrations .....           | 29 |
| Revolutionizing Recycling: New Technique Turns Plastic Waste Into Wealth .....                      | 31 |
| Finger wrap uses sweat to provide health monitoring at your fingertips--literally .....             | 33 |
| Novel glass-forming liquid electrolyte shows glass transition across broad range.....               | 34 |

## CURIOSITIES

|   |    |
|---|----|
| Giant gold nuggets could be born from earthquakes and electricity .....                   | 37 |
| An Over-the-Counter Pain & Fever Medicine Has Been Recalled Nationwide .....              | 38 |
| Weight Loss Drug Shows Potential Benefit for Type 2 Diabetes .....                        | 39 |
| Molecular 'cage' approach could advance selective elimination of cancer cells .....       | 40 |
| Hydrogen stored in iron: A cheap, scalable grid battery for the winter .....              | 42 |
| Assorted, distinctive behavior of molten uranium salt revealed by neutrons .....          | 44 |
| Deadly Snail Venom Could Hold the Key to New Diabetes Treatments .....                    | 46 |
| Low-energy electrons in cosmic ice spring surprise by generating prebiotic molecules..... | 49 |
| How fish guts might play a role in future skin care products.....                         | 51 |
| Peptides and AI Unveil New Pathways in Drug Design .....                                  | 52 |

## TECHNICAL NOTES

|   |    |
|---|----|
| (Note: Open your Web Browser and click on Heading to link to section) ... | 55 |
| CHEMICAL EFFECTS.....   | 55 |

## Bulletin Board

## Contents

SEP. 06, 2024

|                                 |    |
|---------------------------------|----|
| ENVIRONMENTAL RESEARCH.....     | 55 |
| PHARMACEUTICAL/TOXICOLOGY ..... | 55 |
| OCCUPATIONAL.....               | 55 |

# Bulletin Board

## Regulatory Update

SEP. 06, 2024

### ASIA PACIFIC

#### Version 3 of the AICIS Categorisation Guidelines will be published on 24 September 2024

2024-08-30

A new version of the Industrial Chemicals Categorisation Guidelines will be published on 24 September 2024.

Version 3 will include revisions and updates that we originally announced in March 2024, but delayed by 6 months to give introducers time to prepare for the changes. It will also include updates prompted by the recent vaping reforms.

Differences between version 3 and the current Categorisation Guidelines

List of chemicals with high hazards for categorisation

We will add entries to the list of chemicals with high hazards for categorisation (the list) that introducers may need to check during the AICIS categorisation process. This was announced in our response to feedback on proposed changes to AICIS Categorisation Guidelines (March 2024). The changes include:

- almost 600 unique entries added to the list, based on current sources
- the European Commission Endocrine Disruptor List (List I) added as a source

These changes are the first (and probably largest) of what will likely be annual updates to the list. The list is a collation of chemicals that trusted national and international sources consider to be highly hazardous. These updates ensure that the list is consistent with the national and international regulatory status of these highly hazardous chemicals.

This follows the changes that came into place with version 2 of the Categorisation Guidelines that reduced the burden involved in the requirement to check salts and esters of chemicals on the list. In version 1, introducers had to check for salts and esters of all the chemicals on the list. Since version 2 was published, this checking is only required for chemicals that are specified within part 6 of the Categorisation Guidelines.

# Bulletin Board

## Regulatory Update

SEP. 06, 2024

Read More

AICIS, 30-08-24

<https://www.industrialchemicals.gov.au/news-and-notice/version-3-aicis-categorisation-guidelines-will-be-published-24-september-2024>

#### OCEAN ENERGY EVENT IS COMING DOWN UNDER

2024-08-24

The 2024 International Conference on Ocean Energy (ICOE 2024) will bring together in Melbourne, ocean energy leaders, decision-makers and researchers from every corner of the globe for a rich and exciting programme of sessions, workshops, networking, technical site visits and an insight into Australasia's rapidly evolving ocean energy activities.

Australia has moved from a target of 26% carbon emissions reduction to a 43% reduction by 2030 and net zero by 2050. The ocean energy sector has a pivotal role to play and ICOE 2024 will bring together all the key players in the sector to meet this transformational shift.

Read More

ICOE, 30-08-24

<https://icoe2024melbourne.com/>

#### Community invited to have their say on new thresholds for PFAS in regulated waste

2024-08-30

Queenslanders are invited to have their say on proposed changes to the state's environmental regulations that will amend threshold levels for PFAS in regulated waste.

Currently, waste that contains any level of per and poly-fluoroalkyl substances, commonly known as PFAS, is considered regulated waste and must be transported by a licenced transporter and be safely handled, stored, and disposed of by a licenced facility.

Regulated waste is subject to more stringent management requirements than other waste to ensure the environment and public health are not compromised.

The proposed changes will allow waste with very low levels of PFAS to no longer be categorised as regulated waste, providing greater management

# Bulletin Board

## Regulatory Update

SEP. 06, 2024

options for low-risk material, and reducing waste management costs, without causing risks to the community or the environment.

The proposed limits are extremely low and have been developed using the best available scientific research.

In liquid waste, for example, the proposed threshold is the equivalent of one drop of water in 20 Olympic-sized swimming pools.

[Read More](#)

Queensland Government, 30-08-24

<https://www.desi.qld.gov.au/our-department/news-media/mediareleases/community-invited-have-say-new-thresholds-pfas-regulated-waste>

## AMERICA

### State sets new limits for toxic chemicals in water

2024-08-14

#### PFAS, 6PPD-quinone among chemicals listed

Washington's waters have new protections, thanks to a major update to state water quality rules. The updates protect aquatic life, such as fish and invertebrates, from the effects of toxic chemicals in the water.

The Washington Department of Ecology developed these changes to the state's aquatic life toxics criteria based on updated science and new research, new methods and modeling tools, and recommendations from the U.S. Environmental Protection Agency (EPA) and Tribal governments.

Once the new criteria are approved by EPA, Ecology will use them to identify polluted waters and develop clean up plans. Ecology will also use the approved criteria when updating water quality permits for facilities discharging those chemicals.

"By using innovative methods and new scientific studies we can better protect salmon, shellfish and all aquatic life from the toxic chemicals they face every day," said Vince McGowan, Ecology's Water Quality program manager. "The new limits are customized to Washington's unique environment and the species we need to protect."

# Bulletin Board

## Regulatory Update

SEP. 06, 2024

[Read More](#)

Department of Ecology, State of Washington, 14-08-24

<https://ecology.wa.gov/about-us/who-we-are/news/2024-news-stories/aug-14-aquatic-life-toxics-criteria>

### EPA's Final Formaldehyde IRIS Assessment Ignores Peer Reviews and Best Available Science

2024-08-19

Today, the American Chemistry Council's (ACC) Formaldehyde Panel issued the following statement on the U.S. Environmental Protection Agency's (EPA) Final Integrated Risk Information System (IRIS) Assessment of Formaldehyde:

"As required under the Toxic Substances Control Act (TSCA), any assessment of formaldehyde must begin with the best available science. This assessment fails that test and is therefore unfit for regulatory decision-making. EPA's final assessment fails to reflect fundamental criticism from multiple peer review bodies or public comments provided by hundreds of experts, stakeholders, and other agencies. The Agency is on a path to ignore applicable scientific standards and procedural requirements, and issue unscientific and legally unsound regulatory actions based on this flawed assessment under TSCA and other laws later this year.

"If EPA continues on its current path, formaldehyde manufacturing and many of its downstream uses could be severely restricted or potentially banned in the U.S., with an overwhelmingly negative impact on the environment, human health, national security, and the economy.

[Read More](#)

American Chemistry Council, 19-08-24

<https://www.americanchemistry.com/chemistry-in-america/news-trends/press-release/2024/epa-s-final-formaldehyde-iris-assessment-ignores-peer-reviews-and-best-available-science>

# Bulletin Board

## Regulatory Update

SEP. 06, 2024

### EUROPE

#### Degraded ecosystems to be restored across Europe as Nature Restoration Law enters into force

2024-08-15

The regulation sets binding targets to restore degraded ecosystems, particularly those with the most potential to capture and store carbon and to prevent and reduce the impact of natural disasters.

The Regulation on Nature Restoration (Nature Restoration Law) came into effect on Sunday (18 August).

Full implementation of the law is crucial to restore the EU's biodiversity and stop further biodiversity loss, to reach climate neutrality by 2050 and adapt to climate change, and to enhance food security for EU citizens. In doing so, the law will support the achievement of other European ambitions, such as water security.

It is also a key instrument to help the EU and its Member States meet international biodiversity commitments under the Kunming-Montreal Global Biodiversity Framework.

The law sets in motion a process for continuous and sustained recovery of nature across the EU's land and sea while supporting more sustainable economic development and agricultural production and working hand in hand with the development of renewable energy.

As an overall target to be reached at the EU level, Member States will put in place restoration measures in at least 20% of the EU's land areas and 20% of its sea areas by 2030. By 2050, such measures should be in place for all ecosystems that need restoration.

The law includes requirements to put in place restoration measures to achieve the good condition of key habitat types and habitats of species on land and at sea. It also requires maintaining urban green space and urban tree canopy cover and increasing this after 2030.

Read More

European Commission, 15-08-24

[https://environment.ec.europa.eu/news/nature-restoration-law-enters-force-2024-08-15\\_en](https://environment.ec.europa.eu/news/nature-restoration-law-enters-force-2024-08-15_en)

# Bulletin Board

## Regulatory Update

SEP. 06, 2024

#### Is a blanket ban on plastic packaging really viable? Why automation can help reduce the environmental impact of packaging

2024-08-14

Every year, the UK produces around 2.4 million tonnes of plastic packaging waste, a significant portion of which comes from the food and beverage industry. Only 44.2 per cent of this packaging was recycled last year, with the rest ending up in landfills, incineration or the environment. Here Stephen Hayes, managing director of automation and control technology specialist Beckhoff UK, explains how food and beverage manufacturers can tackle demands for more productive and efficient packaging designs.

It's clear that food and beverage packaging has a huge impact on the environment. It's estimated that 70 per cent of all litter found in UK coastal areas was related to food and drink packaging. On top of this, the producing and disposing of single-use plastics generates substantial greenhouse gas emissions. The UK's overall carbon footprint from packaging waste is estimated to be the equivalent to 700,000 tonnes of CO2 annually.

The UK Government is currently considering a ban on fruit and vegetable plastic packaging for supermarkets, returning to traditional greengrocer methods. However, there are several implications relating to this.

Plastic packaging extends the shelf life of fresh produce by providing a barrier against moisture and air, which can lead to spoilage. With the average household in the UK already throwing away £700 of food annually, a blanket ban for supermarkets could cause this to increase further.

Plastic packaging also protects produce during transportation and provides a hygienic barrier to contaminants such as dirt and bacteria. It provides space for labelling, which can include important information such as nutritional content, origin and usage instructions. It can also encourage healthier eating habits for consumers by making it more straightforward to prepare and consume fresh produce, especially if it arrives pre-washed, pre-cut or portioned.

# Bulletin Board

## Regulatory Update

SEP. 06, 2024

[Read More](#)

Process and Control Today, 14-08-24

<https://www.pandct.com/news/is-a-blanket-ban-on-plastic-packaging-really-viable-why-automation-can-help-reduce-the-environmental-impact-of-packaging>

## INTERNATIONAL

### Researchers show that pesticide contamination is more than apple-skin deep

2024-08-07

Pesticides and herbicides are critical to ensuring food security worldwide, but these substances can present a safety risk to people who unwittingly ingest them. Protecting human health, therefore, demands sensitive analytical methods to identify even trace levels of potentially harmful substances. Now, researchers reporting in Nano Letters have developed a high-tech imaging method to detect pesticide contamination at low levels, and its application on fruits reveals that current food safety practices may be insufficient.

The analytical method called surface-enhanced Raman spectroscopy (SERS) is gaining popularity as a nondestructive method for detecting chemicals from modern farming on produce. With SERS, metal nanoparticles or nanosheets are used to amplify the signals created by molecules when they are exposed to a Raman laser beam. The patterns created by the metal-enhanced scattered light serve as molecular signatures and can be used to identify small amounts of specific compounds.

Looking to improve SERS sensitivity for pesticide detection, Dongdong Ye, Ke Zheng, Shaobo Han and colleagues designed a metal-coated membrane they could lay atop farm-grown produce. They also wanted to develop the material to be versatile enough to accommodate an array of other applications.

[Read More](#)

Phys.org, 07-08-24

<https://phys.org/news/2024-08-pesticide-contamination-apple-skin-deep.html>

# Bulletin Board

## Regulatory Update

SEP. 06, 2024

### Medical Product Alert N°3/2024: Falsified (contaminated) Oxymorphone Hydrochloride 40mg

2024-08-05

#### Alert Summary

This WHO Medical Product Alert refers to one batch of falsified Oxymorphone Hydrochloride 40mg. The falsified product was detected in the unregulated supply chain in Finland and reported to WHO in July 2024 by the Finnish Medicines Agency (FIMEA).

Oxymorphone Hydrochloride is a semi-synthetic opioid used to treat moderate to severe pain. Laboratory analysis of samples of the falsified product, however, found that the tablets contained metonitazene instead.

Metonitazene is a potent psychoactive synthetic opioid drug, with no officially recognized or authorized medicinal or therapeutic use. It is under international control as a Schedule I narcotic drug following recommendations of the WHO Expert Committee on Drug Dependence in 2021. Small doses can result in serious adverse effects such as respiratory depression, severe sedation, addiction, and an overdose may be fatal.

#### How to identify this falsified product

This product is confirmed as falsified because it deliberately misrepresents its identity, composition, and source.

The falsified product imitates Oxymorphone Hydrochloride marketed by AUROLIFE PHARMA LLC., who have confirmed that the product, subject of this Alert, is falsified and was not produced by their company.

To identify this falsified product check for the following:

- The falsified version label does not have a barcode on the bottle.
- The falsified version is labelled 40mg. AUROLIFE PHARMA Oxymorphone Hydrochloride is only available as 5mg and 10mg doses.
- The falsified versions of the tablets lack embossed letters/numbers.
- The falsified product's label is missing the National Drug Code of the United States of America.

Please refer to the Annex of this Alert for full details of the falsified product.

# Bulletin Board

## Regulatory Update

SEP. 06, 2024

Read More

WHO, 05-08-24

[https://www.who.int/news/item/05-08-2024-medical-product-alert-n-3-2024--falsified-\(contaminated\)-oxymorphone-hydrochloride-40mg](https://www.who.int/news/item/05-08-2024-medical-product-alert-n-3-2024--falsified-(contaminated)-oxymorphone-hydrochloride-40mg)

### Why Denmark is ramping up its support for UNEP and building resilience

2024-08-16

A key aim of Denmark's development cooperation strategy is to protect nature and help countries build their resilience to climate change.

To achieve that goal, Denmark has partnered closely with the United Nations Environment Programme (UNEP) and is one of the organization's strongest financial supporters.

Danish environment minister Magnus Heunicke said there is a simple reason for that collaboration.

UNEP, he believes, is uniquely placed to address the triple planetary crisis of climate change, nature and biodiversity loss, and pollution and waste, which is imperiling lives around the world.

"We are facing an existential threat to humanity," Heunicke said earlier this year at UNEP headquarters in Nairobi, Kenya. "That is why we need UNEP. We need someone to lay out the facts [and] get countries to work together."

Read More

UNEP, 16-08-24

<https://www.unep.org/news-and-stories/story/why-denmark-ramping-its-support-unep-and-building-resilience>

# Bulletin Board

## REACH Update

SEP. 06, 2024

### Nine intentions have been submitted

2024-08-28

Nine intentions have been submitted for:

- Rosin, maleated (EC 232-480-4, CAS 8050-28-0)
- Reaction products of tall oil fatty acids and tall oil rosin with maleic anhydride (EC -, CAS -)
- Rosin, fumarated (EC 266-040-8, CAS 65997-04-8)
- Resin acids and Rosin acids, fumarated, esters with glycerol (EC 307-051-0, CAS 307-051-0)
- Rosin, oligomers (EC 500-163-2, CAS 65997-05-9)
- cobalt bis(2-ethylhexanoate) [1]; cobalt hydroxide oxide [2]; cobalt dihydroxide [3]; cobalt oxide [4]; cobalt(II) 4-oxopent-2-en-2-olate [5]; cobalt trihydroxide [6]; cobalt sulphide [7]; cobalt(2+) propionate [8] (EC -, CAS -)
- decan-1-ol (EC 203-956-9, CAS 112-30-1)
- Resin acids and Rosin acids, maleated, esters with pentaerythritol (EC 305-516-2, CAS 94581-17-6)
- Rosin (EC 232-475-7, CAS 8050-09-7)

A proposal has been submitted for:

- 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno[5,6-c]pyran galaxolide (HHCB) (EC 214-946-9, CAS 1222-05-5)

A withdrawal has been received for:

- bis(4-methylbenzoyl)peroxide (EC 407-950-9, CAS 895-85-2)

Read More

ECHA, 28-08-24

<https://echa.europa.eu/>

## Bulletin Board

## Janet's Corner

SEP. 06, 2024

## Air Conditioning

2024-09-06

What do you call oxygen and nitrogen  
training together?



[www.periodictable.co.za](http://www.periodictable.co.za)

Air conditioning

<https://www.periodictable.co.za/blog/chemistry-jokes>

## Bulletin Board

## Hazard Alert

SEP. 06, 2024

## Zinc Phosphide

2024-09-06

## USES [2,3]

Zinc phosphide is used for rodent control on crops including grapes, sugarcane, artichoke, sugar beet, alfalfa, barley, berries, oats, sugar maple, wheat, corn, and hay. It is also used on grasses such as home lawns, rangeland, and golf courses. Zinc phosphide targets household rodent pests, such as mice and rats, in addition to field rodents including voles, ground squirrels, pocket gophers, prairie dogs, and jack rabbits.

## EXPOSURE SOURCES &amp; ROUTES OF EXPOSURE [3]

Exposure Sources

Exposure can occur via contact to a pesticide containing zinc phosphide including contact with skin, breathe it in, or if you accidentally eat or drink a product containing it. This can happen if you get some on your hands and eat or smoke without washing your hands first. Young children and pets are most likely to be exposed to zinc phosphide by eating the bait pellets if they find them. Baits often have peanut butter, molasses, or other flavours that may attract dogs or children. You may also be exposed if you apply bait with your bare hands, or breathe in any dust or crumbled, powdery bait.

Routes of Exposure

The main routes of exposure to zinc phosphide are:

- Inhalation
- Skin contact
- Eye contact
- Ingestion

## HEALTH EFFECTS [4]

Acute Health Effects

- Zinc phosphide dust may release phosphine once it contacts the moist tissues of the respiratory tract if the dust is inhaled, resulting in pulmonary oedema and cardiotoxicity.

**Zinc phosphide is an inorganic compound with the molecular formula  $Zn_3P_2$  that combines phosphorus with zinc. [1] The IUPAC chemical name is trizinc diphosphide, and the CAS registry number is 1314-84-7. Zinc phosphide is a grey-black powder with an odour similar to garlic. It is practically insoluble in water and insoluble in alcohol. [1,2]**



# Bulletin Board

## Hazard Alert

SEP. 06, 2024

- If ingested, zinc phosphide releases phosphine in the gut and may cause headache, dizziness, fatigue, nausea and vomiting, cough, dyspnea, chest tightness, and thirst. Other signs include liver failure, jaundice, loss of ability to urinate, tetany, delirium, convulsions, coma, and death.
- Death in humans from fatal doses may be delayed for 30 hours after exposure, with the majority of tissue damage occurring in the liver, kidneys and heart.
- Victims of lethal phosphine exposure were found to have liver, myocardial, and alveolar cell necrosis, pulmonary oedema and microscopic pulmonary congestion, and anoxic damage in the brain.
- Hyperglycaemia following exposure to phosphine has also been reported. Elevated levels of the enzyme creatine phosphokinase were found in two instances of severe poisoning by phosphine.<sup>28,29</sup>
- Phosphine have been shown to interfere with acetylcholinesterase in humans, but the impact of this inhibition on the toxicity is not clear.

### Carcinogenicity

- The U.S. EPA determined that chronic exposure to zinc phosphide should be negligible and therefore waived carcinogenicity testing requirements for reregistration.
- No human data were found on carcinogenic effects of zinc phosphide or phosphine.

### **SAFETY**

#### First Aid Measures [5]

- Move victim to fresh air. Emergency personnel should avoid self-exposure to zinc phosphide.
- Evaluate vital signs including pulse and respiratory rate and note any trauma. If no pulse is detected, provide CPR. If not breathing, provide artificial respiration. If breathing is laboured, administer 100% humidified oxygen or other respiratory support.
- Rush to a health care facility.
- Obtain authorisation and/or further instructions from the local hospital for performance of other invasive procedures.

#### Workplace Controls & Practices [4]

Control measures include:

# Bulletin Board

## Hazard Alert

SEP. 06, 2024

- Use only in a well ventilated area.
- After handling zinc phosphide and before eating, drinking or smoking, wash hands, arms and face thoroughly with soap and water.

### Personal Protective Equipment [5]

The following personal protective equipment is recommended when handling zinc phosphide:

- PVC gloves.
- Full face-piece respirator with combined dust and gas cartridge or supplied air respirator. For help in selecting a suitable mask consult AS/NZS 1715.
- After each day's use, wash gloves and respirator and if rubber, wash with detergent and warm water.

### **REGULATION**

#### United States

No occupational exposure limits have been established for zinc phosphide. However, as zinc phosphide can be converted to phosphine gas the following exposure limits apply to phosphine:

OSHA Permissible Exposure Limit (PEL):

- **General Industry:** 29 CFR 1910.1000 Table Z-1 -- 0.3 ppm, 0.4 mg/m<sup>3</sup> TWA
- **Construction Industry:** 29 CFR 1926.55 Appendix A -- 0.3 ppm, 0.4 mg/m<sup>3</sup> TWA
- **Maritime:** 29 CFR 1915.1000 Table Z-Shipyards -- 0.3 ppm, 0.4 mg/m<sup>3</sup> TWA

American Conference of Governmental Industrial Hygienists (ACGIH) Threshold Limit Value (TLV): 0.3 ppm, 0.42 mg/m<sup>3</sup> TWA; 1 ppm, 1.4 mg/m<sup>3</sup> STEL

National Institute for Occupational Safety and Health (NIOSH) Recommended Exposure Limit (REL): 0.3 ppm, 0.4 mg/m<sup>3</sup> TWA; 1 ppm, 1 mg/m<sup>3</sup> STEL

### **REFERENCES**

1. <http://npic.orst.edu/factsheets/znpngen.html>
2. <http://npic.orst.edu/factsheets/znpstech.html>

# Bulletin Board

## Hazard Alert

SEP. 06, 2024

3. <http://www.toxipedia.org/display/toxipedia/Zinc+Phosphide>
4. <http://extoxnet.orst.edu/pips/zincphos.htm>
5. [http://www.pesticideinfo.org/Detail\\_Chemical.jsp?Rec\\_Id=PC34737](http://www.pesticideinfo.org/Detail_Chemical.jsp?Rec_Id=PC34737)
6. [http://www.animalcontrol.com.au/pdf/MOUSEOFF\\_ZP\\_2013.pdf](http://www.animalcontrol.com.au/pdf/MOUSEOFF_ZP_2013.pdf)
7. <http://nj.gov/health/eoh/rtkweb/documents/fs/2041.pdf>

# Bulletin Board

## Gossip

SEP. 06, 2024

All-in-one solution captures and destroys 'forever chemicals' using light

2024-08-30

Proposed methods of removing toxic 'forever chemicals' from water have either only trapped the chemicals or broken them down. A new study has demonstrated a method that does both – quickly and cheaply.

Per- and polyfluoroalkyl substances, more commonly called PFAS or 'forever chemicals,' are a group of synthetic chemicals that resist degradation – hence the forever moniker – and pose a risk to the environment and us.

Now, chemical engineers at the University of British Columbia (UBC) in Canada have come up with an all-in-one solution for trapping and breaking down these forever chemicals into harmless components. Their method is explained in a recently published study.

"PFAS are notoriously difficult to break down, whether they're in the environment or in the human body," said Dr Johan Foster, an associate professor of chemical and biological engineering in UBC's faculty of applied science and the study's co-corresponding author. "Our system will make it possible to remove and destroy these substances in the water supply before they can harm our health."

Activated carbon is commonly used to absorb PFAS from drinking water due to its high surface area and strong affinity for organic compounds. However, one drawback of activated carbon is that additional steps are needed to dispose of the adsorbed chemicals. So, the researchers turned their minds to developing a means of destroying them in situ.

Photocatalytic degradation is a promising way of breaking down PFAS using light energy. Various metal oxides have emerged in recent years as potential options for eliminating the chemicals under UV irradiation. To that end, the researchers developed an iron oxide/graphemic carbon hybrid photocatalyst and found that it trapped PFAS chemicals and broke them down into harmless components.

"The whole process is fairly quick, depending on how much water you're treating," Foster said. "We can put huge volumes of water through this catalyst, and it will adsorb the PFAS and destroy it in a quick two-step process. Many existing solutions can only adsorb, while others are designed to destroy the chemicals. Our catalyst system can do both,

## Bulletin Board

## Gossip

SEP. 06, 2024

making it a long-term solution to the PFAS problem instead of just kicking the can down the road."

New Atlas, 30 August 2024

<https://newatlas.com>

### Can supercapacitors be the next energy superheroes?

2024-07-22

How many batteries do you own? The count in my own house includes phones, tablets, laptops, cameras and seemingly hundreds of kid's toys and gadgets. That's a lot of different lithium-based storage devices.

Batteries – in particular lithium-ion ones – are an almost inescapable facet of modern life. I even travel with a portable power pack to charge the other ones. They power our devices and will help smooth the transition to more. But how many capacitors do you own? In my case, the answer could be zero, but I simply don't know. The countless circuits in those battery-powered devices listed above almost certainly contain quite a few, but I've never knowingly bought one on its own, or as the key component of something else.

Could that be about to change? Supercapacitors offer a glimpse of an energy storage future different from – or complementary to – batteries. Unlike batteries, capacitors store charge on two closely spaced surfaces, and thus do not rely on redox chemistry. That means they can be charged and discharged extremely quickly, and they don't suffer the deterioration from structural chemical changes during those charging cycles that cause batteries to lose storage. Those are attractive benefits, as anyone with a smartphone more than two or three years old will appreciate.

There are of course downsides, which is why supercapacitors have not taken over the world and earned a Nobel prize. The main one is their energy density, or rather a lack of it. For any given size, supercapacitors currently hold far less energy than an equivalent battery.

As James Mitchell Crow's feature details, however, plenty of research is underway to rectify that. Many decades of research on battery-related or porous materials means there are plenty of groups out there with the skillsets to find the new compounds needed. Hopefully, in a few years' time, we'll all be as au fait with our capacitors as we are with our batteries today. renewable, but intermittent, sources of energy – besides the devices

## Bulletin Board

## Gossip

SEP. 06, 2024

listed above, there are many more kilowatt-hours of battery storage in my garage, hooked up to the solar panels on the roof.

Chemistry World, 22 July 2024

<https://chemistryworld.com>

### Chemists create industrially important alkyl amines from dinitrogen and alkenes

2024-09-05

A critical chemical bond can be assembled using dinitrogen (N<sub>2</sub>)—a molecule freely available in the air around us—chemists at RIKEN have shown in a new article published in Nature.

This demonstration has the potential to make the synthesis of industrially important compounds such as polymers and drugs much more energy efficient.

Dinitrogen is everywhere, making up nearly 80% of the air we breathe. But despite dinitrogen's high availability, it is challenging to use it directly in chemical reactions. That's because the molecule's strong triple bond needs to be severed.

For applications such as the synthesis of alkyl amines for making drugs and polymers, dinitrogen is first split in two to generate ammonia, in an additional step called the Haber–Bosch process. The easily accessible alkene component also has to be pre-activated by converting it into an alcohol or carboxylic acid. These extra steps add time and inefficiency to the process.

They have another disadvantage. "Synthesizing these nitrogen and carbon sources also consumes a lot of energy," notes Takanori Shima of the RIKEN Center for Sustainable Resource Science.

Researchers are searching for better alternatives to this approach. "It would be better to directly use dinitrogen and alkenes to synthesize alkyl amines under mild conditions," he adds. "But such a reaction was unknown and expected to be highly challenging."

Previously, Shima and his collaborators had discovered a way to overcome these challenges using titanium polyhydrides, which are chemical complexes of titanium atoms bridged by hydrogen atoms.

## Bulletin Board

## Gossip

SEP. 06, 2024

“We have found that titanium polyhydride exhibits extremely high reactivity toward stable small molecules such as dinitrogen and benzene,” says Shima.

Now, Shima and his team have shown that the multiple titanium–hydride units within titanium polyhydride can work cooperatively to generate alkyl amines from dinitrogen and alkenes.

“When we reacted alkenes with titanium polyhydride, the alkenes were activated—but many titanium–hydride units remained after the reaction,” Shima says.

When the team then added dinitrogen, the free titanium–hydride units cooperatively cleaved the dinitrogen molecule, and then clipped the activated carbon and nitrogen species together via a new nitrogen–carbon bond, producing the alkyl amine.

A computational analysis revealed that the key to the reaction is that after activating both substrates, the formation of nitrogen–carbon bonds selectively occurs in the titanium polyhydride framework. That is because the formation of nitrogen–carbon bonds is much more energetically favorable than other possible pathways, such as nitrogen–hydrogen or carbon–hydrogen bond formations.

Shima and his team are now exploring ways to turn this transformation into a catalytic process.

Phys Org, 5 September 2024

<https://phys.org>

### Hotter Than Lava: The Surprising Science of Molten Uranium

2024-09-04

Researchers at Oak Ridge National Laboratory have uncovered groundbreaking chemistry in molten uranium trichloride, challenging conventional knowledge and paving the way for advancements in nuclear reactor design and waste management.

The Department of Energy’s Oak Ridge National Laboratory is a world leader in molten salt reactor technology development — and its researchers additionally perform the fundamental science necessary to enable a future where nuclear energy becomes more efficient. In a recent paper published in the *Journal of the American Chemical Society*,

## Bulletin Board

## Gossip

SEP. 06, 2024

researchers have documented for the first time the unique chemistry dynamics and structure of high-temperature liquid uranium trichloride (UCl<sub>3</sub>) salt, a potential nuclear fuel source for next-generation reactors.

“This is a first critical step in enabling good predictive models for the design of future reactors,” said ORNL’s Santanu Roy, who co-led the study. “A better ability to predict and calculate the microscopic behaviors is critical to design, and reliable data help develop better models.”

#### The Push for Modern Nuclear Solutions

For decades, molten salt reactors have been expected to possess the capacity to produce safe and affordable nuclear energy, with ORNL prototyping experiments in the 1960s successfully demonstrating the technology. Recently, as decarbonization has become an increasing priority around the world, many countries have re-energized efforts to make such nuclear reactors available for broad use.

Ideal system design for these future reactors relies on an understanding of the behavior of the liquid fuel salts that distinguish them from typical nuclear reactors that use solid uranium dioxide pellets. The chemical, structural and dynamical behavior of these fuel salts at the atomic level are challenging to understand, especially when they involve radioactive elements such as the actinide series — to which uranium belongs — because these salts only melt at extremely high temperatures and exhibit complex, exotic ion-ion coordination chemistry.

#### High-Tech Tools for Advanced Material Insights

The research, a collaboration among ORNL, Argonne National Laboratory, and the University of South Carolina, used a combination of computational approaches and an ORNL-based DOE Office of Science user facility, the Spallation Neutron Source, or SNS, to study the chemical bonding and atomic dynamics of UCl<sub>3</sub> in the molten state.

The SNS is one of the brightest neutron sources in the world, and it allows scientists to perform state-of-the-art neutron scattering studies, which reveal details about the positions, motions, and magnetic properties of materials. When a beam of neutrons is aimed at a sample, many neutrons will pass through the material, but some interact directly with atomic nuclei and “bounce” away at an angle, like colliding balls in a game of pool.

Using special detectors, scientists count scattered neutrons, measure their energies and the angles at which they scatter, and map their final positions. This makes it possible for scientists to glean details about

## Bulletin Board

## Gossip

SEP. 06, 2024

the nature of materials ranging from liquid crystals to superconducting ceramics, from proteins to plastics, and from metals to metallic glass magnets.

**Breakthrough in Actinide Chemistry**

Each year, hundreds of scientists use ORNL's SNS for research that ultimately improves the quality of products from cell phones to pharmaceuticals — but not all of them need to study a radioactive salt at 900 degrees Celsius, which is as hot as volcanic lava. After rigorous safety precautions and special containment developed in coordination with SNS beamline scientists, the team was able to do something no one has done before: measure the chemical bond lengths of molten UCl<sub>3</sub> and witness its surprising behavior as it reached the molten state.

"I've been studying actinides and uranium since I joined ORNL as a postdoc," said Alex Ivanov, who also co-led the study, "but I never expected that we could go to the molten state and find fascinating chemistry."

What they found was that, on average, the distance of the bonds holding the uranium and chlorine together actually shrunk as the substance became liquid — contrary to the typical expectation that heat expands and cold contracts, which is often true in chemistry and life. More interestingly, among the various bonded atom pairs, the bonds were of inconsistent size, and they stretched in an oscillating pattern, sometimes achieving bond lengths much larger than in solid UCl<sub>3</sub> but also tightening to extremely short bond lengths. Different dynamics, occurring at ultra-fast speed, were evident within the liquid.

**Conclusions on Molten UCl<sub>3</sub> and Future Research Implications**

"This is an uncharted part of chemistry and reveals the fundamental atomic structure of actinides under extreme conditions," said Ivanov.

The bonding data were also surprisingly complex. When the UCl<sub>3</sub> reached its tightest and shortest bond length, it briefly caused the bond to appear more covalent, instead of its typical ionic nature, again oscillating in and out of this state at extremely fast speeds — less than one trillionth of a second.

This observed period of an apparent covalent bonding, while brief and cyclical, helps explain some inconsistencies in historical studies describing the behavior of molten UCl<sub>3</sub>. These findings, along with the broader results of the study, may help improve both experimental and computational approaches to the design of future reactors.

## Bulletin Board

## Gossip

SEP. 06, 2024

Moreover, these results improve fundamental understanding of actinide salts, which may be useful in tackling challenges with nuclear waste, pyroprocessing, and other current or future applications involving this series of elements.

Sci Tech Daily, 4 September 2024

<https://scitechdaily.com>

**Simple technique removes over 98% of nanoplastic particles from water**

2024-08-26

Microplastics. We've found them in the Arctic sea and even frozen into the ice. The Mariana Trench, the deepest part of all our oceans, is polluted with plastic debris. Mount Everest has microplastic contamination. Our drinking water and food, especially processed foods in single-use packaging, are contaminated with microplastics. Recent studies have found microplastics in our blood, lungs, liver, and kidneys ... They've even been found in the placentas of unborn babies.

Studies on the adverse health effects of microplastics in the human body have only recently been done. Respiratory, gastrointestinal, endocrine, developmental and reproductive issues, and even cancers are starting to be linked to the consumption and inhalation of microplastics. Micro and nanoplastics are inescapable. But now researchers from the University of Missouri have developed a relatively simple and safe method of extracting over 98% of nanoplastic particles from water.

Using non-toxic, hydrophobic natural ingredients, researchers were able to create a liquid solvent that floats atop water like oil. When emulsified into the water and then allowed to re-separate, the solvent will then float back to the surface carrying more than 98% of the nanoplastic contaminants back to the surface with it, where it can simply be skimmed off the water. Given its hydrophobic nature, there's little risk of leaving further contamination from the eutectic solvent behind.

"Our strategy uses a small amount of designer solvent to absorb plastic particles from a large volume of water," says Gary Baker, an associate professor in Mizzou's Department of Chemistry. "Currently, the capacity of these solvents is not well understood. In future work, we aim to determine the maximum capacity of the solvent. Additionally, we will explore methods to recycle the solvents, enabling their reuse multiple times if necessary."

# Bulletin Board

## Gossip

SEP. 06, 2024

We currently have some ways of removing microplastics from our drinking water, depending on the size. Basic activated carbon filters – like you'd find in a Britta – aren't specifically made to remove them, but are fairly effective at removing anything larger than five microns in size. Multi-stage sediment filters with a one-micron pore size are quite good. Reverse osmosis, which squeezes water through pores as small as one ten thousandth of a micron is one of the very best methods for removing contaminants of any sort from water – however, these become clogged and need to be cleaned regularly. Distilling water is nearly 100% effective, but also strips away any healthy minerals that our bodies need.

This new approach adds another arrow to the quiver, and works in both fresh and seawater.

The team's study was published in ACS Applied Engineering Materials.

New Atlas, 26 August 2024

<https://newatlas.com>

### **New process vaporizes plastic bags and bottles, yielding gases to make new, recycled plastics**

2024-08-29

A new chemical process can essentially vaporize plastics that dominate the waste stream today and turn them into hydrocarbon building blocks for new plastics.

The catalytic process, developed at the University of California, Berkeley, works equally well with the two dominant types of post-consumer plastic waste: polyethylene, the component of most single-use plastic bags; and polypropylene, the stuff of hard plastics, from microwavable dishes to luggage. It also efficiently degrades a mix of these types of plastics.

The process, if scaled up, could help bring about a circular economy for many throwaway plastics, with the plastic waste converted back into the monomers used to make polymers, thereby reducing the fossil fuels used to make new plastics. Clear plastic water bottles made of polyethylene terephthalate (PET), a polyester, were designed in the 1980s to be recycled this way. But the volume of polyester plastics is minuscule compared to that of polyethylene and polypropylene plastics, referred to as polyolefins.

"We have an enormous amount of polyethylene and polypropylene in everyday objects, from lunch bags to laundry soap bottles to milk jugs

# Bulletin Board

## Gossip

SEP. 06, 2024

-- so much of what's around us is made of these polyolefins," said John Hartwig, a UC Berkeley professor of chemistry who led the research. "What we can now do, in principle, is take those objects and bring them back to the starting monomer by chemical reactions we've devised that cleave the typically stable carbon-carbon bonds. By doing so, we've come closer than anyone to give the same kind of circularity to polyethylene and polypropylene that you have for polyesters in water bottles."

Hartwig, graduate student Richard J. "RJ" Conk, chemical engineer Alexis Bell, who is a UC Berkeley Professor of the Graduate School, and their colleagues will publish the details of the catalytic process in the xx issue of the journal Science.

### **A circular economy for plastics**

Polyethylene and polypropylene plastics constitute about two-thirds of post-consumer plastic waste worldwide. About 80% ends up in landfills, is incinerated or simply tossed into the streets, often ending up as microplastics in streams and the ocean. The rest is recycled as low-value plastic, becoming decking materials, flowerpots and sporks.

To reduce this waste, researchers have been looking for ways to turn the plastics into something more valuable, such as the monomers that are polymerized to produce new plastics. This would create a circular polymer economy for plastics, reducing the need to make new plastics from petroleum, which generates greenhouse gases.

Two years ago, Hartwig and his UC Berkeley team came up with a process for breaking down polyethylene plastic bags into the monomer propylene -- also called propene -- that could then be reused to make polypropylene plastics. This chemical process employed three different bespoke heavy metal catalysts: one to add a carbon-carbon double bond to the polyethylene polymer and the other two to break the chain at this double bond and repeatedly snip off a carbon atom and, with ethylene, make propylene (C<sub>3</sub>H<sub>6</sub>) molecules until the polymer disappeared. But the catalysts were dissolved in the liquid reaction and short-lived, making it hard to recover them in an active form.

In the new process, the expensive, soluble metal catalysts have been replaced by cheaper solid ones commonly used in the chemical industry for continuous flow processes that reuse the catalyst. Continuous flow processes can be scaled up to handle large volumes of material.

## Bulletin Board

## Gossip

SEP. 06, 2024

Conk first experimented with these catalysts after consulting with Bell, an expert on heterogeneous catalysts, in the Department of Chemical and Biomolecular Engineering.

Synthesizing a catalyst of sodium on alumina, Conk found that it efficiently broke or cracked various kinds of polyolefin polymer chains, leaving one of the two pieces with a reactive carbon-carbon double bond at the end. A second catalyst, tungsten oxide on silica, added the carbon atom at the end of the chain to ethylene gas, which is constantly streamed through the reaction chamber to form a propylene molecule. The latter process, called olefin metathesis, leaves behind a double bond that the catalyst can access again and again until the entire chain has been converted to propylene.

The same reaction occurs with polypropylene to form a combination of propene and a hydrocarbon called isobutylene. Isobutylene is used in the chemical industry to make polymers for products ranging from footballs to cosmetics and to make high-octane gasoline additives.

Surprisingly, the tungsten catalyst was even more effective than the sodium catalyst in breaking polypropylene chains.

"You can't get much cheaper than sodium," Hartwig said. "And tungsten is an earth-abundant metal used in the chemical industry in large scale, as opposed to our ruthenium metal catalysts that were more sensitive and more expensive. This combination of tungsten oxide on silica and sodium on alumina is like taking two different types of dirt and having them together disassemble the whole polymer chain into even higher yields of propene from ethylene and a combination of propene and isobutylene from polypropylene than we did with those more complex, expensive catalysts."

#### Like a string of pearls

One key advantage of the new catalysts is that they avoid the need to remove hydrogen to form a breakable carbon-carbon double bond in the polymer, which was a feature of the researchers' earlier process to deconstruct polyethylene. Such double bonds are an Achilles heel of a polymer, in the same way that the reactive carbon-oxygen bonds in polyester or PET make the plastic easier to recycle. Polyethylene and polypropylene don't have this Achilles heel -- their long chains of single carbon bonds are very strong.

## Bulletin Board

## Gossip

SEP. 06, 2024

"Think of the polyolefin polymer like a string of pearls," Hartwig said. "The locks at the end prevent them from falling out. But if you clip the string in the middle, now you can remove one pearl at a time."

The two catalysts together turned a nearly equal mixture of polyethylene and polypropylene into propylene and isobutylene -- both gases at room temperature -- with an efficiency of nearly 90%. For polyethylene or polypropylene alone, the yield was even higher.

Conk added plastic additives and different types of plastics to the reaction chamber to see how the catalytic reactions were affected by contaminants. Small amounts of these impurities barely affected the conversion efficiency, but small amounts of PET and polyvinyl chloride -- PVC -- significantly reduced the efficiency. This may not be a problem, however, because recycling methods already separate plastics by type.

Hartwig noted that while many researchers are hoping to redesign plastics from the ground up to be easily reused, today's hard-to-recycle plastics will be a problem for decades.

"One can argue that we should do away with all polyethylene and polypropylene and use only new circular materials. But the world's not going to do that for decades and decades. Polyolefins are cheap, and they have good properties, so everybody uses them," Hartwig said. "People say if we could figure out a way to make them circular, it would be a big deal, and that's what we've done. One can begin to imagine a commercial plant that would do this."

Other co-authors of the paper are graduate students Jules Stahler, Jake Shi, Natalie Lefton and John Brunn of UC Berkeley and Ji Yang of Lawrence Berkeley National Laboratory. Shi, Hartwig and Bell are also affiliated with Berkeley Lab. The work was funded by the Department of Energy (DE-AC02-05CH11231).

Science Daily, 29 August 2024

<https://sciencedaily.com>

#### New filter removes chemical contaminants from water even at very low concentrations

2024-09-05

Pharmaceuticals and personal care products pose a major environmental threat. These chemicals, found in everyday items like medicines and

# Bulletin Board

## Gossip

SEP. 06, 2024

cosmetics, can pollute waterways, harming the plants and animals living in the waterways and the humans who use the water.

The pollutants are often present at very low concentrations, and existing filtration methods aren't always selective enough to remove the chemicals that cause environmental damage.

A team of researchers from Japan and the United States, led by Professor Shuhei Furukawa from the Institute for Integrated Cell-Material Sciences (WPI-iCeMS) at Kyoto University, have developed a new method for removing these chemicals from water.

"Current workflows for water treatment involve steps for pollutant detection and pollutant removal, and the two steps are normally conducted separately through different materials or industrial set-up," explains Professor Furukawa. "We developed new membrane materials that can simultaneously detect and remove trace-level pollutants."

The new approach uses a polymer membrane that houses an interconnected network of pores constructed from metal-organic polyhedra, which are like tiny cages to filter and capture the targeted chemical molecules.

The design of the pores is critical to the effectiveness of the membrane. The chemicals in pharmaceuticals and personal care products are relatively large, and most current adsorbents have pores that are too small to capture these molecules.

The researchers tested the pore-networked membrane against 13 different pharmaceuticals and personal care products at different concentrations, and they compared its performance to a variety of existing filtration systems.

They found that the new membrane was better at filtering out these chemicals than existing systems, and it could also be refined to selectively adsorb particular pharmaceutical products, even at incredibly low concentrations.

The findings are published in the journal *Communications Materials*.

"An optimized pore-networked membrane detected and removed target drugs below the parts-per-billion level in real water samples, demonstrating the potential for its use in real water-treatment workflows," says Dr. Idaira Pacheco-Fernández, an environmental scientist from WPI-iCeMS, Kyoto University, who contributed to this project for water analysis.

# Bulletin Board

## Gossip

SEP. 06, 2024

The new membrane is also designed so the captured molecules can be extracted into solution for testing, enabling real-time monitoring of contamination.

The next step for the researchers is to vary the pore-networked membrane design by using other types of porous fillers which could filter out different types and sizes of molecules. They're also interested in whether this approach could capture and detect small molecules from other liquids, such as blood.

Phys Org, 5 September 2024

<https://phys.org>

### Revolutionizing Recycling: New Technique Turns Plastic Waste Into Wealth

2024-08-30

Chemical recycling offers a sustainable alternative to traditional plastic recycling by breaking down plastics into high-quality products. Researchers have optimized this process with a new mathematical formula.

Each year, hundreds of millions of tons of plastic waste are produced globally. In response, scientists are diligently developing innovative methods to recycle a significant portion of this waste into high-quality products, aiming to create a truly circular economy.

However, current recycling practices fall short of this goal. Most plastic waste is recycled mechanically: shredded and then melted down. Although this process does result in new plastic products, their quality deteriorates with each recycling step.

An alternative to this is chemical recycling, which avoids loss of quality. This method involves breaking down long-chain plastic molecules (polymers) into their fundamental building blocks (monomers), which can be reassembled into new, high-quality plastics, creating a truly sustainable cycle.

#### Fuels from plastic waste

As the approach of chemical recycling develops, the initial focus is on breaking down these long polymer chains into shorter-chain molecules that can be used as liquid fuels, say, or lubricants. This gives plastic waste a second life as petrol, jet fuel, or engine oil. Scientists at ETH Zurich have



# Bulletin Board

## Gossip

SEP. 06, 2024

now laid down important foundations for developing this process. These enable the global scientific community to engage in more targeted and effective recycling development work.

Researchers in the group led by Javier Pérez-Ramírez, Professor of Catalysis Engineering, investigated how to break down polyethylene and polypropylene with hydrogen. Here, too, the first step is to melt the plastic in a steel tank. Gaseous hydrogen is then introduced into the molten plastic.

A crucial step involves adding a powdered catalyst containing metals such as ruthenium. By carefully selecting a suitable catalyst, researchers can increase the efficiency of the chemical reaction, promoting the formation of molecules with specific chain lengths while minimizing byproducts such as methane or propane.

### Rotational speed and geometry are key

“The molten plastic is a thousand times thicker than honey. The key is how you stir it in the tank to ensure the catalyst powder and hydrogen get mixed right through,” explains Antonio José Martín, a scientist in Pérez-Ramírez’s group. Through experiments and computer simulations, the research team demonstrated that the plastic is best stirred using an impeller with blades parallel to the axis. Compared to a propeller with angled blades or a turbine-shaped stirrer, this results in more even mixing and fewer flow vortices. The stirring speed is equally crucial. It must be neither too slow nor too fast; the ideal speed is close to 1,000 revolutions per minute.

The researchers successfully developed a mathematical formula to describe the entire chemical recycling process with all its parameters. “It’s every chemical engineer’s dream to have a formula like this at hand for their process,” Pérez-Ramírez says. All scientists in the research field can now precisely calculate the effect of the stirrer’s geometry and speed.

With this formula, future experiments can focus on directly comparing different catalysts with the influence of mixing under control. In addition, the principles developed here are central for scaling up the technology from the laboratory to large recycling plants. “But for now, our focus remains on researching better catalysts for the chemical recycling of plastics,” Martín says.

Sci Tech Daily, 30 August 2024

<https://scitechdaily.com>

# Bulletin Board

## Gossip

SEP. 06, 2024

### Finger wrap uses sweat to provide health monitoring at your fingertips--literally

2024-09-03

A sweat-powered wearable has the potential to make continuous, personalized health monitoring as effortless as wearing a Band-Aid. Engineers at the University of California San Diego have developed an electronic finger wrap that monitors vital chemical levels -- such as glucose, vitamins, and even drugs -- present in the same fingertip sweat from which it derives its energy.

The advance was published Sept. 3 in Nature Electronics by the research group of Joseph Wang, a professor in the Aiiso Yufeng Li Family Department of Chemical and Nano Engineering at UC San Diego.

The device, which wraps snugly around the finger, draws power from an unlikely source -- the fingertip’s sweat. Fingertips, despite their small size, are among the body’s most prolific sweat producers, each packed with over a thousand sweat glands. These glands can produce 100 to 1000 times more sweat than most other areas of the body, even during rest. This constant trickle of natural perspiration -- without any stimuli or physical activity -- offers a reliable energy source, fueling the device even during periods of inactivity or sleep.

The device is constructed from several electronic components printed onto a thin, flexible and stretchable polymer material. Its design allows it to conform to the finger while being durable enough to withstand repeated bending, stretching and movement. “It is based on a remarkable integration of energy harvesting and storage components, with multiple biosensors in a fluidic microchannel, along with the corresponding electronic controller, all at the fingertip,” said Wang.

Central to its operation are biofuel cells that are positioned where the device contacts the fingertip. These cells have been specially engineered to efficiently collect and convert chemicals in sweat into electricity. This electricity is stored in a pair of stretchable, silver chloride-zinc batteries, which power a suite of sensors -- four in total -- each tasked with monitoring a specific biomarker: glucose, vitamin C, lactate and levodopa, a drug used for treating Parkinson’s disease. As sweat is wicked through tiny paper microfluidic channels to these sensors, the device analyzes the biomarker levels, all while drawing energy it needs from the very sweat it’s sampling. A small chip processes signals from the sensors and wirelessly

## Bulletin Board

## Gossip

SEP. 06, 2024

transmits the data via Bluetooth low energy to a custom-designed smartphone or laptop application.

“This is automatic health monitoring at your fingertips,” said study co-first author Shichao Ding, a postdoctoral researcher in Wang’s research group at the UC San Diego Jacobs School of Engineering. “The wearer can be resting or asleep, and the device can still harvest energy and track biomarker levels.”

In tests, a subject wore the device throughout the day to track glucose levels during meals, lactate levels during both desk work and exercise, vitamin C levels while drinking orange juice, and levodopa levels after eating fava beans, a natural source of the compound.

Ding and co-first author Tamoghna Saha say that the device can be customized to cater to individual health needs by detecting different sets of biomarkers. The researchers are working on developing a closed-loop system that not only monitors biomarkers, but also administers treatments based on the collected data. For instance, in the case of diabetes, such a device could continuously monitor glucose levels and automatically deliver insulin as needed, then assess the treatment’s effectiveness by further monitoring biomarker levels.

“Autonomous power, sensing and treatment all in one device -- that’s the ultimate goal,” said Ding.

Science Daily, 3 September 2024

<https://sciencedaily.com>

### Novel glass-forming liquid electrolyte shows glass transition across broad range

2024-09-04

As the world shifts towards a more sustainable future, the development of advanced electrochemical devices, such as rechargeable batteries with higher energy densities and efficient electrodeposition capabilities, has become increasingly crucial. In recent years, ultra-concentrated electrolyte solutions, where metal salts are dissolved at concentrations two to three times higher than those in a single solvent, or mixtures where metal salts are excessively dissolved in a single solvent, have gained attention as new electrolyte solutions.

These solutions remain liquid at room temperature and enable high ion conduction and high-efficiency, high-quality metal film formation.

## Bulletin Board

## Gossip

SEP. 06, 2024

However, the physicochemical or thermodynamic definition of these liquids remains unclear. Moreover, identifying the dissolved species and understanding their structures, which are crucial for their use as electrolytes, is extremely challenging.

A research team from Niigata University, led by Prof. Yasuhiro Umabayashi and Dr. Jihae Han, along with Dr. Hikari Watanabe from Tokyo University of Science, from a solution chemistry perspective, has been studying the mechanisms of specific lithium-ion conduction in lithium solvate ionic liquids and highly concentrated electrolyte solutions. They found a novel glass-forming liquid electrolyte, a two-component mixture of cyclic sulfone and lithium salt, which exhibits a glass transition across a broad compositional range.

Furthermore, to elucidate the uniquely high Li<sup>+</sup> transference number in these mixtures, speciation and dipole reorientation dynamics were studied to provide evidence of large-size aggregate formation in these mixtures. These findings have been published in the Faraday Discussions on 10 June 2024.

The thermophysical properties of both lithium salt-1,3-propanesultone (PS) and lithium salt-sulfolane (SL) binary mixtures showed that only glass transition was observed in a certain lithium salt concentration range. Raman spectroscopy revealed that lithium ions exist in solution as contact ion pairs (CIPs) and aggregates (AGG) in solution.

In addition, two-dimensional correlation analysis of Raman spectra and dielectric relaxation spectra (DRS) successfully attributed the observed relaxation in DRS. It suggests that AGGs generated at high lithium salt concentration have a large spatial scale and play an important role in the specific lithium-ion conduction.

To achieve the Sustainable Development Goals (SDGs) and the objectives of Society-5, there is a growing demand for next-generation energy storage devices that can store electric energy efficiently and are tailored for specific applications. The development of these devices, utilizing both liquid and solid electrolytes, has become more advanced.

“Our research into glass-formed liquid electrolytes marks a significant leap towards bridging the gap between traditional liquid and solid electrolytes,” explains Professor Yasuhiro Umabayashi, the corresponding author. “These materials offer unique advantages in terms of efficiency and application-

# Bulletin Board

## Gossip

SEP. 06, 2024

specific adaptability, paving the way for next-generation energy storage devices.”

Phys Org, 4 September 2024

<https://phys.org>

# Bulletin Board

## Curiosities

SEP. 06, 2024

### Giant gold nuggets could be born from earthquakes and electricity

2024-09-02

Stumbling on a giant gold nugget and never working again is something we've all daydreamed about, but how exactly do they form? A new experiment has found that earthquakes and electricity might be key ingredients.

Gold doesn't form here on Earth – it's thought to be forged in supernovae and collisions between neutron stars. These cataclysms then scatter it through the cosmos, so the shiny stuff then turns up in the dusty discs from which planets form. As such, trace amounts of gold have been present on Earth for billions of years. The heavy element sinks deep into the planet, but seismic activity can push it back up near the surface, while asteroid strikes can deliver more.

Most of the time, gold takes the form of small flakes, but on rare occasions it can form larger nuggets weighing up to a few dozen kilograms. Exactly how it clumps together into these nuggets remains a bit of a mystery.

“The standard explanation is that gold precipitates from hot, water-rich fluids as they flow through cracks in the Earth's crust,” said Dr. Chris Voisey, lead author of the study. “As these fluids cool or undergo chemical changes, gold separates out and becomes trapped in quartz veins. While this theory is widely accepted, it doesn't fully explain the formation of large gold nuggets, especially considering that the concentration of gold in these fluids is extremely low.”

For the new study, researchers at Monash University investigated a new suspect you might not expect: electricity. Quartz is piezoelectric, meaning it produces an electric charge when mechanical stress is applied, a phenomenon that's used in things like watches and lighters. The team wondered if this effect could be causing gold to clump together into nuggets, with the mechanical stress coming from earthquakes.

To test the idea, the researchers submerged quartz crystals in a fluid that was rich in gold, then used a motor to simulate the kind of stress the mineral might experience from earthquakes. Afterwards, they used a microscope to check the growth of gold.

“The results were stunning,” said Professor Andy Tomkins, co-author of the study. “The stressed quartz not only electrochemically deposited gold onto its surface, but it also formed and accumulated gold nanoparticles.”

# Bulletin Board

## Curiosities

SEP. 06, 2024

Remarkably, the gold had a tendency to deposit on existing gold grains rather than forming new ones."

The key seems to be that quartz is an insulator, while gold is famously a great conductor of electricity. Each of these little piezoelectric zaps pulls more dissolved gold out of the surrounding fluids to settle on the grains already there.

"In essence, the quartz acts like a natural battery, with gold as the electrode, slowly accumulating more gold with each seismic event," said Dr. Voisey. "Our discovery provides a plausible explanation for the formation of large gold nuggets in quartz veins."

The research was published in the journal Nature Geoscience.

**Source:** Monash University via Scimex

New Atlas, 2 September 2024

<https://newatlas.com>

### An Over-the-Counter Pain & Fever Medicine Has Been Recalled Nationwide

2024-09-03

The pills were labeled with the wrong drug facts, according to the FDA, which could lead to overdose or other complications.

It's reported a drug maker based in Illinois is scrambling to reach customers after a labeling mixup that could put some consumers in danger.

If you typically turn to Tylenol or any other brand of acetaminophen products to relieve your pain, you'll want to check some details. The US Food and Drug Administration (FDA) has announced that Libertyville, IL-based A-S Medication Solutions LLC is working via email, fax, letter, telephone calls, and in-person visits to alert buyers that their 500 milligram acetaminophen pain reliever may have been mislabeled with drug facts that represent those of 81 milligram aspirin, also commonly referred to as "baby aspirin."

This affects 429 bottles of acetaminophen product that were distributed nationwide with the reported lot code 4138197 and expiration date of 10/31/2025. While no specific retailer is named as the seller(s), this follows a 2021 recall for nearly 200,000 bottles of acetaminophen made by the

# Bulletin Board

## Curiosities

SEP. 06, 2024

same company that USA Today reported had been distributed to Humana health plan members.

So what's the danger of mixing up aspirin and the active ingredient in Tylenol? A big one is dosage. Five hundred milligrams of acetaminophen tends to be a generous dose, with higher dosages typically requiring prescription. One reason is that the drug can be hard on the liver. A consumer who reads the bottle and believes they're taking only 81 milligrams, as baby aspirin labels suggest, could easily try to multiply that dosage to get faster or more effective pain relief, only to overdose.

Another difference between the two, as the University of Tennessee Medical Center explains, is that aspirin is an anti-inflammatory. In contrast, acetaminophen's mechanism is not to minimize inflammation, but instead to alter how the body perceives pain.

The recall was originally initiated in June 2024, but this week the FDA has given it a Class I risk level, meaning using the drug could lead to serious health consequences or death.

The Healthy, 3 September 2024

<https://thehealthy.com>

### Weight Loss Drug Shows Potential Benefit for Type 2 Diabetes

2024-08-22

Researchers at the University of Liverpool have found that the weight loss drug, Tirzepatide is associated with significantly reduced risk of developing type 2 diabetes (T2D).

Obesity is a major worldwide health concern. Current global estimates of the number of adults living with obesity is at 650 million, with a further 340 million children and adolescents. Overweight and obesity represent the primary risk factors for the development of T2D, with T2D driving excess morbidity and mortality.

The study published in The Lancet's eClinicalMedicine used anonymised electronic medical records from a global federated database. Two cohorts of individuals were generated from this data; group one was those without pre-existing T2D, the second with T2D. Using real world data, Tirzepatide was tested in comparison to another weight loss drug, Semaglutide.

# Bulletin Board

## Curiosities

SEP. 06, 2024

Compared to Semaglutide, Tirzepatide was found to be associated with significantly reduced risk of developing T2D in people living with obesity, and a reduction in major adverse cardiovascular events in people with T2D.

Dr Uazman Alam, Diabetes & Obesity Research, Institute of Life Course and Medical Sciences, University of Liverpool and Liverpool University Hospital NHS Foundation Trust said: "Around 1 in every 4 adults is living with obesity which is a major risk factor for diabetes. Around 4 million people have type 2 diabetes in the UK, with diabetes complications costing £6.2 billion a year for the UK healthcare system. These findings are incredibly positive in helping us address this significant health challenge."

Dr Matthew Anson, Clinical Research Fellow, University of Liverpool added: "In part, weight loss as a result of the drug may have played a role in the reduction of developing type 2 diabetes and also reducing cardiovascular complications. Now, definitive randomised control trials are needed to better understand how Tirzepatide could be used to prevent T2D in a population at higher risk of developing it."

Technology Networks, 22 August 2024

<https://technologynetworks.com>

### Molecular 'cage' approach could advance selective elimination of cancer cells

2024-09-04

Chemotherapy saves the lives of cancer patients. However, these treatments are not without side effects and other limitations, which encourages basic research to focus on these challenges. A recent study published in Cell Reports Physical Science, which proposes the use of molecular "cages" (made of pseudopeptides) to selectively eliminate cancer cells in acidic microenvironments.

To achieve this, an extensive study was conducted using a broad family of "cages" to understand how they act. This research was led by a scientific team from the Institute for Advanced Chemistry of Catalonia (IQAC-CSIC) of the Spanish National Research Council (CSIC), in collaboration with the University of Burgos and with the participation of the Institute of Environmental Assessment and Water Studies (IDAEA-CSIC).

# Bulletin Board

## Curiosities

SEP. 06, 2024

These results are relevant for the preclinical development of new ionophores (ion-transporting molecules) with potential therapeutic applications in cancer treatment.

### Challenges in the fight against cancer

Chemotherapy against cancer faces two main challenges: lack of selectivity, which causes undesirable side effects, and the emergence of chemoresistance, since cells can develop resistance to the chemical agents used in chemotherapy, rendering ineffective treatments for some patients.

Additionally, one characteristic of cancer cells is that their metabolism creates an acidic pH in the environment of solid tumors. This gives these cells special characteristics, making them more resistant and capable of migrating to other areas of the body (a process known as metastasis).

There is increasing evidence of the potential of ionophores (ion-transporting molecules) as new chemotherapeutic agents in cancer. However, controlling their activity to limit toxicity has become a challenge so far. The use of molecular "cages" that selectively act in the slightly acidic pH of the solid tumor microenvironment is a way to overcome these hurdles and advance their development.

### Molecular 'cages' to eliminate cancer cells

These "cages," derived from fluorine-substituted amino acids, kill cancer cells at slightly acidic pH levels (below 7, as observed around tumors), but are harmless at the physiological pH of healthy tissues.

"In a previous study published in 2019, we designed a molecule with a three-dimensional 'cage' structure that showed good selectivity for killing cancer cells in slightly acidic environments," explains Ignacio Alfonso, a researcher at IQAC-CSIC and the lead author of the study.

These "cages" had a fluorine atom at each of the three side chains and efficiently encapsulated a chloride ion in acidic environments. Furthermore, they were able to transport chloride across lipid bilayers, and this transport was more efficient when there was a pH gradient with an acidic environment, making them more toxic to cells in a slightly acidic pH, like the microenvironment of a solid tumor.

"In this work, we wanted to go one step further and understand the mechanism of action of these molecules," explains the IQAC-CSIC researcher.

# Bulletin Board

## Curiosities

SEP. 06, 2024

“For this, we have conducted an exhaustive study with a broad family of ‘cages’ with different numbers of fluorine atoms in various positions to understand the chloride capture capacity, the transport process, and the toxicity at different pHs in cell cultures,” Alfonso clarifies.

The process has been extensively studied at the molecular level using cutting-edge theoretical and experimental approaches (fluorescence, nuclear magnetic resonance, and computational studies). The results showed the effect of fluorine on these molecules and, therefore, have allowed researchers to understand the mechanism of action and the identification of a cage with even higher selectivity to kill cancer cells in acidic environments.

“These results will help to understand and improve the design of these ionophores with potential therapeutic applications in cancer treatment,” concludes Roberto Quesada, a researcher at the University of Burgos.

Phys Org, 4 August 2024

<https://phys.org>

### Hydrogen stored in iron: A cheap, scalable grid battery for the winter

2024-08-30

While hydrogen’s high energy per mass makes it an excellent fuel, it’s awfully hard and expensive to store long-term. That could change, thanks to the work of researchers at Switzerland’s ETH Zurich. They’ve worked out a way to store hydrogen in ordinary steel-walled containers for months without losing it into the atmosphere – using iron.

#### Discovering solutions in the past

The research team led by Wendelin Stark, Professor of Functional Materials at ETH Zurich, hit upon this method by drawing from the steam-iron process of producing hydrogen, first invented in 1784.

The group’s storage solution is especially suitable in places like Switzerland, where solar power is abundant in the summer, and scarce in the winter.

Surplus solar power is used to split water to produce hydrogen in the summer; it’s then streamed into stainless steel reactors filled with iron ore at 752 °F (400 °C). The hydrogen extracts oxygen from the iron oxide,

# Bulletin Board

## Curiosities

SEP. 06, 2024

so you’re left with iron and water in the reactor, ready to store without expending a lot of energy.

Steam is fed into the reactor to retrieve the stored hydrogen when needed; it can then be converted into electricity or heat easily enough.

There are also several other advantages of using this method:

- The iron ore used in the reactors is cheap, plentiful, and doesn’t require processing.
- The reactors themselves are simply made of stainless steel.
- The charging process occurs at ambient pressure – negating the need for high pressure tanks (350-700 bar) typically necessary to store hydrogen gas.

#### Testing a centuries-old idea

The research team piloted its tech on ETH’s Hönggerberg campus, using three stainless steel reactors. Each of them have a capacity of 1.4 cubic meters, and are filled with 2-3 tons of iron ore. The test plant can store about 10 megawatt hours of hydrogen for extended periods, and that’ll yield between 4-6 megawatt hours of electrical energy. That’s enough to run three to five Swiss homes in the winter. The pilot project is set to grow by 2026, with the team looking to meet one-fifth of the winter electricity needs of the campus using solar power from summer months.

According to the team’s research paper published last November, utilizing this system for a single home is currently more expensive than powering it with electricity from the grid. Scaling it up to 100 homes brings the energy cost nearly in line with that of the grid, and it’s estimated that it’ll only get cheaper as the system expands.

#### Powering Switzerland and beyond

The researchers note that expanding storage capacity just means adding more reactors, with the processing material serving its charging-discharging cycle duties for years before it needs to be replaced.

In order to provide all of Switzerland with power through the winter months, the team estimates that you’ll need about 15–20 TWh of green hydrogen a year, and roughly 10,000,000 cubic meters of iron ore (or 2% of what Australia’s iron mines produce).

You’ll also need about 10,000 reactor systems, each capable of storing 1GWh. That works out to an area of land equivalent to about 1 square meter per inhabitant of Switzerland.

# Bulletin Board

## Curiosities

SEP. 06, 2024

It's hard to arrive at a clear leveled cost of storage from this small pilot project. And while Switzerland plans to go solar for more than 40% of its electricity needs by 2050, we don't know if it'll invest in hydrogen storage at a national scale. Still, this clever technology from hundreds of years ago seems promising for our seasonal energy requirements in the future.

**Source:** ETH Zurich

New Atlas, 30 September 2024

<https://newatlas.com>

### Assorted, distinctive behavior of molten uranium salt revealed by neutrons

2024-09-03

The Department of Energy's Oak Ridge National Laboratory is a world leader in molten salt reactor technology development -- and its researchers additionally perform the fundamental science necessary to enable a future where nuclear energy becomes more efficient. In a recent paper published in the *Journal of the American Chemical Society*, researchers have documented for the first time the unique chemistry dynamics and structure of high-temperature liquid uranium trichloride (UCl<sub>3</sub>) salt, a potential nuclear fuel source for next-generation reactors.

"This is a first critical step in enabling good predictive models for the design of future reactors," said ORNL's Santanu Roy, who co-led the study. "A better ability to predict and calculate the microscopic behaviors is critical to design, and reliable data help develop better models."

For decades, molten salt reactors have been expected to possess the capacity to produce safe and affordable nuclear energy, with ORNL prototyping experiments in the 1960s successfully demonstrating the technology. Recently, as decarbonization has become an increasing priority around the world, many countries have re-energized efforts to make such nuclear reactors available for broad use.

Ideal system design for these future reactors relies on an understanding of the behavior of the liquid fuel salts that distinguish them from typical nuclear reactors that use solid uranium dioxide pellets. The chemical, structural and dynamical behavior of these fuel salts at the atomic level are challenging to understand, especially when they involve radioactive elements such as the actinide series -- to which uranium belongs --

# Bulletin Board

## Curiosities

SEP. 06, 2024

because these salts only melt at extremely high temperatures and exhibit complex, exotic ion-ion coordination chemistry.

The research, a collaboration among ORNL, Argonne National Laboratory and the University of South Carolina, used a combination of computational approaches and an ORNL-based DOE Office of Science user facility, the Spallation Neutron Source, or SNS, to study the chemical bonding and atomic dynamics of UCl<sub>3</sub> in the molten state.

The SNS is one of the brightest neutron sources in the world, and it allows scientists to perform state-of-the-art neutron scattering studies, which reveal details about the positions, motions and magnetic properties of materials. When a beam of neutrons is aimed at a sample, many neutrons will pass through the material, but some interact directly with atomic nuclei and "bounce" away at an angle, like colliding balls in a game of pool.

Using special detectors, scientists count scattered neutrons, measure their energies and the angles at which they scatter, and map their final positions. This makes it possible for scientists to glean details about the nature of materials ranging from liquid crystals to superconducting ceramics, from proteins to plastics, and from metals to metallic glass magnets.

Each year, hundreds of scientists use ORNL's SNS for research that ultimately improves the quality of products from cell phones to pharmaceuticals -- but not all of them need to study a radioactive salt at 900 degrees Celsius, which is as hot as volcanic lava. After rigorous safety precautions and special containment developed in coordination with SNS beamline scientists, the team was able to do something no one has done before: measure the chemical bond lengths of molten UCl<sub>3</sub> and witness its surprising behavior as it reached the molten state.

"I've been studying actinides and uranium since I joined ORNL as a postdoc," said Alex Ivanov, who also co-led the study, "but I never expected that we could go to the molten state and find fascinating chemistry."

What they found was that, on average, the distance of the bonds holding the uranium and chlorine together actually shrunk as the substance became liquid -- contrary to the typical expectation that heat expands and cold contracts, which is often true in chemistry and life. More interestingly, among the various bonded atom pairs, the bonds were of inconsistent size, and they stretched in an oscillating pattern, sometimes achieving bond lengths much larger than in solid UCl<sub>3</sub> but also tightening to

# Bulletin Board

## Curiosities

SEP. 06, 2024

extremely short bond lengths. Different dynamics, occurring at ultra-fast speed, were evident within the liquid.

“This is an uncharted part of chemistry and reveals the fundamental atomic structure of actinides under extreme conditions,” said Ivanov.

The bonding data were also surprisingly complex. When the UCl<sub>3</sub> reached its tightest and shortest bond length, it briefly caused the bond to appear more covalent, instead of its typical ionic nature, again oscillating in and out of this state at extremely fast speeds -- less than one trillionth of a second.

This observed period of an apparent covalent bonding, while brief and cyclical, helps explain some inconsistencies in historical studies describing the behavior of molten UCl<sub>3</sub>. These findings, along with the broader results of the study, may help improve both experimental and computational approaches to the design of future reactors.

Moreover, these results improve fundamental understanding of actinide salts, which may be useful in tackling challenges with nuclear waste, pyroprocessing, and other current or future applications involving this series of elements.

The research was part of DOE's Molten Salts in Extreme Environments Energy Frontier Research Center, or MSEE EFRC, led by Brookhaven National Laboratory. The research was primarily conducted at the SNS and also used two other DOE Office of Science user facilities: Lawrence Berkeley National Laboratory's National Energy Research Scientific Computing Center and Argonne National Laboratory's Advanced Photon Source. The research also leveraged resources from ORNL's Compute and Data Environment for Science, or CADES.

Science Daily, 3 September 2024

<https://sciencedaily.com>

### Deadly Snail Venom Could Hold the Key to New Diabetes Treatments

2024-08-20

Scientists are finding clues for how to treat diabetes and hormone disorders in an unexpected place: a toxin from one of the most venomous animals on the planet.

# Bulletin Board

## Curiosities

SEP. 06, 2024

A multinational research team led by University of Utah scientists has identified a component within the venom of a deadly marine cone snail, the geography cone, that mimics a human hormone called somatostatin, which regulates the levels of blood sugar and various hormones in the body. The hormone-like toxin's specific, long-lasting effects, which help the snail hunt its prey, could also help scientists design better drugs for people with diabetes or hormone disorders, conditions that can be serious and sometimes fatal.

### A blueprint for better drugs

The somatostatin-like toxin the researchers characterized could hold the key to improving medications for people with diabetes and hormone disorders.

Somatostatin acts like a brake pedal for many processes in the human body, preventing the levels of blood sugar, various hormones, and many other important molecules from rising dangerously high. The cone snail toxin, called consomatin, works similarly, the researchers found—but consomatin is more stable and specific than the human hormone, which makes it a promising blueprint for drug design.

By measuring how consomatin interacts with somatostatin's targets in human cells in a dish, the researchers found that consomatin interacts with one of the same proteins that somatostatin does. But while somatostatin directly interacts with several proteins, consomatin only interacts with one. This fine-tuned targeting means that the cone snail toxin affects hormone levels and blood sugar levels but not the levels of many other molecules.

In fact, the cone snail toxin is more precisely targeted than the most specific synthetic drugs designed to regulate hormone levels, such as drugs that regulate growth hormone. Such drugs are an important therapy for people whose bodies overproduce growth hormone. Consomatin's effects on blood sugar could make it dangerous to use as a therapeutic, but by studying its structure, researchers could start to design drugs for endocrine disorders that have fewer side effects.

Consomatin is more specific than top-of-the-line synthetic drugs—and it also lasts far longer in the body than the human hormone, thanks to the inclusion of an unusual amino acid that makes it difficult to break down. This is a useful feature for pharmaceutical researchers looking for ways to make drugs that will have long-lasting benefits.

### Learning from cone snails



# Bulletin Board

## Curiosities

SEP. 06, 2024

Finding better drugs by studying deadly venoms may seem unintuitive, but Helena Safavi, PhD, associate professor of biochemistry in the Spencer Fox Eccles School of Medicine (SFESOM) at the University of Utah and the senior author on the study, explains that the toxins' lethality is often aided by pinpoint targeting of specific molecules in the victim's body. That same precision can be extraordinarily useful when treating disease.

"Venomous animals have, through evolution, fine-tuned venom components to hit a particular target in the prey and disrupt it," Safavi says. "If you take one individual component out of the venom mixture and look at how it disrupts normal physiology, that pathway is often really relevant in disease." For medicinal chemists, "it's a bit of a shortcut."

Consomatin shares an evolutionary lineage with somatostatin, but over millions of years of evolution, the cone snail turned its own hormone into a weapon.

For the cone snail's fishy prey, consomatin's deadly effects hinge on its ability to prevent blood sugar levels from rising. And importantly, consomatin doesn't work alone. Safavi's team had previously found that cone snail venom includes another toxin which resembles insulin, lowering the level of blood sugar so quickly that the cone snail's prey becomes nonresponsive. Then, consomatin keeps blood sugar levels from recovering.

"We think the cone snail developed this highly selective toxin to work together with the insulin-like toxin to bring down blood glucose to a really low level," says Ho Yan Yeung, PhD, a postdoctoral researcher in biochemistry in SFESOM and the first author on the study.

The fact that multiple parts of the cone snail's venom target blood sugar regulation hints that the venom could include many other molecules that do similar things. "It means that there might not only be insulin and somatostatin-like toxins in the venom," Yeung says. "There could potentially be other toxins that have glucose-regulating properties too." Such toxins could be used to design better diabetes medications.

It may seem surprising that a snail is able to outperform the best human chemists at drug design, but Safavi says that the cone snails have evolutionary time on their side. "We've been trying to do medicinal chemistry and drug development for a few hundred years, sometimes badly," she says. "Cone snails have had a lot of time to do it really well."

# Bulletin Board

## Curiosities

SEP. 06, 2024

Or, as Yeung puts it, "Cone snails are just really good chemists."

Technology Networks, 20 August 2024

<https://technologynetworks.com>

### Low-energy electrons in cosmic ice spring surprise by generating prebiotic molecules

2024-09-02

Electrons likely play a much more significant role than photons in the synthesis of prebiotic molecules in space, according to findings out of Wellesley College, US, presented at the recent American Chemical Society meeting in Denver. The work, which was discussed by undergraduate student Kennedy Barnes, explores the relative importance of low-energy electrons versus photons in initiating the chemical reactions responsible for the extraterrestrial synthesis of the molecules that could have helped spawn the first living organisms.

Previous research in this area has indicated that both electrons and photons can catalyse the same reactions, but this study suggests that the prebiotic molecule yield from low-energy electrons and photons could be significantly different in space. The Wellesley College team's calculations suggest that the number of cosmic-ray-induced electrons within interstellar ice could be much greater than the number of photons striking this ice. This indicates that electrons play a more significant role than photons in the extraterrestrial synthesis of prebiotic molecules such as the amino acid glycine, which was detected on comet 67P in 2016. Other examples of such prebiotic molecules include glycolaldehyde, the simplest monosaccharide sugar and a precursor to ribose, and glycerol phosphates, which serve as the backbone for phospholipids and are critical components of cell membranes.

The team, spearheaded by Barnes with fellow undergraduate Rong Wu and mentored by team leaders Christopher Arumainayagam and physicist James Battat, demonstrated for the first time that high-energy galactic cosmic rays can trigger a cascade of low-energy secondary electrons that could be a significant contributor to the interstellar synthesis of prebiotic molecules. These molecules could even have been brought to Earth via comets, meteorites and interplanetary dust particles and may have kick-started the development of life.

Barnes notes that there is a debate in the astrochemistry community about how important these low-energy electrons are and whether they

## Bulletin Board

## Curiosities

SEP. 06, 2024

are really doing any chemistry. 'There are a lot of people who said no, and so we did calculations to show that there is sufficient energy for these electrons to do a lot of chemistry and potentially create these complex organic molecules that have been detected,' she says.

Arumainayagam agrees that the chemistry happening here is special. 'What we are talking about is not electrons hitting the ices, but rather cosmic rays travelling through these ices, producing a cascade of low energy that's less than 20eV electrons which go on to create new molecules, and that's where the chemistry is,' he says.

'It started off with us wanting to investigate the difference between radiation chemistry – the chemistry from electrons – and the photochemistry – the chemistry induced by photons,' Barnes recalls. The researchers were able to simulate the conditions of interstellar space to compare the impact of low energy electrons with photons, thanks in part to an electron gun that Barnes installed to do the first experiments with water ices in an ultra-high vacuum chamber.

'What's neat about this vacuum chamber is that we can cool down our substrate to 10K – that is the temperature of the ices that are found in pre-stellar-cores in the interstellar medium,' Arumainayagam explains. He calls pre-stellar cores the birthplace of stars, as well as molecules.

More recently, the Wellesley team has also found separate and, as yet, unpublished evidence of low-energy electron-stimulated formation of hydrogen peroxide and hydroperoxyl radicals in these cosmic ices. Hydrogen peroxide has been identified on the surface of Jupiter's moon Europa, Arumainayagam notes, but his group's experiments suggest that it should also be there in the gas phase. That could be confirmed in a few years when Nasa's Europa Clipper mission arrives at the Jupiter system in 2030.

The researchers hope their findings will inspire colleagues to incorporate low-energy electrons into their astrochemistry models that simulate what happens within cosmic ices. 'Right now, a lot of the models are over-simplified, and I think a lot of that has to do with computational power,' Barnes tells Chemistry World. 'But these low-energy electrons can do important chemistry and I think there's a huge gap in the simulations by not incorporating them.'

Paul Rimmer, a prebiotic and atmospheric chemist at the University of Cambridge, is enthusiastic about the work. 'What I find especially interesting is Kennedy Barnes's experimental work, actually shooting a

## Bulletin Board

## Curiosities

SEP. 06, 2024

beam of low-energy electrons on interstellar ice analogues to find out what happens,' he says. Rimmer says Barnes is 'completely correct' that these interactions are understudied, though he notes that the work has not yet been published or peer reviewed. 'The specific reproducible results, whatever they turn out to be, could be of significant interest both for astrochemistry and prebiotic chemistry. I will watch this space.'

Chemistry World, 2 September 2024

<https://chemistryworld.com>

### How fish guts might play a role in future skin care products

2024-09-05

There are some pretty strange ingredients in cosmetics and skin care products. One example is snail mucin—also known as snail slime—which is used for its moisturizing and antioxidant properties. But researchers reporting in ACS Omega might have found something even weirder to put on your face: molecules made by fish gut bacteria.

In cultured cells, the compounds had skin-brightening and anti-wrinkle properties, making them potential ingredients for your future skin care routine.

Though fish guts might seem like the absolute last place to look for cosmetic compounds, it's not a completely far-fetched idea. Many important drugs have been found in bizarre places—famously, penicillin's antibiotic properties were discovered after a failed experiment got moldy.

More recently, the brain cancer drug candidate Marizomib was derived from microbes unearthed in marine sediments at the bottom of the ocean. Two potentially untapped sources of new compounds could be the gut microbes of the red seabream and the blackhead seabream, fish found in the western Pacific Ocean.

Although these microbes were first identified in 1992 and 2016, respectively, no studies have been performed on the compounds they make. So, Hyo-Jong Lee and Chung Sub Kim wanted to see if these bacteria produce any metabolite compounds that could have cosmetic benefits.

The team identified 22 molecules made by the gut bacteria of the red seabream and blackhead seabream. They then evaluated each compound's ability to inhibit tyrosinase and collagenase enzymes in lab-

# Bulletin Board

## Curiosities

SEP. 06, 2024

grown mouse cells. (Tyrosinase is involved in melanin production, which causes hyperpigmentation in aging skin. Collagenase breaks down the structural protein collagen, causing wrinkles.)

Three molecules from the red seabream bacteria inhibited both enzymes the best without damaging the cells, making them promising anti-wrinkle and skin-brightening agents for future cosmetic products.

Phys Org, 5 September 2024

<https://phys.org>

### Peptides and AI Unveil New Pathways in Drug Design

2024-09-02

Chinese scientists have explored how peptides aggregate, revealing that amino acid composition significantly affects their structure and behavior.

#### Understanding Peptide Aggregation: Key to Advances in Medicine and Materials

Researchers from China have investigated how short peptide chains aggregate together in order to deepen our understanding of the process, which is crucial for drug stability and material development. Their study, published in *JACS Au*, provides valuable insights into how short proteins called peptides interact, fold, and function. These findings have significant implications for medicine, material science, and biotechnology.

Peptides are short chains of amino acids that play essential roles in the body by building structures, speeding up chemical reactions, and supporting our immune system. The specific function of a protein is determined by how its amino acids interact with each other and aggregate into a three-dimensional structure.

#### AI and Molecular Dynamics: Predicting Peptide Behavior

The research team used molecular dynamics simulations together with advanced AI techniques, including deep learning models like Transformer Regression Networks, to predict how various peptides of four or five amino acids (tetrapeptides and pentapeptides, respectively) would aggregate based on their amino acid sequence.

By analyzing 160,000 tetrapeptides and 3.2 million pentapeptides, they discovered that certain amino acids, particularly aromatic ones like tryptophan, phenylalanine, and tyrosine, significantly enhance aggregation, especially when located towards one end (the C-terminus)

# Bulletin Board

## Curiosities

SEP. 06, 2024

of the peptide chain. This is probably because aromatic amino acids have ring-shaped structures that attract each other through their electron clouds, normally termed as " $\pi$ - $\pi$ " interactions, which helps them clump together. By contrast, hydrophilic amino acids, such as aspartic acid and glutamic acid, inhibit aggregation due to the strong interaction with water molecules that prevents the peptides from sticking together.

#### Peptide Characteristics and Their Impact on Aggregation

The study also showed that changing the amino acid sequence affects aggregation. For example, adding aromatic amino acids to the end of the peptide chain increases aggregation, while placing negatively charged amino acids at the beginning reduces it. The team also found that peptides clump together into different shapes based on the types and positions of their amino acids.

"Amino acids with a charge generally cause peptides to form long, thread-like structures, while those that avoid water tend to create round, ball-like clusters," explains Dr. Wenbin Li, an assistant professor at Westlake University and corresponding author of the study. "We also discovered that by understanding how tetrapeptides stick to each other, we can predict how pentapeptides will behave, making it easier to predict how longer peptides will clump together."

#### Implications for Biotechnology and Disease Treatment

The findings provide important guidelines for predicting and managing how peptides aggregate. "This knowledge could help in creating new materials, designing more stable drugs and drug delivery systems, and understanding diseases linked to peptide aggregation, such as Alzheimer's disease, where clumped amyloid-beta peptides form damaging plaques in the brain," says Dr. Jiaqi Wang, an assistant professor at Xi'an Jiaotong-Liverpool University (XJTLU) and first author of the study.

It can also improve biotechnology, such as semiconductors, biosensors, and diagnostics, ensuring these tools work accurately and consistently.

"By offering new insights into peptide aggregation, this research is set to advance biochemistry, materials science, and computational biology. It also demonstrates the integration of AI into scientific discovery. These

# Bulletin Board

## Curiosities

SEP. 06, 2024

advances could lead to breakthroughs in medical treatments, eco-friendly products, and innovative technologies.

Sci Tech Daily, 2 September 2024

<https://scitechdaily.com>

# Bulletin Board

## Technical Notes

SEP. 06, 2024

(NOTE: OPEN YOUR WEB BROWSER AND CLICK ON HEADING TO LINK TO SECTION)

### CHEMICAL EFFECTS

[Contrasting effects of iron oxides on soil organic carbon accumulation in paddy and upland fields under long-term fertilization](#)

[Persistent endocrine-disrupting chemicals and incident uterine leiomyomata: A mixtures analysis](#)

[Extracellular vesicles-derived long noncoding RNAs participated in benzene hematotoxicity by mediating apoptosis and autophagy](#)

### ENVIRONMENTAL RESEARCH

[Photodegradation Processes and Weathering Products of Microfibers in Aquatic Environments](#)

[The influence of environmental factors related to Juvenile Dermatomyositis \(JDM\), its course and refractoriness to treatment](#)

### PHARMACEUTICAL/TOXICOLOGY

[Eganelisib combined with immune checkpoint inhibitor therapy and chemotherapy in frontline metastatic triple-negative breast cancer triggers macrophage reprogramming, immune activation and extracellular matrix reorganization in the tumor microenvironment](#)

[A Phase I Trial of Apelisib Combined With Capecitabine in Patients With HER2-Negative Metastatic Breast Cancer](#)

[The toxic effect of 2,6-di-tert-butylphenol on embryonic development in zebrafish \(Danio rerio\): Decreased survival rate, morphological abnormality, and abnormal vascular development](#)

### OCCUPATIONAL

[Workplace Exposures Vary Across Neighborhoods in the US: Implications on Social Vulnerability and Racial/Ethnic Health Disparities](#)

[Occupational agents-mediated asthma: From the perspective of autophagy](#)