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\* While Chemwatch has taken all efforts to ensure the accuracy of information in this publication, it is not intended to be comprehensive or to render advice. Websites rendered are subject to change.

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# Bulletin Board

## **Regulatory Update**

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## **ASIA PACIFIC**

### Proposed decisions on the reconsiderations of paraguat and diquat

### 2024-07-03

The Australian Pesticides and Veterinary Medicines Authority (APVMA) has published its proposed decisions on the reconsiderations of paraquat and diguat, non-selective herbicides used to control weeds in various agricultural, horticultural, and commercial situations.

The APVMA is proposing to:

- vary and affirm paraguat and diquat chemical product registrations and associated label approvals where at least one use pattern is proposed to be supported
- vary and affirm paraquat and diquat active constituent approvals to update the conditions of approval
- cancel 2 diquat chemical product registrations and associated label approvals that do not meet the statutory safety, trade or labelling criteria.

The proposed decision includes consideration of all current approved paraguat and diguat active constituents, registered chemical products, and approved labels.

A summary of risk assessment outcomes for paraguat and diquat uses, and whether they are proposed to be supported or not, is available on the APVMA website. Summaries of the underlying risk assessments have also been published in the Paraguat Review Technical Report and Diguat **Review Technical Report** 

#### Read More

APVMA, 30-07-24

https://www.apvma.gov.au/sites/default/files/2024-07/APVMA%20 Special%20Gazette%2C%2030%20July%202024.pdf

## **Regulatory Update**

CHEMWATCH

### Chemical added to the Inventory following issue of an assessment certificate (early listing) - 29 July 2024

#### 2024-07-29

The following industrial chemical has been added to the Australian Inventory of Industrial Chemicals in accordance with section 83 of the Industrial Chemicals Act 2019.

CAS Number	24128
Chemical Name	.alphaD-Glucan, (1 fwdarw.6)-, 2-hydro (trimethylammonio chloride
Molecular Formula	C6H16NO2.xCl.xUn
Defined Scope of Assessment	The chemical has b imported into Aust tonnes per annum imported as a comp formulations conta concentration for lo into finished cosme containing the asse to 2% concentratio professional use imported as a comp laundry products a concentration for c
Listing date	25 July 2024

#### Read More

AICIS, 29-07-24

https://www.industrialchemicals.gov.au/news-and-notices/chemicaladded-inventory-following-issue-assessment-certificate-early-listing-29july-2024



#### 33-99-7

I.fwdarw.2),(1. oxy-3o)propyl ether,

#### specified

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ponent of ining at up to 33.5% ocal reformulation etic products essed polymer at up n for consumer and

ponent of finished t up to 0.68% onsumer use only.



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## **Regulatory Update**

**AMERICA** 

### **Biden-Harris Administration Proposes Ban on** Numerous Consumer and Workplace Uses of Cancercausing 1-Bromopropane to Protect Public Health 2024-08-01

Today, July 31, the U.S. Environmental Protection Agency announced a proposed rule under the Toxic Substances Control Act (TSCA) to safeguard public health and protect consumers and workers, with this latest proposal focused on the solvent 1-bromopropane (1-BP). Exposure to this chemical can cause serious health effects such as skin, lung, and intestinal cancer; damage to the liver, kidneys, and nervous system; and effects on the reproductive systems that lead to reduced fertility. If finalized, the rule would prohibit all but one consumer use of 1-BP, as well as some workplace uses.

EPA is also proposing worker protections for most industrial and commercial uses that would not be banned under the rule. These protections would help keep both workers and consumers safe from the harmful effects of 1-BP exposure and align with President Biden's Cancer Moonshot, a whole-of-government approach to end cancer as we know it. This is the seventh existing chemical for which EPA has proposed a rule to address unreasonable risks under TSCA section 6(a) since Congress amended the law in 2016.

"The science shows that 1-BP can cause cancer and other serious health problems, and today's action is an important step to use the power of our nation's chemical safety law to finally protect people from this dangerous chemical and prevent cancer-causing exposure," said Assistant Administrator for the Office of Chemical Safety and Pollution Prevention Michal Freedhoff. "Our proposal would end all unsafe consumer exposures from this chemical and put strict protections in place for workers to ensure critical uses can continue safely."

1-BP is a solvent that is widely used in cleaning and degreasing operations, spray adhesives and dry cleaning. 1-BP is also used in insulation for building and construction materials and in the manufacture of other chemicals. Consumer uses of 1-BP include aerosol degreasers, spot cleaners, stain removers and insulation.

EPA is proposing to protect the public from exposure to 1-BP by banning all consumer uses of this chemical except in insulation (because EPA

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**Regulatory Update** 

## AUG. 09, 2024

determined that this use did not contribute to the unreasonable risk to people). The ban on consumer uses would begin to go into effect within six months after the final rule is published and would come fully into force within 15 months.

#### Read More

US EPA, 01-08-24

https://www.epa.gov/assessing-and-managing-chemicals-under-tsca/riskmanagement-1-bromopropane-1-bp

### 2023 TRI Preliminary Dataset

#### 2024-08-31

The 2023 Toxics Release Inventory (TRI) preliminary dataset contains data about chemical releases, waste management and pollution prevention activities that took place during calendar year 2023 at more than 20,000 federal and industrial facilities across the country.

The TRI preliminary dataset is available each July through September, giving the public access to the most recent TRI information, prior to EPA finalizing the National Analysis dataset in October. EPA publishes the National Analysis report, based on the October dataset, early the following calendar year.

Users should note that while these preliminary data have undergone the basic data quality checks included in the online TRI reporting software, they have not undergone the complete TRI data guality process. In addition, EPA does not aggregate or summarize these data, or offer any analysis or interpretation of them.

You can use the TRI preliminary dataset to:

- Identify how many TRI facilities operate in a certain geographic area (e.g., a ZIP code),
- Identify which chemicals are being managed by TRI facilities and in what quantities, and
- Find out if a particular facility initiated any pollution prevention activities in the most recent calendar year.





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# **Regulatory Update**

#### Read More

US EPA, 31-08-24

https://www.epa.gov/toxics-release-inventory-tri-program/2023-tripreliminary-dataset

### **EPA Announces Next Steps to Protect People from Sulfuryl Fluoride used to Fumigate Residential Structures**

#### 2024-08-30

Today, the U.S. Environmental Protection Agency (EPA) is announcing that it has approved additional safety measures to prevent deaths and serious injuries when people re-enter homes fumigated with sulfuryl fluoride. EPA has approved new product labels containing additional protective measures. This is a result of the June 2023 final early mitigation decision for sulfuryl fluoride, which instructed companies to submit amended product labels that contained additional protective measures within 12 months.

Sulfuryl fluoride is the only fumigant registered for use in residential structures, and it is used to control pests such as termites, powder post beetles, old house borers, bedbugs, carpet beetles, moths, cockroaches, rats, and mice. Some of these pests, such as cockroaches and rats, pose significant public health risks. Sulfuryl fluoride is a restricted use pesticide, meaning it can only be used by a certified applicator or someone under the certified applicator's direct supervision. To use sulfuryl fluoride, a residential structure is covered with a tent to contain the gas, then it is filled with sulfuryl fluoride gas to kill the pests. Once the fumigation is complete, the structure is aired out, and the inside air is tested using a "clearance device" to ensure that the amount of sulfuryl fluoride is at or below the "clearance level" that EPA has determined as a safe for humans to re-enter.

#### **Read More**

#### US EPA, 30-08-24

https://www.epa.gov/ingredients-used-pesticide-products/sulfurylfluoride

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# **Canada Requests Information on 312 PFAS; Responses**

**Regulatory Update** 

#### Due January 29, 2025 2024-07-27

On July 27, 2024, Canada's Minister of the Environment published a Canada Gazette notice announcing a mandatory survey to obtain information on the manufacture, import, and use of 312 specific perand polyfluoroalkyl substances (PFAS). Canada's "Guidance manual for responding to the: Notice with respect to certain per- and polyfluoroalkyl substances (PFAS)" (Guidance Manual) states that the purpose of the notice is to collect information on certain PFAS substances, either alone, in mixtures, products, or manufactured items in Canadian commerce for the calendar year 2023. Canada will use this information to establish baseline commercial use data and support future activities related to the class of PFAS. The list of specific PFAS "is focused on those substances known, or anticipated to be in Canadian commerce that have not been recently surveyed." Responses are due January 29, 2025.

#### Read More

B&C, 27-07-24

https://www.lawbc.com/canada-requests-information-on-312-pfasresponses-due-january-29-2025/

### **Bill mandating end to use of PFAS-containing** firefighting foams becomes law in Alaska 2024-07-26

Alaska firefighting departments will have to stop using fire-suppression foams containing contaminants known as "forever chemicals," under a law that went into effect on Monday.

The new law is the product of a bill, Senate Bill 67, that legislators passed nearly unanimously. It went into effect without Gov. Mike Dunleavy's signature.

The new law targets Per- and Polyfluoroalkyl Substances, known as PFAS. They have qualities making them resistant to fire, water and oil. They are linked to numerous poor health effects, including developmental delays, compromised immune systems, reproductive problems and certain cancers according to the Environmental Protection Agency and U.S. Centers for Disease Control and Prevention.





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## **Regulatory Update**

The compounds number in the thousands and have been widely used since the mid-20th century in a wide variety of consumer and industrial products, including cookware, textiles, building materials, body care products like shampoo and dental floss and packing material. They have seeped into the environment - in water bodies, soil and the air - and are found in the blood of people and animals around the world, according to the EPA.

The number of PFAS compounds now exceeds 12,000, according to Alaska Community Action on Toxics.

#### Read More

Alasks Public Media, 26-07-24

https://alaskapublic.org/2024/07/26/bill-mandating-end-to-use-of-pfascontaining-firefighting-foams-becomes-law-in-alaska

## **EUROPE**

## Safety of a feed additive consisting of sepiolite for all animal species (Sepiol S.A. and Tolsa S.A.)

2024-07-17

Abstract

Following a request from the European Commission, EFSA was asked to deliver a scientific opinion on the safety of sepiolite as a technological feed additive for all animal species. In 2022, the Panel on Additives and Products or Substances used in Animal Feed (FEEDAP) delivered an Opinion on the safety and efficacy of the same additive. The Panel concluded that sepiolite used as a feed additive is safe for the consumers and the environment, and efficacious as a thickener-suspending agent, binder and anticaking agent in feed for all animal species under the proposed conditions of use. The additive was not considered an eye or skin irritant. However, it was considered a respiratory irritant, a respiratory and dermal sensitiser; owing to the dusting potential and its silica content, the additive was considered a risk by inhalation. Regarding the target species, in the previous Opinion, the Panel concluded on the safety of the additive for dairy ruminants. However, no conclusion could be drawn for all other species/categories. Based on the tolerance studies in chickens for fattening, weaned piglets and trout evaluated in the current assessment, and the one in dairy cows previously assessed, the Panel concluded that

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the inclusion of sepiolite at the maximum recommended level of 20,000 mg/kg complete feed is safe for all animal species.

#### Read More

EFSA, 17-07-24

https://www.efsa.europa.eu/en/efsajournal/pub/8850

### Export and import of hazardous chemicals – review of the list of chemicals subject to international trade rules 2024-07-29

The Commission intends to update the list of hazardous chemicals subject to certain rules when internationally traded.

The aim is to support non-EU countries in preventing unwanted imports, and to ensure that information on hazards, risks and safe handling is exchanged when these chemicals are exported. Once a chemical has been put on the list, it can only be exported if certain conditions are met.

The Commission would like to hear your views.

This draft act is open for feedback for 4 weeks. Feedback will be taken into account for finalising this initiative. Feedback received will be published on this site and therefore must adhere to the feedback rules.

#### More about draft acts

In order to contribute you'll need to register or login using your existing social media account.

#### Read More

Europa, 29-07-24

https://ec.europa.eu/info/law/better-regulation/have-your-say/ initiatives/14128-Export-and-import-of-hazardous-chemicals-review-ofthe-list-of-chemicals-subject-to-international-trade-rules\_en





# Bulletin Board

## **Regulatory Update**

Public consultation on the evaluation of Regulation (EU) 1025/2012 on European standardisation Supporting document from ANEC

#### 2024-07-29

ANEC does not believe a total revision of Regulation (EU) 1025/2012 is needed. Instead a targeted amendment is needed to address aspects of the Regulation, especially in the obligations on Member States to provide the political and financial frameworks needed at the national level to ensure the participation of all stakeholders in European standardisation. Indeed, some of our comments - for example, on the Standardisation Request (SReg) - may be better addressed in the supporting architecture and implementation of the Regulation, such as the Vademecum.

A legislative proposal should demonstrate the New Legislative Framework, and use of harmonised standards, is the correct tool to use to achieve the intended goal. We believe there should be an independent evaluation of the suitability of the New Legislative Framework once a proposal has been drafted.

ANEC believes the EC must have the right to direct whether a harmonised standard can be offered to ISO/IEC for development at international level, or needs to be developed within the ESS in order to safeguard European values or ethics. This is of utmost importance given the ECJ "James Elliott" ruling that harmonised standards form a part of European law, confirmed by its later ruling in "Public Resource" that citizens should have freelyavailable access to the texts of harmonised standards given their legal effect. We also consider the ESOs must be responsible for ensuring ENs reflect (and are developed in line with) the provisions of Regulation (EU) 1025/2012, including the effective participation of the Annex III organisations.

Standardisation Requests (SRegs) must not delegate political decisions (e.g. on safety limits) to ESOs, and be comprehensively drafted to ensure clear understanding by the ESOs of what they are required to do.

Similarly, we believe there should a limit to domains standardisation can cover. We consider (harmonised) standards should not address the definition or legal interpretation of ethical values; the definition or the legal interpretation of rights enshrined in the EU Charter of Fundamental Rights; matters of religion or ideology; the domains of the social partners. Neither the EC nor the ESOs should promote or support standardisation work at the international level that covers such domains.

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## **Regulatory Update**

Read More

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ANEC, 29-07-24

https://www.anec.eu/images/Publications/position-papers/Horizontal/ ANEC-WP1-2024-G-061\_.pdf

## Paris 2024: Olympics-themed water bottles recalled in France over harmful levels of banned chemical BPA

2024-08-01

A week before the Olympic games kick off in Paris, France has recalled a line of Olympics-themed water bottles for children.

According to Rappel Conso, the official consumer recall agency, the nowrecalled bottles contain unsafe levels of the chemical Bisphenol A (BPA). A statement on the agency's website asserts the "levels of Bisphenol A are not in line with regulations" on the chemical.

The bottles, which were made by the Vilac Company, have an image of the Olympic rings and either the flame or the Paris Olympics mascot. They were released in August 2023 and had been sold until last month.

BPA has been widely used in making food containers and other plastics since the 1950s. However, in recent years, it's been the subject of multiple safety investigations, as research has demonstrated that it can seep into food. If products containing BPA are warmed, the chemical may be released more easily.

#### Read More

msn, 01-08-24

https://www.msn.com/en-us/sports/other/paris-2024-olympics-themedwater-bottles-recalled-in-france-over-harmful-levels-of-banned-chemicalbpa/ar-BB1qz4bF





# **Bulletin Board**

## **Regulatory Update**

**INTERNATIONAL** 

### IARC Monographs Volume 133: Anthracene, 2-bromopropane, butyl methacrylate, and dimethyl hydrogen phosphite

#### 2024-07-15

The International Agency for Research on Cancer (IARC) is pleased to announce that Volume 133 of the IARC Monographs, Anthracene, 2-bromopropane, butyl methacrylate, and dimethyl hydrogen phosphite, is now available online.

2-Bromopropane is a solvent used in dry cleaning and in adhesive production and application, and it also occurs as an impurity of 1-bromopropane (used since the 1990s as a substitute for ozone-depleting solvents).

Anthracene is a high-production-volume polycyclic aromatic hydrocarbon that is mainly used as an intermediate in the manufacture of dyes and pigments, pyrotechnics, coatings, wood preservatives, pesticides, and organic chemicals. Also formed by tobacco smoke, biomass burning (indoor and outdoor), traffic and industry emissions, and contaminated food, it is ubiquitous in the environment and is a widespread environmental pollutant.

Butyl methacrylate is a high-production-volume chemical used in coatings, polyvinyl chloride plastics, polypropylene non-woven materials, glues, caulks, inks and paints, pesticides, and health-care materials.

Dimethyl hydrogen phosphite is a high-production-volume chemical used as an intermediate in the manufacture of adhesives, lubricants, pesticides, and pharmaceuticals, and as a stabilizer in oil and plaster, a steel corrosion inhibitor, and a flame retardant.

For all of these agents, data on exposure levels were sparse, and the cancer evidence in humans was inadequate because no epidemiological studies on cancer were available.

The Working Group classified anthracene, butyl methacrylate, and dimethyl hydrogen phosphite as possibly carcinogenic to humans (Group 2B) on the basis of sufficient evidence for cancer in experimental animals. For each of these agents, there was limited or inadequate mechanistic evidence. 2-Bromopropane was classified as probably carcinogenic to humans (Group 2A) on the basis of sufficient evidence for cancer in

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experimental animals (noting an unusually high degree of carcinogenic activity) and strong mechanistic evidence in experimental systems, supported by suggestive mechanistic evidence in exposed humans.

#### Read More

#### WHO, 15-07-24

https://www.iarc.who.int/news-events/iarc-monographs-volume-133-anthracene-2-bromopropane-butyl-methacrylate-and-dimethylhydrogen-phosphite/

# In Brazil, urban agriculture offers path to sustainable food systems

#### 2024-07-18

The United Nations Environment Programme (UNEP) is supporting Brazil with the establishment of green spaces and farms in and around cities. The process is known as urban and peri-urban agriculture. It can help Brazil improve food availability, bolster community resilience and reduce greenhouse gas emissions when implemented into government policies. Experts say this can provide a much-needed boon to the country, which has 27 million people grappling with food insecurity.

"Urban and peri-urban agriculture can help feed urban dwellers while reducing extreme temperatures in cities, preventing floods and providing a green belt to halt urban sprawl," said Ruth Do Coutto, Chief, Mitigation Branch in UNEP's Climate Change Division. "This can unlock economic and social benefits and improve quality of life in and around cities in Brazil and beyond."

To maximize the potential of urban and peri-urban agriculture in Brazil, UNEP is working with government entities, academia and community stakeholders.

#### Read More

#### UNEP, 18-07-24

https://www.unep.org/technical-highlight/brazil-urban-agriculture-offers-path-sustainable-food-systems



# **Bulletin Board**

## **REACH Update**

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### **Rolling List of (groups of) substances for restriction** updating Annex I to the Restrictions Roadmap under the Chemicals Strategy for Sustainability SWD(2022)128

### 2024-07-03

Document date: 03/07/2024 - Created by GROW.F.1 - Publication date: n/a -Last update: 03/07/2024

Rolling List of (groups of) substances for restriction updating Annex I to the Restrictions Roadmap under the Chemicals Strategy for Sustainability SWD(2022)128

#### Read More

European Commission, 03-07-24

https://ec.europa.eu/docsroom/documents/60674



## **Janet's Corner**

### **Mozart the Worm** 2024-08-09



https://www.facebook.com/beatricebiologist/



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# Bulletin Board

## **Hazard Alert**

### Toxaphene

2024-08-09

### **USES** [2,3]

Toxaphene was used as a nonsystemic stomach and contact insecticide from the late 1940s until 1982 (peaking in 1975), when the EPA cancelled all uses of it as a pesticide or pesticide ingredient. It was used mainly on cotton, but also on flowers because it was persistent and relatively nontoxic to bees. Toxaphene was used to control insects on cotton, corn, fruit, vegetables, and small grains as well as to protect livestock from such pests as lice, fleas, ticks, mange, and scab mites. Up through the early 1970s, Toxaphene, often mixed with rotenone, was used widely in lakes and rivers to eradicate fish that were considered a detriment to sport fishing. This occurred most often in Canada and the Northern United States. Its use as a pesticide was cancelled in 1982, all uses were banned in 1990, and existing stocks were not to be sold in the United States after 1 March 1990. It is currently used only for the following:

- Scabies control in cattle (as a dip)
- Insect control for pineapples in Puerto Rico and for bananas in the Virgin Islands
- Emergency treatment of cotton, corn, and small grains
- "Toxaphene-like pesticides" are still produced and used in other countries including in India, parts of Eastern Europe, Latin America, and Africa.

#### **EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]**

#### **Exposure Sources**

People may be exposed to Toxaphene if they live near a location with heavy contamination, such as a hazardous waste site. The exposure may occur at higher levels through breathing contaminated air or through direct skin contact with contaminated soil or water. In addition, people who consume large quantities of fish, shellfish, or wild game animals from areas contaminated with Toxaphene may have higher exposure to this substance since these animals tend to accumulate Toxaphene in fatty tissues. Individuals may be exposed to Toxaphene through drinking water contaminated with Toxaphene runoff from contaminated soils.

**Toxaphene** (also known as chlorinated camphene) is a mixture of approximately 200 organic compounds, formed by the chlorination of camphene (C10H16) to an overall chlorine content of 67-69 % by weight. The bulk of the compounds (mostly chlorobornanes, chlorocamphenes, and other bicyclic chloroorganic compounds) found in Toxaphene have chemical formulas ranging from C10H11Cl5 to C10H6Cl12, with a mean formula of C10H10Cl8.

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## **Hazard Alert**

#### **Routes of Exposure**

- Inhalation There is some potential for inhalation exposure among populations living near waste sites that contain Toxaphene and its degradation products.
- Oral Potential routes of exposure are via consumption of food sources (e.g., fish and aquatic mammals) that contain Toxaphene residues, or via Toxaphene-contaminated drinking water.

#### **HEALTH EFFECTS** [4]

#### **Acute Health Effects**

Acute oral exposure to Toxaphene in humans results in central nervous system (CNS) stimulation, with the major effect being convulsive seizures. The dose necessary to induce nonfatal convulsions in humans is approximately 10 milligrams per kilogram body weight per day (mg/kg/ day). No studies are available on the effects of acute inhalation exposure to Toxaphene in humans or animals. Animal studies have reported effects on the liver, kidney, and CNS from acute oral exposure to Toxaphene.

#### Carcinogenicity

Several human studies examined the incidence of cancer associated with inhalation exposure to Toxaphene. However, these studies were inconclusive due to lack of information on exposure levels and concurrent exposure to other pesticides. A study by the National Toxicology Program (NTP) reported an increase in liver tumours in male and female mice and an increase in thyroid tumours in male and female rats when fed Toxaphene in the diet. EPA considers Toxaphene to be a probable human carcinogen (cancer-causing agent) and has classified it as a Group B2 carcinogen.

#### **Other Effects**

No information is available on the developmental or reproductive effects of Toxaphene in humans following inhalation or oral exposure. Animal studies have reported developmental effects, including behavioural effects and immunosuppression, in the offspring of rats exposed orally to Toxaphene. Several studies have reported no reproductive effects from oral exposure to Toxaphene in animals.



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## **Hazard Alert**

#### SAFETY

### First Aid Measures [5]

- Inhalation: Remove to fresh air.
- Skin Contact: Flush with water.
- Eye Contact: Immediately flush with water for a minimum of 15 minutes.
- Ingestion: Methanol may be fatal or cause blindness. Seek immediate medical attention.
- Note to Physician: Effects may be delayed. Ethanol may inhibit methanol metabolism.
- After following first aid measures, seek medical attention.

### Workplace Controls & Practices [4]

#### Storage & handling include:

- Keep container tightly closed.
- Avoid contact with skin and eyes.
- Store at 2-6°C.
- Avoid sources of ignition.
- Handle in accordance with good laboratory practices. This product is intended for use only by people trained in the safety and handling of chemicals and laboratory preparations.

### Personal Protective Equipment [5]

- Handle in accordance with good laboratory practices.
- Respiratory Protection: Not normally needed. If exposure limits are exceeded, use approved/certified respirator.
- Eye Protection: Splash goggles.
- Skin Protection: Neoprene or other chemical resistant gloves. Disposable nitriles are acceptable for light intermittent exposure.
- Engineering Controls: Work in a fume hood or use general or other local exhaust ventilation to meet Exposure Limits.

### REGULATION

#### **United States**

OSHA: The Occupational Safety & Health Administration has set the following Permissible Exposure Limit (PEL) for Toxaphene:

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## **Hazard Alert**

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- General Industry: 29 CFR 1910.1000 Z-1 Table -- 0.5 mg/m3 TWA; Skin
- Construction Industry: 29 CFR 1926.55 Appendix A -- 0.5 mg/m3 TWA; Skin
- Maritime: 29 CFR 1915.1000 Table Z-Shipyards -- 0.5 mg/m3 TWA; Skin
- ACGIH: The American Conference of Governmental Industrial Hygienists has set a Threshold Limit Value (TLV) for Toxaphene of 0.5 mg/m3 TWA; 1 mg/m3 STEL; Skin; Appendix A3 - Confirmed Animal Carcinogen with Unknown Relevance to Humans
- NIOSH: The National Institute for Occupational Safety and Health has identified Toxaphene as a Potential Occupational Carcinogen

### REFERENCES

- 1. http://en.wikipedia.org/wiki/Toxaphene
- 2. http://www.atsdr.cdc.gov/toxfaqs/tfacts94.pdf
- 3. http://www.atsdr.cdc.gov/toxguides/toxguide-94.pdf
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Scientists Use Carbon Isotopes To Track Spread of "Forever Chemicals"

#### 2024-08-08

Organofluorine compounds — sometimes called 'forever chemicals' — are increasingly turning up in our drinking water, oceans and even human blood, posing a potential threat to the environment and human health.

Now, researchers at The University of Texas at Austin have developed a way to fingerprint them, which could help authorities trace them to their source when they end up in aquifers, waterways or soil.

The technique involves passing samples through a strong magnetic field then reading the burst of radio waves their atoms emit. This reveals the composition of carbon isotopes in the molecule and gives the chemical its fingerprint, a feat that had not previously been achieved with forever chemicals.

The work is important because it allows scientists to track the spread of forever chemicals in the environment, said Cornelia Rasmussen, a research assistant professor at the University of Texas Institute for Geophysics at the Jackson School of Geosciences.

"Ultimately we will be able to trace molecules and see how they move," said Rasmussen, who co-led development of the technique. "For example, whether they just stay where they got dumped or whether they're moving downstream."

The new technique was described in a paper published in the journal Environmental Science & Technology.

The super strong molecular bonds that give forever chemicals their handy characteristics — which are put to use in everything from fire retardants to non-stick surfaces and slow-release drugs — also keep them from breaking down in the environment, causing them to build up as pollution in soil and organic material to which they easily stick.

The U.S. Environmental Protection Agency plans to regulate forever chemicals, which include PFAS, and eliminate most of them from drinking water. However, the molecular bonds of the chemicals also make them difficult to trace. That's because conventional chemical fingerprinting involves breaking molecules apart in a mass spectrometer which doesn't work well with the tough molecular bonds of forever chemicals.

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Instead, the researchers turned to a technology called nuclear magnetic resonance (NMR) spectroscopy, which measures a molecule's structure and identifies its isotopes without breaking it apart.

Isotopes refer to chemical elements with differences in the number of neutrons in its atoms. Forever chemicals are made by bonding carbon isotopes to the element fluorine, which almost never happens in nature. Once the molecular bonds form, they are virtually unbreakable.

The researchers' technique uses the NMR instrument alongside their own computational tools to determine the mix of carbon isotopes at each position in the molecule. Because the mix of carbon isotopes bonding to each fluorine atom is unique to how the chemical was manufactured, this information can be used like a fingerprint to trace a chemical.

It's like a built-in barcode for molecules, said coauthor, David Hoffman, an associate professor at the Department of Molecular Biosciences in UT's College of Natural Sciences.

"Part of the reason this has worked out so well is because we're assembling tools from different areas of science [chemistry and geosciences] that don't normally mix and using them to do something no one's really done before," he said.

The researchers tested their technique on samples that included pharmaceuticals and a common pesticide. Rasmussen and Hoffman are now conducting a pilot study to see how the technique will fare on pollutants that show up in the city of Austin's creeks and wastewater. If successful, the technique could be useful for state and federal agencies who want to track the spread of water-borne forever chemicals.

Rasmussen said that the work has opened up a new layer of isotope information in organic chemistry that could find many applications beyond tracking forever chemicals, such as detecting counterfeit drugs or astrobiology. Her ultimate goal, however, is to take the technique even further afield.

"It's given us a whole range of possibilities to learn really interesting things about metabolism on early Earth," she said. "It could even tell us whether organics on Mars are the last remnants of some ancient Martian life."

Credit: Rasmussen C, Hoffman D. Fingerprinting Organofluorine Molecules via position-specific isotope analysis. Environ Sci Technol. 2024:acs. est.4c02250. doi: 10.1021/acs.est.4c02250



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Technology Networks, 8 August 2024

https://technologynetworks.com

# Study finds a new pathway connecting diet, genetics and body weight

#### 2024-08-08

A new biochemical pathway linked to diet and body weight hints at the possibility of a new class of anti-obesity drugs, Stanford Medicine researchers and their colleagues have found.

The study, conducted in mice, found a relationship between a previously unstudied body weight-associated gene called PTER and an amino acid called taurine, which has been associated in some studies with reductions in body weight and improvements in endurance exercise.

The newly identified relationship highlights a body weight-regulating metabolic pathway independent of the mechanisms of weight loss drugs like Ozempic or Wegovy, suggesting the two approaches could work in tandem to one day provide additional options for weight control in people.

"This is an additional branch of a very complex system of feeding and body weight regulation," said Jonathan Long, Ph.D., an assistant professor of pathology.

"We all want to know, 'What should I eat? When should I eat it? How does it affect me?' But many diet-based studies offer confusing information. We are trying to answer this question in a more concrete way—starting with molecules, then pathways, then working our way up to the physiology."

Long is the senior author of the study, which was published Aug. 7 in Nature. Postdoctoral scholar Wei Wei, Ph.D., is the lead author of the research.

#### Weight, nutrition and hunger: A complex relationship

The complicated web of interactions that govern when we get hungry, what and how much we eat, and how much we weigh is exceedingly

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difficult to untangle. Previous research in Long's laboratory uncovered a relationship between an "anti-hunger" molecule called lac-phe produced after vigorous exercise and the diabetes drug metformin that can cause moderate weight loss.

In the new study, Wei and Long focused on taurine, which is abundant in protein-rich foods such as meat and shellfish. Taurine supplementation in mice can lower body weight and enhance exercise performance.

Conversely, mice genetically engineered to have low levels of taurine show muscle atrophy and a decreased capacity for exercise. But exactly how taurine has these effects has been unclear.

"Taurine does all sorts of stuff in our bodies, and is metabolized in many different ways," Long said. "It's a complicated soup."

One byproduct, or metabolite, of taurine is called N-acetyltaurine, which is formed when taurine and another molecule called acetate are combined. Levels of N-acetyltaurine in the body fluctuate in response to physiological changes—including endurance exercise and diet—that affect taurine and acetate levels.

As they were exploring taurine metabolism and its relationship to body weight, Wei and Long identified an enzyme called PTER, for phosphotriesterase-related, that converts N-acetyltaurine back into taurine. (Many metabolic pathways can run both forward and backward—a molecular seesaw that allows the body to respond nimbly to changes in diet, exercise and other variables.)

The gene that encodes PTER is part of a panel of genes that have been associated with body mass index in humans. Mutations in one, MC4R, cause people to feel hungry all the time and are strongly associated with obesity. But many of the others, including PTER, have remained mysterious.

"Despite this genetic association, no one really knew what PTER did or why it was linked to body mass index in humans," Long said. "It was an orphan gene that encoded an orphan enzyme. Now we know that PTER breaks down, or hydrolyzes, N-acetyltaurine."

### **Teasing out molecular effects**

When Long and Wei studied mice in which the PTER gene had been knocked out, they found that the animals had higher levels of



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N-acetyltaurine in their blood and tissues than control mice—a not unexpected finding when PTER is missing.

When they were fed a diet high in fat, and given taurine in their drinking water, the mice without PTER ate and weighed significantly less than the control animals after eight weeks. The difference in body weight was due entirely to a reduction of fat mass in the knockout animals, the researchers found.

Next, they tested whether giving the mice N-acetyltaurine directly had a similar effect. They found that a daily dose of N-acetyltaurine reduced body weight and food intake in both PTER knockout mice and the control animals fed a high-fat diet.

Further studies showed that the PTER pathway is independent of the pathway used by the GLP1 receptor agonists, such as Ozempic, currently on the market.

"This is a complicated interaction of genetics and diet that can regulate the body weight of these animals," Long said. "This is a fundamental advance in understanding how we eat affects our weight and our bodies."

Interestingly, it's not clear how N-acetyltaurine is made. It is possible that the gut microbiome plays a role. The researchers found that mice treated with antibiotics for one week to kill off much of their gut bacteria had 30% less N-acetyltaurine circulating in their bodies than before treatment.

"This possible role of the gut microbiome is interesting in the context of research into the rational manipulation of our intestinal bacteria for health," Long said. "Perhaps we could one day have probiotic or dietary interventions that promote the formation of N-acetyltaurine to reduce body weight. But much more work needs to be done."

Long and his colleagues are continuing their studies of PTER and taurine metabolites in people. The task is daunting but exciting.

"All of the stuff we eat, and we eat a lot of stuff, can interact with our bodies at a molecular and genetic level," Long said. "It's not a simple code. But we're starting to understand these intersecting pathways at a much more granular level than ever before."

Phys Org, 8 August 2024

https://phys.org

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### Engineering researchers crack the code to boost solar cell efficiency and durability

#### 2024-08-01

Photovoltaic (PV) technologies, which convert light into electricity, are increasingly applied worldwide to generate renewable energy. Researchers at the School of Engineering of the Hong Kong University of Science and Technology (HKUST) have developed a molecular treatment that significantly enhances the efficiency and durability of perovskite solar cells. Their breakthrough will potentially accelerate the large-scale production of this clean energy.

A key to the solution was their successful identification of critical parameters that determine the performance and lifespan of halide perovskites, a next-generation photovoltaic material which has emerged as one of the most promising materials in PV devices for its unique crystal structure. The findings have been published in Science.

Led by Assistant Professor LIN Yen-Hung of the Department of Electronic and Computer Engineering and the State Key Laboratory of Advanced Displays and Optoelectronics Technologies, the research team investigated various ways of passivation, a chemical process that reduces the number of defects or mitigates their impact in materials, thereby enhancing the performance and longevity of devices comprising these materials. They focused on the "amino-silane" molecular family for passivating perovskite solar cells.

"Passivation in many forms has been very important in improving the efficiency of perovskite solar cells over the last decade. However, passivation routes that lead to the highest efficiencies often do not substantially improve long-term operational stability," Prof. Lin explained the problem.

For the first time, the research team showed how different types of amines (primary, secondary, and tertiary) and their combinations can improve perovskite films' surfaces where many defects form. They achieved this using both "ex-situ" (outside the operating environment) and "in-situ" (within the operating environment) methods to observe molecules' interactions with perovskites. From there, they identified molecules that substantially increase photoluminescence quantum yield (PLQY), i.e. the quantity of photons emitted during materials excitation, indicating fewer defects and better quality.



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"This approach is crucial for the development of tandem solar cells, which combine multiple layers of photoactive materials with different bandgaps. The design maximizes the use of the solar spectrum by absorbing different parts of sunlight in each layer, leading to higher overall efficiency," Prof. Lin elaborated on the application.

In their solar cell demonstration, the team fabricated devices of medium (0.25 cm<sup>2</sup>) and large (1 cm<sup>2</sup>) sizes. The experiment achieved low photovoltage loss across a broad range of bandgaps, maintaining a high voltage output. These devices reached high open-circuit voltages beyond 90% of the thermodynamic limit. Benchmarking against about 1,700 sets of data from existing literature showed that their result was among the best reported to date in terms of efficiency in energy conversion.

Even more critically, the study demonstrated remarkable operational stability for amino-silane passivated cells under the International Summit on Organic Solar Cells (ISOS)-L-3 protocol, a standardized testing procedure for solar cells. Approximately 1,500 hours into the cell aging process, the maximum power point (MPP) efficiency and power conversion efficiency (PCE) remained at high levels. For the bestpassivated cells to decrease to 95% of their initial values, the champion MPP efficiency and the champion PCE were recorded at 19.4% and 20.1% respectively -- among the highest (when factored for the bandgap) and the longest metrics reported to date.

Prof. Lin emphasized that their treatment process not only boosts the efficiency and durability of perovskite solar cells, but is also compatible with industrial-scale production.

"This treatment is similar to the HMDS (hexamethyldisilazane) priming process widely used in the semiconductor industry," he said. "Such similarity suggests that our new method can be easily integrated into existing manufacturing processes, making it commercially viable and ready for large-scale application."

The team included Electronic and Computer Engineering PhD student CAO Xue-Li, Senior Manager of the State Key Laboratory of Advanced Displays and Optoelectronics Technologies Dr. Fion YEUNG, along with collaborators from Oxford University and the University of Sheffield.

Science Daily, 1 August 2024

https://sciencedaily.com

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### 3D-Printed Ceramic Ink Removes "Forever Chemicals" From Water

#### 2024-08-02

Engineers have invented a new way to remove health-harming 'forever chemicals' from water – using 3D printing.

Researchers at the University of Bath say their method, using ceramicinfused lattices (or 'monoliths'), removes at least 75% of perfluorooctanoic acid (PFOA), one of the most common perfluoroalkyl and polyfluoroalkyl substance (PFAS), from water, and could become an important tool in future efforts to eliminate the chemicals from water supplies.

Their findings were published this week in The Chemical Engineering Journal.

Known as forever chemicals due to the incredibly long time they take to break down – in some cases over 1,000 years – PFAS are man-made and known for causing health issues including harms to reproductive, developmental, cardiovascular systems, and in increasing likelihood of diabetes.

Sources of PFAS include domestic products, often with water-repellent properties, such as non-stick pans, raincoats, paints, fabrics and firefighting foams.

Dr Liana Zoumpouli, a Research Associate in Bath's Department of Chemical Engineering and a member of the Centre for Digital, Manufacturing and Design, says: "PFAS, or 'forever chemicals', are a major focus in water treatment and public health. We have created an efficient way to remove these chemicals from water without using lots of energy.

"Using 3D printing to create the monoliths is relatively simple, and it also means the process should be scalable. 3D printing allows us to create objects with a high surface area, which is key to the process. Once the monoliths are ready you simply drop them into the water and let them do their work. It's very exciting and something we are keen to develop further and see in use."

While legislators around the world, particularly in the US and EU, have brought in some rules on acceptable levels of PFAS and similar chemicals in drinking water, the researchers say further legislation is likely as the scale of health threats comes into clearer focus.



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Co-author Professor Davide Mattia adds: "Currently, these chemicals are not strongly regulated in the UK in drinking water, but there are guidelines, and we expect changes in policy guite soon. Water companies are likely to be looking at integrating systems to deal with them."

Made of ink infused with the ceramic indium oxide, the 4cm monoliths are created by extruding the ink from a 3D printer – like squeezing toothpaste from a tube – and forming it into a lattice shape. Because indium oxide bonds with PFAS, the chemicals immediately stick to the monoliths and can be removed from the water in under three hours, which is compatible with current water treatment plants in the UK and abroad.

While testing has so far found that the monoliths remove 75% of PFAS from water, the team is aiming to increase the efficiency of the process with further refinement. Testing of the monoliths has surprisingly shown they have become more effective under repeated use - they undergo high-temperature thermal 'regeneration' treatment after each use. This is something the researchers are keen to understand more fully with further experimentation.

Reference: Martins AS, Zoumpouli GA, Yi S, Exposito AJ, Wenk J, Mattia D. 3D-printed indium oxide monoliths for PFAS removal. Chem Eng J. 2024;497:154366. doi: 10.1016/j.cej.2024.154366

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Technology Nertworks, 2 August 2024

https://technologynetworks.com

### Chemical production gets a cleaner boost from a new electrochemical method

### 2024-08-07

A new electrochemical method can make chemical production cleaner and more energy-efficient.

Using thin film nickel anodes, a team of Lawrence Livermore National Laboratory (LLNL) scientists and collaborators have figured out how to clean up chemical production.

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When studying a new electrochemical reaction, using thin films is important because they give a consistent surface to work with, making it easier to understand how the catalyst actually works.

"Thin films eliminate complications from porous/rough structures or varying thicknesses, allowing us to focus on the true properties of the catalyst material," said LLNL postdoc Aditya Prajapati, first author of a paper appearing in the journal ACS Catalysis.

A corresponding author and PI of this project, Christopher Hahn, said, "This helps us better understand the chemical reactions and how to improve them, leading to more efficient processes."

Current electrolyzers (which convert electrical energy into molecules with high potential-energy densities) struggle with energy efficiency due to the oxygen evolution at the anode. The team found that replacing this oxygen evolution reaction with biomass oxidation could cut energy use by more than 50%, addressing both efficiency and the need for sustainable biomass conversion.

This process cleans up chemical production by converting 5-Hydroxymethylfurfural (HMF), derived from biomass, into 2,5-Furandicarboxylic acid (FDCA), a valuable building block for sustainable plastics like PEF (a bio-based polymer). The team concluded that the process reduces petroleum dependency and carbon emissions.

"Unlike traditional methods that require high temperatures and produce toxic waste, our electrochemical method is cleaner and more energyefficient," said Nitish Govindarajan, one of the corresponding authors of this work.

By utilizing biomass as the starting material, the process supports the use of renewable feedstock, promoting a circular economy and reducing reliance on finite fossil fuel reserves.

Electrochemical oxidation of HMF to FDCA consumes less energy compared to traditional methods, contributing to lower carbon footprints in chemical production. Additionally, it also has the potential to have a zero-carbon footprint if paired with renewable electricity.





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Other LLNL authors include Wenyu Sun, Jeremy Feaster and Sneha Akhade as well as researchers from Université de Montréal and the University of Bonn.

Phys Org, 7 August 2024

https://phys.org

## Chemical 'waves' used to encode words as Morse code 2024-08-06

Chemical 'waves' can be used to encode information in a similar way to radio waves. The team behind the work, led by Stephen Fletcher from the University of Oxford, developed a controllable reaction network capable of sustained oscillations and then used it to tune the shapes of chemical waves for data transduction.1 'We achieved this by measuring waves of chemical concentration and seeing how different input parameters give different repeating waveforms,' explains first author Michael Howlett. The researchers believe that their new concept could one day be part of technology that is integrated with biological systems and could be included in sensors and other devices.

Reactions that produce chemical waves are very rare and challenging to design, but scientists have long been intrigued by such oscillating processes. Although chemical oscillators based on inorganic redox processes like the Belousov-Zhabotinsky (BZ) reaction have been explored for potential use in molecular communication, information transduction in chemical waves has never been shown before, points out Howlett. 'To effectively encode information, you need reliable, periodic waves, but also a high degree of controllability,' he says. 'A special property of our reaction system is that it's very responsive to experimental changes, but not intolerant of them, which would make the waves unstable.'

Using an oscillator that they developed in 2022 as the starting point,2 the team set out to identify variables that would allow them to produce waves of different amplitudes and frequencies. The new chemically fuelled system has a metabolic reaction network at its core and is centred around thiol–disulfide chemistry. The researchers found that both the rate that hydrogen peroxide (fuel) was injected and the rate of stirring could be used to control the waveforms. 'This enabled us to produce a whole spectrum of chemical wave types,' notes Howlett.

The chemical waves were generated in traditional round bottom flasks with reactants mixed by a magnetic stirring plate. 'When all of the

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reactants had been added, the chemical waves began,' says Howlett. 'This was monitored by manually taking regular samples and measuring the chemical concentrations by liquid chromatography. A plot of these chemical concentrations shows waves and these waves were assigned meaning, such as a letter.'

The scientists managed to communicate using recognisable formats such as Morse code and nucleic acid sequences. To encode a word in Morse code, they carried out a single, continuous reaction where oscillating waveforms were produced over multiple hours. 'We initially found reaction conditions which produced two distinct wave types and ran a chemical reaction where we switched between these conditions with precise timing,' explains Howlett. 'Measuring the chemical concentrations produced a pattern of waves which could be translated by Morse code into a word.' In a similar experiment, they simulated RNA-like instructions, assigning each waveform to a nucleobase. 'This demonstrates that with access to a wide range of waveforms, you can encode much higher levels of information,' says Howlett.

Wilhelm Huck from Radboud University Nijmegen in the Netherlands, who wasn't involved in the study, is impressed by the work. 'One of the key results – I would say real breakthrough and surprising finding – is that the authors developed a chemical system which shows oscillations in batch,' he says. 'This is very unusual, if not unique, for such small systems with just a few feedback loops. The system also appears quite robust, as oscillations persist when experimental conditions are varied. As the periodicity of the oscillations depends on those parameters, it is possible to tune the waveforms, and that's the basis of the concept of information transduction.'

Huck believes that this approach could one day be used to influence the properties of materials or living cells, but the system is still not optimised for practical applications and some problems must be addressed first. Howlett says that the main limitation is the manual sampling of the reactions, which limits the throughput.

Chemistry World, 6 August 2024

https://chemistryworld.com

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New Nano-Scale Materials Mimic Enzymes To Convert CO2 Into Chemical Building Blocks

### 2024-07-19

Montana State University researcher James Crawford recently published a collaborative paper with the National Renewable Energy Laboratory that marks a step forward in their quest for what he calls a "holy grail" of chemistry: converting the greenhouse gas carbon dioxide into chemical building blocks which could be used to create myriad other materials.

That paper, "High Selectivity Reactive Carbon Dioxide Capture over Zeolite Dual-Functional Materials," was published in the June 7 issue of the scientific journal ACS Catalysis. An atom-scale illustration of the carbon dioxide conversion process is featured on the front cover of the journal.

"We have successfully captured carbon dioxide then converted it into methane and carbon monoxide using functionalized microporous materials," said Crawford, an assistant professor of chemical and biological engineering in MSU's Norm Asbjornson College of Engineering. "Methane is a drop-in energy resource compatible with existing natural gas infrastructure. Carbon monoxide has a bad reputation but turns out to be an essential reactant in generating synthetic fuels and chemicals."

The element carbon is found in all living things. It's the second most abundant element in the human body and the fourth most in the universe. It's found in biofuels, chemicals, textiles and building materials. It's also a titular element in carbon dioxide, commonly known as CO2, which makes up less than 1% of Earth's atmosphere. In addition to being exhaled byhumans, the colorless, odorless, heat-trapping gas is one byproduct of burning fossil fuels like oil, natural gas, gasoline and coal.

Existing methods for removing carbon dioxide from the atmosphere mostly result in storing the gas, rather than converting it into new products.

"What we're trying to do is introduce another way to capture CO2 by locking it up with chemical bonds," said Crawford, who is also affiliated with MSU's Energy Research Institute and the Center for Biofilm Engineering. "If you can convert atmospheric gases like carbon dioxide and water into carbon monoxide and hydrogen, you can then combine them to make pretty much any hydrocarbon."

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Hydrocarbons are organic compounds composed entirely of hydrogen and carbon, which makes them useful as the building block for many chemical compounds and materials.

"Biological catalysts, or enzymes, have been upcycling atmospheric gases for billions of years," he said. "My group is interested in learning about enzymes and copying their function in robust, solid-state catalysts. This would enable their use in harsh industrial processes."

His team is interested in materials that can selectively wick CO2 from the air and enable the reactions that change the chemical identity of the molecule. "These catalysts must have CO2 attachment sites, as well as reactive structures that permit chemical reconstruction to take place," Crawford said.

This requires materials with customizable, nano-scale structures, with dimensions measured in billionths of a meter. He is interested in two materials specifically: zeolites, which are ceramic-like materials, and metal-organic frameworks, which have metal nodes connected with organic linkers. Both materials have micropores and chemical "tunability" to create CO2 capture and conversion sites.

"We generate zeolites and metal-organic frameworks in the lab using a process that combines solvents, heat and pressure to drive the formation of our catalysts," Crawford said.

Building on these emerging technologies, Crawford, who earned a bachelor's degree in chemical and biological engineering at MSU before getting his doctorate from the Colorado School of Mines, said he hopes his research will one day lead to designing more efficient nano-catalysts with "biomimetic" properties, meaning they mimic biological processes.

"Biology has figured a lot of this out," Crawford said. "We are making biomimetic materials that will, one day, be able to steer the CO2 conversion process to generate the chemicals we need the most."

Reference: Crawford JM, Rasmussen MJ, McNeary WW, et al. Exploring electrocortical signatures of gait adaptation: differential neural dynamics in slow and fast gait adapters. ACS Catal. 2024;14(11):8541-8548. doi:10.1021/acscatal.4c01340

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Technology Networks, 19 July 2024

https://technologynetworks.com/a>

### 3D-printed blood vessels bring artificial organs closer to reality

#### 2024-08-07

Growing functional human organs outside the body is a long-sought "holy grail" of organ transplantation medicine that remains elusive. New research from Harvard's Wyss Institute for Biologically Inspired Engineering and John A. Paulson School of Engineering and Applied Science (SEAS) brings that guest one big step closer to completion.

A team of scientists has created a new method to 3D-print vascular networks that consist of interconnected blood vessels possessing a distinct "shell" of smooth muscle cells and endothelial cells surrounding a hollow "core" through which fluid can flow, embedded inside a human cardiac tissue. This vascular architecture closely mimics that of naturally occurring blood vessels and represents significant progress toward being able to manufacture implantable human organs.

#### The achievement is published in Advanced Materials.

"In prior work, we developed a new 3D bioprinting method, known as 'sacrificial writing in functional tissue' (SWIFT), for patterning hollow channels within a living cellular matrix. Here, building on this method, we introduce coaxial SWIFT (co-SWIFT) that recapitulates the multilayer architecture found in native blood vessels, making it easier to form an interconnected endothelium and more robust to withstand the internal pressure of blood flow," said first author Paul Stankey, a graduate student at SEAS in the lab of co-senior author and Wyss Core Faculty member Jennifer Lewis, Sc.D.

The key innovation developed by the team was a unique core-shell nozzle with two independently controllable fluid channels for the "inks" that make up the printed vessels: a collagen-based shell ink and a gelatin-based core ink. The interior core chamber of the nozzle extends slightly beyond the shell chamber so that the nozzle can fully puncture a previously printed vessel to create interconnected branching networks for sufficient oxygenation of human tissues and organs via perfusion. The size of the

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vessels can be varied during printing by changing either the printing speed or the ink flow rates.

To confirm the new co-SWIFT method worked, the team first printed their multilayer vessels into a transparent granular hydrogel matrix. Next, they printed vessels into a recently created matrix called uPOROS, composed of a porous collagen-based material that replicates the dense, fibrous structure of living muscle tissue. They were able to successfully print branching vascular networks in both of these cell-free matrices. After these biomimetic vessels were printed, the matrix was heated, which caused collagen in the matrix and shell ink to crosslink, and the sacrificial gelatin core ink to melt, enabling its easy removal and resulting in an open, perfusable vasculature.

Moving into even more biologically relevant materials, the team repeated the printing process using a shell ink that was infused with smooth muscle cells (SMCs), which comprise the outer layer of human blood vessels. After melting out the gelatin core ink, they then perfused endothelial cells (ECs), which form the inner layer of human blood vessels, into their vasculature. After seven days of perfusion, both the SMCs and the ECs were alive and functioning as vessel walls-there was a three-fold decrease in the permeability of the vessels compared to those without ECs.

Finally, they were ready to test their method inside living human tissue. They constructed hundreds of thousands of cardiac organ building blocks (OBBs)—tiny spheres of beating human heart cells, which are compressed into a dense cellular matrix. Next, using co-SWIFT, they printed a biomimetic vessel network onto the cardiac tissue. Finally, they removed the sacrificial core ink and seeded the inner surface of their SMC-laden vessels with ECs via perfusion and evaluated their performance.

Not only did these printed biomimetic vessels display the characteristic double-layer structure of human blood vessels, but after five days of perfusion with a blood-mimicking fluid, the cardiac OBBs started to beat synchronously-indicative of healthy and functional heart tissue. The tissues also responded to common cardiac drugs—isoproterenol caused them to beat faster, and blebbistatin stopped them from beating. The team even 3D-printed a model of the branching vasculature of a real patient's left coronary artery into OBBs, demonstrating its potential for personalized medicine.

"We were able to successfully 3D-print a model of the vasculature of the left coronary artery based on data from a real patient, which demonstrates the potential utility of co-SWIFT for creating patient-specific, vascularized



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human organs," said Lewis, who is also the Hansjörg Wyss Professor of Biologically Inspired Engineering at SEAS.

In future work, Lewis's team plans to generate self-assembled networks of capillaries and integrate them with their 3D-printed blood vessel networks to more fully replicate the structure of human blood vessels on the microscale and enhance the function of lab-grown tissues.

"To say that engineering functional living human tissues in the lab is difficult is an understatement. I'm proud of the determination and creativity this team showed in proving that they could indeed build better blood vessels within living, beating human cardiac tissues. I look forward to their continued success in their quest to one day implant lab-grown tissue into patients," said Wyss Founding Director Donald Ingber, M.D., Ph.D. Ingber is also the Judah Folkman Professor of Vascular Biology at HMS and Boston Children's Hospital and Hansjörg Wyss Professor of Biologically Inspired Engineering at SEAS.

Additional authors of the paper include Katharina Kroll, Alexander Ainscough, Daniel Reynolds, Alexander Elamine, Ben Fichtenkort, and Sebastien Uzel.

Phys Org, 7 August 2024

https://phys.org

### Revolutionizing THC Testing: Detecting Cannabis With Just a Few Drops of Saliva

#### 2024-07-27

European universities have developed a new method for quickly and accurately detecting THC in small saliva samples.

This technique simplifies traditional processes into two main steps and utilizes mass spectrometry for rapid analysis. It represents a significant advancement in drug testing technology.

Cannabis is the most widely used illegal drug in Europe. It is estimated that around 8% of adults used cannabis in 2022. Widespread abuse of this substance has health consequences, and is viewed as an important social problem. A fundamental resource to control its use and avoid these health problems would be a quick, simple, non-invasive, and reliable form of analysis that uses a fluid that is easy to extract, such as saliva.

**Innovative Saliva-Based Analysis** 

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In order to expedite this type of analysis and make it effective in smaller saliva samples, the FQM-215 – Affordable and Sustainable Sample Preparation group at the University of Cordoba worked together with the GICAPC group at the University of Valencia to design a new analysis technique that simplifies processing of the sample and makes it possible to verify the presence of THC (Tetrahydrocannabinol) with only 0.25 mL of saliva.

#### **Dispersive Microextraction Technique**

To this end, a technique known as dispersive microextraction by sorption, with a miniaturized stirrer bar, is used, which "consists of the addition of a material capable of extracting the analytes in the sample (in this case, the tetrahydrocannabinol in the saliva), which has magnetic properties, in such a way that when a very small magnet (the stirrer bar) is placed into the device in which the saliva is located, a magnetic agitation occurs causing a vortex to form, dispersing those particles that interact with the analytes in the sample. When the agitation is stopped, the particles with the analytes are attracted to the magnet again," explained UCO researcher Jaime Millán Santiago.

In this way, the THC molecules in the saliva can be extracted very quickly. "We have reduced to 2 steps what would otherwise be 5," said UCO professor Marisol Cárdenas.

#### **Streamlined THC Detection**

After the sample preparation step comes the second one: "We transfer the miniaturized magnet, coated with the particles that have trapped the THC that was in the sample, and transfer it to a needle, to which we apply a high voltage and add an organic solvent capable of interrupting the interaction between the extractant material and the THC, generating an electrospray that is introduced into the mass spectrometer" the researcher explained.

In just two steps, and with a very small sample of saliva, the concentration of cannabis in saliva can be determined in just a few minutes. This technology, as Professor Rafael Lucena explained, "could already be incorporated into the analysis methods of routine laboratories" and stands out for its sensitivity, sensibility, precision, and accuracy.

#### **Collaborative Innovation**

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This technology is possible thanks to the combination of two innovations developed by the teams in Cordoba and Valencia. While the step of

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extracting and preparing the sample was designed by the University of Valencia, the method of analysis was devised by this team in the Department of Analytical Chemistry at the University of Cordoba.

"We use stainless steel needles (an inexpensive and available material) and we take advantage of the non-metallic part of the needle (luer cavity) to couple the magnet with THC, retained on the extractant material, and, to immobilize it, we use another external magnet, thus allowing the flow of the solvent to pass and elute the analytes, which come out of the tip of the needle as a spray that enters the analytical instrument, where the concentration of THC is measured," explained Jaime Millán, one of the creators of this method.

Sci Tech Daily, 27 July 2024

https://scitechdaily.com

### Mucus-based bioink could be used to print and grow lung tissue

#### 2024-07-30

Lung diseases kill millions of people around the world each year. Treatment options are limited, and animal models for studying these illnesses and experimental medications are inadequate. Now, writing in ACS Applied Bio Materials, researchers describe their success in creating a mucus-based bioink for 3D printing lung tissue. This advancement could one day help study and treat chronic lung conditions.

While some people with lung diseases receive transplants, donor organs remain in short supply. As an alternative, medications and other treatments can be used to manage symptoms, but no cure is available for disorders such as chronic obstructive pulmonary disease and cystic fibrosis. Researchers continue to seek better medications, often relying on testing in rodents. But these animal models may only partially capture the complexities of pulmonary diseases in humans, and they might not accurately predict the safety and efficacy of new drugs.

Meanwhile, bioengineers are exploring the production of lung tissue in the lab, either as a more accurate model to study human lungs or as a potential material to use in implants. One technique involves 3D printing structures that mimic human tissue, but designing a suitable bioink to support cell growth remains challenging. So, Ashok Raichur and colleagues set out to overcome this obstacle.

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The team began with mucin, a mucus component that hasn't been widely explored for bioprinting. Segments of this antibacterial polymer's molecular structure resemble epidermal growth factor, a protein that promotes cell attachment and growth. Raichur and colleagues reacted mucin with methacrylic anhydride to form methacrylated mucin (MuMA), which they then mixed with lung cells.

Hyaluronic acid—a natural polymer found in connective and other tissues—was added to increase the bioink's viscosity and enhance cell growth and adhesion to MuMA. After the ink was printed in test patterns including round and square grids, it was exposed to blue light to crosslink the MuMA molecules. The crosslink bonds stabilized the printed structure in the form of a porous gel that readily absorbed water to support cell survival.

The researchers found that the interconnected pores in the gel facilitated diffusion of nutrients and oxygen, encouraging cell growth and formation of lung tissue. The printed structures were nontoxic and slowly biodegraded under physiological conditions, making them potentially suitable as implants in which the printed scaffold would gradually be replaced by newly grown lung tissue. The bioink could also be used to make 3D models of lungs to study lung disease processes and evaluate potential treatments.

#### Phys Org, 30 July 2024

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https:// https://phys.org/news/2024-07-mucus-based-bioink-lung-tissue. html

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# Scientists Identify New Class of Semiconductor Nanocrystals

### 2024-08-01

U.S. Naval Research Laboratory (NRL) scientists confirm the identification of a new class of semiconductor nanocrystals with bright ground-state excitons, a significant advancement in the field of optoelectronics, in an article recently published in the American Chemical Society (ACS) journal ACS Nano.

The groundbreaking theoretical research could revolutionize the development of highly efficient light-emitting devices and other technologies.

Generally, the lowest-energy exciton in nanocrystals is poorly emitting, earning the name "dark" exciton. Because it slows the emission of light, the dark exciton limits the performance of nanocrystal-based devices like lasers or light-emitting diodes (LEDs). Scientists have long sought to overcome the dark exciton.

"We set out to find new materials in which the exciton ordering is inverted, so that the lowest-energy exciton is bright," said John Lyons, Ph.D., from the Theory of Advanced Functional Materials Section. "Searching through open-source databases of materials using criteria informed by our theoretical modeling, we identified over 150 targets. We further narrowed this list with advanced first-principles calculations, ending up with 28 candidates for bright-exciton nanomaterials."

More detailed modeling of these materials indicates that at least four can yield bright ground-state excitons in nanocrystals. "This discovery, made in collaboration with Prof. David Norris from Federal Institute of Technology (ETH) Zurich and Peter Sercel, Ph.D., from the Center for Hybrid Organic-Inorganic Semiconductors for Energy (CHOISE), could pave the way for the development of ultrabright and highly efficient light-emitting devices, lasers, and other technologies," Lyons said.

Alexander Efros, Ph.D., a senior scientist, Materials Science division and the senior author on the paper, elaborated on the implications of the research. "In our research, we have identified several bright-exciton materials that can emit light across a broad spectrum, from infrared to ultraviolet," said Efros. "This versatility makes them very useful for optoelectronic applications. The capability to engineer nanocrystals with bright excitonic states across this wide range opens new avenues for creating better and more efficient LEDs, solar cells, and photodetectors."

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By resolving the dark-exciton problem, NRL scientists hope to stimulate the large nanomaterial community to attack bright-exciton nanostructures, an area that has been stalled for too long. Today, three of these materials are being grown at NRL as part of the Nanoscience Institute Program's Bright Nanocrystal Emitters initiative aiming to conclusively demonstrate bright-exciton behavior in the lab and leverage it for future naval technologies.

"Our findings demonstrate the power of combining high-throughput computational screening, pen-and-paper theory, and high-accuracy calculations of electronic structure" said Michael Swift, Ph.D. "No one technique would be enough on its own, but together we discovered new ultrabright nanocrystals and unlocked the power of the bright exciton across unexplored classes of materials."

Reference: Swift MW, Sercel PC, Efros AL, Lyons JL, Norris DJ. Identification of semiconductor nanocrystals with bright ground-state excitons. ACS Nano. 2024;18(30):19561-19567. doi: 10.1021/acsnano.4c02905

Technology Networks, 1 August 2024

https://technologynetworks.com

### New membrane technology could lead to more effective and efficient water purification systems 2024-08-08

A team of NYU Abu Dhabi (NYUAD) researchers has developed a novel approach that utilizes microwave technology to more easily synthesize and fine-tune a new type of membrane which effectively purifies water from a wide range of contaminants.

The membrane synthesis technique takes a few minutes, making it one of the fastest methods for creating covalent organic framework (COF) membranes. These membranes act as filters in devices designed to clean polluted water from specific contaminants, allowing its reuse in different applications—an important discovery at a time when efficient wastewater treatment becomes vital in a world threatened by water scarcity.

The new type of dual-faced membrane, characterized by its unique superhydrophilic and near-hydrophobic surfaces, enables efficient removal of contaminants like oils and dyes from water. This dual functionality not only enhances the filtration process but also endows

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the membranes with strong antibacterial properties, crucial for long-term usability and effectiveness.

Published in the Journal of the American Chemical Society, the study titled "Tunable Wettability of a Dual-Faced COF Membrane for Enhanced Water Filtration" presents this novel approach developed by Farah Benyettou and Asmaa Jrad under the leadership of Ali Trabolsi, Professor of Chemistry and Co-Principal Investigator at the NYUAD Water Research Center. The team's method involves a one-step microwave-mediated synthesis that occurs at the liquid-water vapor interface, allowing precise control over the membrane's properties without the need for subsequent modifications.

"By fine-tuning the reaction time, we can adjust the membrane's thickness and its hydrophilic and hydrophobic characteristics," explained Benyettou.

"This capability allows us to tailor the membrane specifically for various types of water pollutants, significantly enhancing both the efficiency and speed of water purification," explained Jrad.

The COF membranes developed by the NYU Abu Dhabi team demonstrate superior performance in removing oil from oil-in-water mixtures and boast exceptional water flux due to their multilayered structure and consistent porosity. Furthermore, these membranes outperform traditional polymeric ones in resisting organic fouling, a common challenge in membranebased water filtration systems.

This technology represents a significant leap forward in the synthesis of high-quality, crystalline, free-standing COF membranes.

"Our method not only simplifies the production process but also enhances the separation capabilities of the membranes, offering a promising solution to critical water purification challenges worldwide," Trabolsi added.

Phys Org, 8 August 2024

https://phys.org

### Do smells prime our gut to fight off infection? 2024-08-07

Many organisms react to the smell of deadly pathogens by reflexively avoiding them. But a recent study from the University of California, Berkeley, shows that the nematode C. elegans also reacts to the odor

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of pathogenic bacteria by preparing its intestinal cells to withstand a potential onslaught.

As with humans, nematodes' guts are a common target of disease-causing bacteria. The nematode reacts by destroying iron-containing organelles called mitochondria, which produce a cell's energy, to protect this critical element from iron-stealing bacteria. Iron is a key catalyst in many enzymatic reactions in cells -- in particular, the generation of the body's energy currency, ATP (adenosine triphophate).

The presence in C. elegans of this protective response to odors produced by microbes suggests that the intestinal cells of other organisms, including mammals, may also retain the ability to respond protectively to the smell of pathogens, said the study's senior author, Andrew Dillin, UC Berkeley professor of molecular and cell biology and a Howard Hughes Medical Institute (HHMI) investigator.

"Is there actually a smell coming off of pathogens that we can pick up on and help us fight off an infection?" he said. "We've been trying to show this in mice. If we can actually figure out that humans smell a pathogen and subsequently protect themselves, you can envision down the road something like a pathogen-protecting perfume."

So far, however, there's only evidence of this response in C. elegans. Nevertheless, the new finding is a surprise, considering that the nematode is one of the most thoroughly studied organisms in the laboratory. Biologists have counted and tracked every cell in the organism from embryo to death.

"The novelty is that C. elegans is getting ready for a pathogen before it even meets the pathogen," said Julian Dishart, who recently received his UC Berkeley Ph.D. and is the first author of the study. "There's also evidence that there's probably a lot more going on in addition to this mitochondrial response, that there might be more of a generalized immune response just by smelling bacterial odors. Because olfaction is conserved in animals, in terms of regulating physiology and metabolism, I think it's totally possible that smell is doing something similar in mammals as it's doing in C. elegans."

The work was published June 21 in the journal Science Advances.

### Mitochondria communicate with one another

Dillin is a pioneer in studying how stress in the nervous system triggers protective responses in cells -- in particular, the activation of a suite of



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genes that stabilize proteins made in the endoplasmic reticulum. This activation, the so-called unfolded protein response (UPR), is "like a first aid kit for the mitochondria," he said.

Mitochondria are not only the powerhouses of the cell, burning nutrients for energy, but also play a key role in signaling, cell death and growth.

Dillin has shown that errors in the UPR network can lead to disease and aging, and that mitochondrial stress in one cell is communicated to the mitochondria of cells throughout the body.

One key piece of the puzzle was missing, however. If the nervous system can communicate stress through a network of neurons to the cells doing the day-to-day work of protein building and metabolism, what in the environment triggers the nervous system?

"Our nervous system evolved to pick up on cues from the environment and create homeostasis for the entire organism," Dillin said. "Julian actually figured out that smell neurons are picking up environmental cues and which types of odorants from the pathogens turn on this response."

Previous work in Dillin's lab showed the importance of smell in mammalian metabolism. When mice are deprived of smell, he found, they gained less weight while eating the same amount of food as normal mice. Dillin and Dishart suspect that the smell of food may trigger a protective response, like the response to pathogens, in order to prepare the gut for the damaging effects of ingesting foreign substances and converting that food to fuel.

"Surviving infections was the most important thing we did evolutionarily," Dillin said. "And the most risky and taxing thing we do every single day is eat, because pathogens are going to be in our food."

"When you eat food, it's also incredibly stressful, because the body is metabolizing the food but also generating ATP in the mitochondria from the nutrients that they're incorporating. And that generation of ATP causes a by-product called reactive oxygen species, which is very damaging to cells," Dishart said. "Cells have to deal with this increased existence of reactive oxygen species. So perhaps smelling food can prepare us to deal with that enhanced reactive oxygen species load."

Dillin speculates further that mitochondria's sensitivity to the smell of pathogenic bacteria may be a holdover from an era when mitochondria were free-living bacteria, before they were incorporated into other cells as power plants to become eukaryotes some 2 billion years ago. Eukaryotes

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eventually evolved into multicellular organisms with differentiated organs -- so-called metazoans, like animals and humans.

"There's a lot of evidence that bacteria sense their environment in some way, though it's not always clear how they do it. These mitochondria have retained one aspect of that after being subsumed into metazoans," he said.

In his experiments with C. elegans, Dishart found that the smell of pathogens triggers an inhibitory response, which unleashes a signal to the rest of the body. This became clear when he ablated olfactory neurons in the worm and found that all peripheral cells, but primarily intestinal cells, showed the stress response typical of mitochondria that are being threatened. This study and others also showed that serotonin is a key neurotransmitter communicating this information throughout the body.

Dillin and his lab colleagues are tracking the neural circuits that lead from smell neurons to peripheral cells and the neurotransmitters involved along the way. And he's looking for a similar response in mice.

"I always hate it when I get sick. I'm like, 'Body, why didn't you prepare for this better?' It seems really stupid that you turn on response mechanisms only once you're infected," Dillin said. "If there are earlier detection mechanisms to increase our chances of survival, I think that's a huge evolutionary win. And if we could harness that biomedically, that would be pretty wild."

Other UC Berkeley authors of the paper are Corinne Pender, Koning Shen, Hanlin Zhang, Megan Ly and Madison Webb. The work is supported by HHMI and the National Institutes of Health (R01ES021667, F32AG065381, K99AG071935).

Science Daily, 7 August 2024

https://sciencedaily.com

### "Brittility Factor" Explains How Soft Materials Fail **Under Stress** 2024-07-22

Understanding what makes a soft material fail when stressed is a key part of addressing major engineering challenges, such as landslide prevention or creating better industrial materials.

Now, a new study from researchers at the University of Illinois at Urbana-Champaign is transforming how scientists speak about these soft





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materials. By linking a spectrum of other soft material behaviors that were previously thought to be unrelated, the team has identified a new parameter – the "brittility" factor – which they say can help simplify soft material failure models.

#### **Redefining material failure**

The study of soft materials is an important part of engineering due to the knock-on effects for industrial, environmental and biomedical applications. Despite its importance, researchers Simon Rogers, an associate professor of chemical and biomolecular engineering at the University of Illinois Urbana-Champaign, and Krutarth Kamani, a graduate student in the university's Department of Chemical and Biomolecular Engineering, noticed that there was a significant communication breakdown occurring between scientists working in this field.

When soft materials - synthetic or natural - begin to deform under pressure, they eventually reach a point where they either spring back to their original form like a rubber band, or undergo permanent deformation, like that rubber band snapping. This is known as the material's "yielding" behavior. If a material has a slow, gradual yielding transition then it is called a "ductile" material, whereas a material with a very abrupt yielding transition is deemed "brittle".

In a break from this traditional dichotomy, Rogers and Kamani argue that soft materials should not be viewed as being either strictly brittle or ductile. Rather, scientists should consider a wider spectrum of yielding behaviors.

#### Introducing the brittility factor

In their new study, the researchers show that it is possible to account for the different spectrum of yielding behaviors exhibited by real-world materials in a continuum model by introducing a new parameter – the brittility factor. The higher the brittility factor, the less a soft material will deform permanently before it yields.

"We didn't expect this study to explain as much as it does," said Rogers. "What we ended up with was a way to bring a whole bunch of soft material behaviors together under the same physics umbrella. Previously, they'd been studied independently or maybe all been applied simultaneously, but never thought of as being physically or mathematically connected."

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"This single parameter amazingly connects so many puzzling observations researchers have come across over the years," Kamani added.

The team's model was also tested by comparing it to the results of realworld rheometry tests conducted on an array of different soft materials, indicating the general applicability of the brittility factor. Kamani and Rogers believe that the brittility factor could be a simple tool for understanding the yielding transition of different materials under various stresses and strains, and could even explain why some materials are more resistant to rapid yielding than others - a question that has perplexed materials scientists for decades.

"This work marks the point at which we are approaching the crest of the hill in understanding soft materials behavior," Rogers concluded. "We've always felt like each step takes us higher, but with no end in sight. Now we can see the top of the hill, and we are closer to the top and free to move forward in whatever direction we would like."

Reference: Kamani KM, Rogers SA. Brittle and ductile yielding in soft materials. Proc Natl Acad Sci USA. 2024;121(22):e2401409121. doi: 10.1073/pnas.2401409121

Technology Networks, 22 July 2024

https://technologynetworks.com

### Advanced chelators offer efficient and eco-friendly rare earth element recovery 2024-08-06

The world is going to need a lot of weird metals in the coming years, according to chemistry professor Justin Wilson at UC Santa Barbara. But he isn't talking about lithium, cobalt or even beryllium. Wilson's interested in dysprosium, which is so hidden in the periodic table that you'd be forgiven for thinking he made it up.

Rare earth elements (REEs) like dysprosium have a lot of niche uses in modern electronics. So much so that the U.S. Department of Energy classifies them as "critical minerals." And while they aren't guite as rare as noble metals like platinum or gold, they are difficult to obtain from natural deposits. They also share extremely similar chemical properties, making them devilishly difficult to isolate from one another.

But a team led by Wilson and postdoctoral researcher Yangyang Gao has just developed a technique to purify certain REEs at room temperature



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without relying on the toxic and caustic compounds currently used for the task. The results, published in the journal Angewandte Chemie, promise a safer, more effective way to process these metals from mining operations and recover them from electronic waste.

#### Useful elements out of the public eye

Rare earth elements include scandium, yttrium and the lanthanides -- the first of the two rows that publishers excise from the periodic table so that it fits on a single page. The lanthanides (and actinides below them) actually slot in just to the right of the second column. You may be familiar with the REE neodymium as the metal used to make crazy strong magnets. Wilson is interested in neodymium as well.

These elements share many chemical properties, making them tough to separate from one another. They all form ions with a +3 charge, and they all prefer to bond with non-metals in the second row of the periodic table (like oxygen and nitrogen). Fortunately, they differ slightly in their ionic radius, or size. However, their sizes are still fairly similar, with only a 16% change in radius across the series.

Despite their similar physical and chemical properties, the REEs do have their distinguishing features. Differences in the number and arrangement of valence electrons confer each of these elements with distinct magnetic and optical properties. Only by isolating them in pure samples can we take advantage of these unique characteristics.

### Tuning the technique

The current industry standard for separating REEs from one another is called liquid-liquid extraction, which combines an organic solvent (such as a kerosene or benzene) and a water-based solvent. "It's like salad dressing at this point, where you have two phases and they don't mix," Wilson said. So, chemists add molecules called chelators into the organic solvent that are designed to bind to REEs.

The key is that these chelators have a slight preference for smaller atoms, which enables them to separate one type of REE from another based on size. Still the process is rather inefficient: only a couple percent enrichment for each extraction cycle. Obtaining a sufficiently pure sample of a particular element for industrial use requires many liquid-liquid extraction cycles, which generates a lot of chemical waste.

Wilson and his co-authors at Cornell and University of Nevada, Reno, developed more optimized chelators and a process that doesn't require

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an organic solvent. This eliminates substances that are often inflammable, carcinogenic and toxic.

The authors tested their method in a solution of dysprosium (Dy) and neodymium (Nd). They used a specific chelator, called G-macropa, to bind to the larger Nd atoms, and then added sodium bicarbonate (aka baking soda) to cause the smaller Dy to precipitate as a carbonate salt. This can simply be filtered out and processed to recover the pure metal. Decreasing the acidity of the remaining solution enabled them to separate the Nd from the chelator, which can then be reused.

A single cycle of this new process can concentrate dysprosium by a factor of over 800, compared to less than 10 for liquid-liquid extraction.

"[I was very surprised] when my postdoc, Yangyang, showed me the elemental analysis data," Wilson said. After repeating the test to confirm the results, the team realized just how fine-tuned their chelator was for this separation process.

By collaborating with David Cantu, a professor at UN Reno, they were able to understand and compare the efficacy of G-macropa to other chelators at a molecular level. These theoretical studies will help scientists design second-generation analogues.

#### Large applications and small adjustments

This efficiency is important for scaling the process because the G-macropa chelator is more complex, and thus expensive, than the ones in standard use. The team is also exploring chelators that may be less expensive to produce.

Wilson and his co-authors focused on separating Nd from Dy because the two elements are abundant in e-waste, particularly those neodymium magnets. Indeed, they performed their experiments on e-waste to emphasize its potential for making recycling an economically viable source of REEs.

They're working to tailor this technique to other assemblages of rare earth elements as well as ensuring it works with high concentrations of REEs more similar to industrial sources.

Advances in separating rare earth elements could massively impact the supply chain for these metals. The United States has large deposits of REEs, but important environmental and health regulations have prevented



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American industries from competing with China, where these safeguards are much more lax.

"A cleaner and more efficient separation of these elements could potentially open up domestic supplies of the rare earth elements," Wilson said. This would be a win-win for national security and the American economy as these weird metals become ever more important.

Science Daily, 6 August 2024

https://sciencedaily.com

## New ligand-guided technique enhances drug development

#### 2024-8-08

Achieving a level of precision to create complex medicines and materials with extreme accuracy is a longstanding goal of scientists and pharmaceutical companies. If achieved, that precision could lead to the development of more effective drug treatments.

Now, scientists at the University of Rochester—led by Shauna Paradine, an assistant professor in the Department of Chemistry-have developed a groundbreaking method to yield products by using a chemical "helper" to guide reactions in an extremely precise manner. The research, published in Nature Communications, opens the door for more efficient drug development while also providing fundamental advancements in the creation of new materials.

#### **Overcoming molecular bias**

In chemical reactions, there are often multiple ways that two molecules can come together. It is a challenge, however, for scientists to control exactly how these interactions occur. Sometimes molecules have a biasknown as a substrate bias—in the way they interact, preferring to react or combine in a specific way.

"If you can overcome that bias, you have the ability to access configurations of your product molecules that you could not otherwise access," Paradine says.

#### What is a ligand?

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A ligand is an atom, ion, or molecule that binds to a central metal atom or ion. The nature of the ligands and the central metal atom can influence the properties and reactivity of the resulting complex.

Paradine and her team discovered a method to overcome substrate bias using a ligand, making the reaction more precise. Specifically, the ligand was able to switch the direction in which the molecules react, without altering any other part of the chemical process.

The team tested many phosphorus-based ligands, which are commonly used for reactions involving palladium metal. Only one of them was able to switch the selectivity of the reaction.

"It was very much like picking out a needle from a haystack," Paradine says.

#### Transforming ligand chemistry—and drug discovery

Although the researchers used a specific ligand in one particular reaction in this study, they applied the data to create a predictive model to understand the selectivity they were observing in reactions. The model helps determine how different ligands affect a reaction, paving the way for using a ligand-centered approach in other types of chemical reactions.

The research has important implications in drug discovery and development.

"The products we're making contain core structures that are often found in biologically active molecules," Paradine says. "In drug discovery, it's really important to be able to finely tune a molecule to optimize its various properties."

In pharmaceutical research, altering and optimizing a molecule's properties typically requires a complex amount of work. By simply changing a ligand, scientists can now get different configurations of a molecule from the same reaction.

"This approach allows us to guickly and selectively create complex and useful molecules, giving us more options to explore in chemical space," Paradine says.

Phys Org, 8 August 2024

https://phys.org

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Physicists may now have a way to make element 120 – the heaviest ever

#### 2024-07-23

The third-heaviest element in the universe has been made in a way that offers a route for synthesising the elusive element 120, which would be the heaviest element in the periodic table.

"We were very shocked, very surprised, very relieved that we didn't make any bad choices in setting up the instrumentation," says Jacklyn Gates at Lawrence Berkeley National Laboratory (LBNL) in California.

She and her colleagues created the element livermorium by smashing a beam of charged titanium atoms into a piece of plutonium. Titanium has never been used in such an experiment because it is tricky to turn it into a well-controlled beam and it takes millions of trillions of collisions to produce very few new atoms. Yet, physicists think a titanium beam will be crucial for creating the hypothetical element 120, also known as unbinilium, which would have 120 protons in its nucleus.

The researchers started with rare isotopes of titanium, which they vaporised in a special oven at 1650°C (around 3000°F). Next, they used microwaves to turn the hot titanium vapour into a charged beam, which could then be fed into a particle accelerator. When the beam reached roughly 10 per cent of the speed of light and collided with the plutonium target, the resulting debris hit a detector that revealed signatures of exactly two atoms of livermorium.

Each atom rapidly decayed into other elements, as was expected – the stability of atomic nuclei decreases as the mass of an atom increases. But the measurement was so precise that there is only about a one in a trillion chance that the finding was a statistical fluke, says Gates. The researchers presented their findings on 23 July at the Nuclear Structure 2024 conference at Argonne National Laboratory in Illinois.

Michael Thoennessen at Michigan State University says this experiment strengthens the case for the feasibility of creating element 120. "You have to do the groundwork and feel your way up to it. In this sense, this is a really important and necessary experiment," he says.

Thoennessen says that creating unbinilium would have deep implications for our understanding of the strong force, which determines when heavy elements are stable or not. Studying unbinilium could also help us understand how exotic elements may have formed in the early universe.

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The heaviest human-made element so far – element 118, also known as oganesson – has two more protons than livermorium and was first synthesised in 2002. In the intervening years, researchers have struggled to make atoms any heavier because that requires smashing together already very heavy elements, which tend to be unstable themselves. "This is really, really difficult business," says Thoennessen.

But the new experiment makes the LBNL researchers optimistic. They plan to start the experiment aimed at creating element 120 in 2025, once they have replaced the plutonium target with the heavier element californium.

"I think we're a lot closer to knowing what we have to do," says Gates. "And having the chance to put a new element on the periodic table [is exciting]. So few people have that opportunity."

New Scientist, 23 July 2024

https://newscientist.com

## CRISPR Identifies Common Blood Thinner as Snake Venom Antidote

#### 2024-08-03

Each day, 7,400 people are bitten by a snake, resulting in 81,000–138,000 unfortunate deaths per year, according to the World Health Organization (WHO).

While antibody-based antivenoms exist, they can be difficult to access in low-income countries, and are not always effective against local tissue injury, which contributes heavily to mortality rates. In 2017, the WHO added snakebite envenoming to its highest priority neglected tropical disease (NTD).

"Snakebites remain the deadliest of the NTDs, with its burden landing overwhelmingly on rural communities in low- and middle-income countries," said Professor Nicholas Casewell, head of the Centre for Snakebite Research and Interventions at Liverpool School of Tropical Medicine.

Using CRISPR gene-editing technology, researchers at the University of Sydney and Liverpool School of Tropical Medicine have demonstrated how a commonly used blood thinner could be repurposed as a cost-effective and easy-to-access cobra venom antidote. The research is published in Science Translational Medicine.



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#### Repurposing existing drugs for snakebites using CRISPR technology

As the health and economic burden of snakebite envenoming grows, researchers are exploring how drug repurposing could provide readily available and cost-effective treatment approaches. A challenge in this arena is building a knowledge base on how venoms interact with the human body at the molecular level to test appropriate drugs.

CRISPR gene-editing technology is extremely useful in this context. CRISPR screens offer a high-throughput method for evaluating the role of specific genes in cellular processes or phenotypes. Equipped with this knowledge, researchers can evaluate the effectiveness of existing or novel drugs for blocking these interactions.

Tian Du, a PhD student from the University of Sydney, and colleagues conducted a whole-genome CRISPR knockout screen in human cell lines after administering venom from different types of cobras. "We used a functional genomics approach to define venom-target genetic interactions that modify the cytotoxicity caused by spitting cobra venom and then used this information to develop a locally acting venom antidote," the authors said.

"Our findings are exciting because current antivenoms are largely ineffective against severe local envenoming, which involves painful progressive swelling, blistering and/or tissue necrosis around the bite site," said Casewell, who is a co-author of the paper. "This can lead to loss of limb function, amputation and lifelong disability."

#### Heparinoid reduces tissue death after venom injection in mice

Several genes, including EXT1, B4GALT7, EXT2, EXTL3, XYLT2 and NDST1, were highlighted in the CRISPR screens.

These genes encode enzymes that are involved in the production of heparan and heparin; the former is located on the surface of cells and in the extracellular matrix, while the latter is stored in immune cells and released into the bloodstream during an immune response. The similar structure of these molecules means that the snake venom tested was capable of binding to both.

"To validate these results, we generated single knockout cell pools with single guide RNAs that targeted each resistance gene individually and tested cytotoxicity. Targeting each component of the heparan/ heparin biosynthesis pathway conferred some resistance to each venom,

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confirming a role for heparan in cobra venom cytotoxicity," Du and colleagues said.

As heparan is necessary for spitting cobra venom to cause cytotoxicity, flooding the site of the bite with "decoy" heparin, or heparinoids - low molecular weight variants of heparin – could work therapeutically to block it, the researchers hypothesized.

After encouraging results in human cell lines, they moved on to in vivo experiments testing heparin and heparinoids as venom antidotes in mice. The US Food and Drug Administration (FDA)-approved heparinoid, tinzaparin, reduced the size of dermonecrotic lesions when administered subcutaneously at the same time as an intradermal venom injection.

This drug has the most translational value, the researchers argue, given that it already has received approval for human use in other indications.

"Heparin is inexpensive, ubiquitous and a WHO-listed Essential Medicine. After successful human trials, it could be rolled out relatively quickly to become a cheap, safe and effective drug for treating cobra bites," Du said.

As tinzaparin did not block dermonecrosis completely, further preclinical studies evaluating dosing, delivery route and potential toxin-targeting drug combinations are warranted.

Time is of the essence here, Professor Greg Neely, a corresponding author of the study from the Charles Perkins Centre and Faculty of Science at the University of Sydney, emphasized, considering the WHO's 2030 goal: "That target is just five years away now. We hope that the new cobra antidote we found can assist in the global fight to reduce death and injury from snakebite in some of the world's poorest communities."

The research team believe CRISPR screens will prove useful in future studies exploring the molecular mechanisms of envenoming. While this study homed in on the genes involved in heparan and heparin biosynthesis, others were identified in the initial screening process that could be implicated in cytotoxicity.

"Cytotoxicity is only one physiologically relevant impact of snake envenoming, and further CRISPR screening using other functional readouts beyond cell death may provide a more comprehensive understanding of mechanisms of action underlying envenoming," the authors concluded.



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Reference: Du TY, Hall SR, Chung F, et al. Molecular dissection of cobra venom highlights heparinoids as an antidote for spitting cobra envenoming. Sci Trans Med. 16(756):eadk4802. doi: 10.1126/scitranslmed. adk4802

Technologyu Networks.com, 3 August 2024

https://technologynetworks.com

# Engineers develop general, high-speed technology to model, explain catalytic reactions 2024-8-05

Atmospheric nitrogen, with the aid of an iron catalyst, reacts with hydrogen to produce ammonia. That reaction produces lots of ammonia -- worldwide production is 160 million tons every year. Most is used in agriculture, especially as nitrogen fertilizer. It's also used in many industries, including refrigeration for food and beverage production. We all know it as a household cleaner.

A research team led by Qi An, an associate professor of materials science and engineering at Iowa State University, has developed artificial intelligence technology that could find ways to improve researchers' understanding of the chemical reactions involved in ammonia production and other complex chemical reactions.

"Our developed HDRL-FP framework has the potential to contribute significantly to the optimization of this process, potentially reducing production costs and CO2 emission, and facilitating the establishment of smaller and more widespread plants," the researchers wrote in a paper recently published online by the journal Nature Communications. "Therefore, the framework highlights its effectiveness and potential for predicting complex chemical reaction pathways."

HDRL-FP is High-Throughput Deep Reinforcement Learning with First Principles. An and his collaborators and co-authors -- Tian Lan and Huan Wang of Salesforce AI Research in California -- say the technology is full of potential.

"Exploring catalytic reaction mechanisms is crucial for understanding chemical processes, optimizing reaction conditions, and developing more effective catalysts," they wrote.

#### Of rewards and atoms

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An said there are two keys to the researchers' software technology: a type of machine learning called reinforcement learning and connecting the simulation process with the positions of the atoms involved.

An said reinforcement learning is like training a dog by using rewards to encourage actions. In reinforcement learning, computers learn from their actions while seeking appropriate rewards. In this case, the rewards are all about finding the best, most-efficient, lowest-cost reaction path.

The method, when used with graphics processing units and highthroughput strategies, can quickly and automatically identify the optimal reaction pathway from thousands of potential pathways, An said. That effectively identifies viable reaction mechanisms amidst the extremely noisy data in real chemical reactions.

The researchers also built the technology to be useful for general studies of catalytic reactions. Studies start with the positions of atoms mapped on an energy landscape. That's enough -- researchers don't have to start with a more specific representation of the reaction environment, including the states, actions or rewards for a particular reaction.

An and his collaborators have worked on the project for about two years. It started when An moved to Iowa State and has been supported by his university startup funds.

He said the system's calculations for the reaction producing ammonia is considered a proof-of-concept demonstration.

"This allows us to figure out the reaction mechanism," An said. "We're able to see important reaction steps in ammonia synthesis."

The researchers' successful peek inside that reaction "enables the investigation of complex catalytic chemical reactions automatically," they wrote, "offering a promising approach for future research and discoveries."

Science Daily, 5 August 2024

https://sciencedaily.com

Effective new catalyst brings hope for cleaner energy, wastewater treatment, and green chemistry 2024-08-08

A catalyst that significantly enhances ammonia conversion could improve wastewater treatment, green chemical and hydrogen production.



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A team of scientists have developed an effective catalyst with a remarkable ability to enhance the efficiency of ammonia conversion. Published in Advanced Energy Materials, the study reveals the catalyst's potential to significantly advance wastewater treatment, green nitrite and nitrate, as well as hydrogen production.

Catalysts are substances that speed up chemical reactions by providing a more efficient route for a reaction to occur and making it easier to start and finish. Since catalysts are neither consumed nor altered in the reaction, they can be used repeatedly, and they are essential in a variety of industrial, environmental, and biochemical processes.

The team, which included researchers from Japan's Hokkaido University, Australia's University of Technology Sydney and elsewhere, developed the catalyst, called NiOOH-Ni, by combining nickel (Ni) with nickel oxyhydroxide.

Ammonia can cause severe environmental problems, such as excessive algal growth in water bodies, which depletes oxygen and harms aquatic life. At high concentrations, ammonia can harm humans and wildlife. Effective management and conversion of ammonia are thus critical, but its corrosive nature makes it difficult to handle.

The researchers developed NiOOH-Ni using an electrochemical process. Nickel foam, a porous material, was treated with an electrical current while immersed in a chemical solution.

This treatment resulted in the formation of nickel oxyhydroxide particles on the foam's surface. Despite their irregular and non-crystalline structure, these nickel-oxygen particles significantly enhance ammonia conversion efficiency.

The catalyst's design allows it to operate effectively at lower voltages and higher currents than traditional catalysts.

"NiOOH-Ni works better than Ni foam, and the reaction pathway depends on the amount of electricity (voltage) used," explains Professor Zhenguo Huang from the University of Technology Sydney, who led the study. "At lower voltages, NiOOH-Ni produces nitrite, while at higher voltages, it generates nitrate."

This means the catalyst can be used in different ways depending on what is needed. For example, it can be used to clean wastewater by converting ammonia into less harmful substances. But in another process, it can

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also be used to produce hydrogen gas, a clean fuel. This flexibility makes NiOOH-Ni valuable for various applications.

"NiOOH-Ni is impressively durable and stable, and it works well even after being used multiple times," says Associate Professor Andrey Lyalin from Hokkaido University, who was involved in the study. "This makes it a great alternative to traditional, more expensive catalysts like platinum, which aren't as effective at converting ammonia."

The catalyst's long-term reliability makes it suitable for large-scale industrial use, potentially transforming how industries handle wastewater and produce clean energy.

Phys Org, 8 August 2024

https://website





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## **Technical Notes**

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### **ENVIRONMENTAL RESEARCH**

Public drinking water contaminant estimates for birth cohorts in the Environmental Influences on Child Health Outcomes (ECHO) Cohort

Prospects and challenges of nanopesticides in advancing pest management for sustainable agricultural and environmental service

Rapid effects of plastic pollution on coastal sediment metabolism in nature

Ecosystem risk-based prioritization of micropollutants in wastewater treatment plant effluents across China

### PHARMACEUTICAL/TOXICOLOGY

Effects of pesticide exposure on the expression of selected genes in normal and cancer samples: Identification of predictive biomarkers for risk assessment

Innovative techniques for combating a common enemy forever chemical: A comprehensive approach to mitigating per- and polyfluoroalkyl substances (PFAS) contamination

<u>Cross-sectional and longitudinal associations of PAHs exposure with serum</u> <u>uric acid and hyperuricemia among Chinese urban residents: the potential</u> <u>role of oxidative damage</u>

Female teleworkers with pain have the highest presenteeism, where its primary contributing variable was not those of musculoskeletal disability