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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.

CHEMWATCH Bulletin Board

Concrete Reinvented: Al Simulates 4 Billion Atoms To Build Better

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ASIA PACIFIC

Funding unlocks clean drinking water access in regional Vic

2025-08-08

Murray Watt and Gayle Tierney splash \$23.8 million on pipes and plants to secure drinking water for a parched and growing regional Victoria.

New treatment facilities, critical water pipelines and a water supply connection are backing safe water supply for regional Victoria.

A total of \$23.8 million will flow to the water infrastructure projects to benefit growing populations across Glengarry, Toongabbie, Cowwarr, Willung, Rosedale, Allendale, Broomfield, Kingston, Newlyn, Smeaton, Springmount, Ballarat, Nyah and Piangil.

Announcing the funding, Minister for the Environment and Water Murray Watt said the projects would safeguard resources for communities, industries and environments that relied on access to water.

"The Albanese Labor government is pleased to partner with the Allan Labor government," Watt said.

"No matter where you live across Australia, you deserve access to clean drinking water. These projects will ensure new high-quality drinking water supplies for our regional Victorian communities."

Read More

The Mandarin, 08-08-25

https://www.themandarin.com.au/297239-funding-unlocks-cleandrinking-water-access-in-regional-vic/

Public willingness to pay for chemicals regulation policies in South Korea: Insights from socio-economic factors

2025-08-08

This study investigates the socio-economic determinants influencing public willingness to pay (WTP) for reducing health risks from phthalate exposure in South Korea. The study focuses on dibutyl phthalate (DBP), benzyl butyl phthalate (BBP), and di-(2-ethylhexyl) phthalate (DEHP)

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that are currently under regulatory consideration. Using the contingent valuation method, a national survey of 1,000 respondents employed both single-bounded (SBDC) and double-bounded dichotomous choice (DBDC) formats. The estimated mean WTP was 3,400 KRW (2.80 USD) using the SBDC model, closely aligning with theoretical expectations and the openended responses, while the DBDC spike model yielded a higher estimate of 6,071 KRW (5.10 USD). Regression analyses identified household income, education level, media exposure, and household size as significant determinants of WTP, indicating that these socio-economic and informational factors positively influence public willingness to financially support chemical risk reduction. Contrary to initial hypotheses, direct chemical exposure and previous harm experiences did not significantly affect WTP. Furthermore, individual income was not a significant factor, indicating that household-level financial decisions more strongly influence public WTP for chemical risk reduction. The results highlight the crucial role of socio-economic status and informational exposure in shaping public support for chemical regulation policies. This study provides foundational empirical data for effective policy design in South Korea, underscoring the importance of targeted informational campaigns and economic considerations to improve public risk perception and policy acceptance. These insights can inform international comparative analyses and help countries develop regulatory frameworks by assessing the economic values associated with chemical risk management.

Read More

Science Direct, 08-08-25

https://www.sciencedirect.com/science/article/abs/pii/ S0301479725027227

AMERICA

EPA Issues Final SNUR for Graphene Nanoplatelets (Generic)

2025-07-29

On July 29, 2025, the U.S. Environmental Protection Agency (EPA) issued final significant use rules (SNUR) for certain chemical substances, including graphene nanoplatelets (generic), that were the subject of premanufacture notices (PMN) and a Microbial Commercial Activity Notice (MCAN) and are also subject to an Order issued by EPA pursuant to

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the Toxic Substances Control Act (TSCA). 90 Fed. Reg. 35624. The SNURs require persons who intend to manufacture (including import) or process any of the chemical substances for an activity that is designated as a significant new use to notify EPA at least 90 days before commencing that activity. EPA notes that the manufacture or processing for the significant new use may not commence until EPA has conducted a review of the required notification, made an appropriate determination regarding that notification, and taken such actions as required by that determination. The final SNURs will be effective September 29, 2025.

Read More

AUG. 15, 2025

B&C, 29-07-25

https://www.lawbc.com/epa-issues-final-snur-for-graphene-nanoplatelets-generic/

Legislation Banning "Forever Chemicals" in Food Packaging in California by 2028 Will Likely Become Law 2025-08-07

The California Senate recently passed a bill, SB 682, that would essentially eliminate the use of per-and polyfluoroalkyl substances (PFAS), also known as "forever chemicals," in food packaging within the state, as of January 1, 2028. Given the broad support in the Senate for this bill and the fact that the California Assembly and Governor Gavin Newsom have been strong proponents of similar legislation in the past, SB 682 will likely be signed into law by September 2025, when the current legislative session ends.

Per-and polyfluoroalkyl substances (PFAS) are a class of fluorinated chemicals that have been used for over fifty years in a wide range of consumer, commercial, and industrial products, including in grease and water-resistant food packaging. PFAS are sometimes referred to as "forever chemicals," due to the ability of some PFAS to persist in the environment and in the human body. While there is no scientific consensus on the types or magnitude of risk that PFAS may pose to human health or the environment, public concern and media focus on these chemicals have led to significant restrictions on PFAS usage over the past few years, both by regulatory agencies and state legislatures.



California has been at the forefront of these efforts, with the state legislature passing a number of laws intended to reduce, phase out, or ban PFAS in consumer products.

Read More

JD Supra, 07-08-25

https://www.jdsupra.com/legalnews/legislation-banning-forever-chemicals-1919640/

Listing of Color Additives Exempt From Certification; Gardenia (Genipin) Blue; Correction

2025-08-01

The Food and Drug Administration (FDA or we) is correcting the order entitled "Listing of Color Additives Exempt from Certification; Gardenia (Genipin) Blue". In the order, FDA amended the color additive regulations to provide for the safe use of gardenia (genipin) blue in various foods, at levels consistent with good manufacturing practice (GMP). The order inadvertently misstated the methanol specification. This document corrects that error.

DATES:

Effective August 29, 2025.

FOR FURTHER INFORMATION CONTACT:

Stephen DiFranco, Office of Pre-market Additive Safety, Human Foods Program, Food and Drug Administration, 5001 Campus Dr., College Park, MD 20740, 240-402-2710; or Deirdre Jurand, Office of Policy, Regulations, and Information, Human Foods Program, Food and Drug Administration, 5001 Campus Dr., College Park, MD 20740, 240-402-2378.

SUPPLEMENTARY INFORMATION:

In FR Doc. 2025-13175, appearing on page 31586 in the Federal Register of Tuesday, July 15, 2025, the following corrections are made:

1. In the Supplementary Information section, in subsection II: Background, on page 31588, in the first column, in the middle of the first full paragraph, "6 mg/kg (6 ppm)" is corrected to read "300 mg/kg (300 ppm)".

§73.168

[Corrected]

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2. On page 31590, in the second column, in § 73.168, in paragraph (b) (3), "Methanol, not more than 6 mg/kg (6 ppm)." is corrected to read "Methanol, not more than 300 mg/kg (300 ppm)."

Read More

AUG. 15, 2025

US FDA, 01-08-25

https://www.federalregister.gov/documents/2025/08/06/2025-14905/listing-of-color-additives-exempt-from-certification-gardenia-genipin-blue-correction

EUROPE

Securing the forest carbon sink for the European Union's climate ambition

2025-08-01

The European Union (EU) climate policies rely on a functioning forest carbon sink. Forests cover about 40% of the EU area and have absorbed about 436 Mt of carbon dioxide equivalent per year between 1990 and 2022, which is about 10% of the EU's anthropogenic emissions. However, the ability of forests to act as carbon sinks is rapidly declining owing to increasing natural and anthropogenic pressures, threatening the EU's climate goals and calling for prompt actions. Here we provide actionable research recommendations to improve the monitoring and modelling of forest resources and their carbon sink, and to better inform forest management decisions. We suggest a timeline for the development of these measures to better support the implementation of strategies and policies outlined in the European Green Deal.

Read More

European commission, 01-08-25

https://publications.jrc.ec.europa.eu/repository/handle/JRC139211



European Commission calls for stakeholder input on how to help make EU environmental laws faster, easier and cheaper to implement

2025-007-28

On 22 July, the European Commission launched a Call for Evidence to simplify environmental legislation and reduce administrative burdens at implementation level.

The future environmental omnibus proposal will put together a series of measures intended to simplify environmental legislation concerning the circular economy, industrial emissions and waste management. The objective is to identify EU environmental policies that have the potential for real simplification for operators without affecting the EU's environmental objectives or the protection of human health.

The Commission is seeking stakeholder input on how to make EU environmental laws faster, easier and cheaper to implement, thereby making life easier for EU businesses. Measures can include streamlining administrative obligations, eliminating duplicate reporting requirements, promoting further digitalisation of reporting and addressing permitting challenges.

The Commission is also screening environmental legislation to identify legislative acts with administrative simplification potential and will analyse suggestions gathered from current and previous consultation processes.

All stakeholders are encouraged to respond using the Have Your Say portal. The Call for Evidence is open until 10 September.

Read More

European commission, 28-07-25

https://circulareconomy.europa.eu/platform/

EU Court overturns titanium dioxide carcinogen classification despite scientific evidence, marking victory for industry lobbies over public health protection in chemical regulation.

2025-08-07

The European Court of Justice has overturned the EU's 2020 classification of titanium dioxide in certain powdered forms as a suspected carcinogen

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when inhaled. The ruling confirms an earlier decision by the General Court, which considered that European authorities had made a "manifest error" in their assessment. This verdict is a victory for industrial lobby groups who have resisted the classification and a setback for public health.

Industry Challenge Succeeds Despite Scientific Evidence

The legal battle originated when multiple industry groups challenged the classification adopted by the European Commission in 2020 under the EU Regulation on the Classification, Labelling and Packaging of chemicals (CLP). The classification was based on a scientific opinion from the European Chemicals Agency (ECHA), which considered that the available scientific evidence indicated that the inhalation of certain forms of titanium dioxide particles could pose cancer risks to humans.

For foodwatch, the court's final judgment is contradictory and could invite further legal challenges of hazard classifications by industry lobby groups in the future. While the ruling acknowledges that the General Court exceeded its legal competences by questioning the scientific methodology behind ECHA's decision, it nevertheless upholds the annulment of the safety classification.

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FoodWatch, 07-08-25

https://www.foodwatch.org/en/eu-court-overturns-titanium-dioxide-classification

PAN Europe demands EU Commission to act on PFAS pesticides

2025-07-24

PAN Europe is calling out the European Commission for its inaction on PFAS pesticides. These substances break down into trifluoroacetic acid (TFA), a highly persistent, mobile and toxic degradation product. TFA has been detected above legal limits in groundwater across Europe. PAN Europe argues that the Commission is failing to meet its legal obligations under EU law to protect groundwater and public health.

TFA pollution could be Europe's most extensive contamination problem. It is widespread, by far the most frequently detected PFAS in our environment, is contaminating drinking water, and concentrations are rising, with PFAS pesticides identified as the main source. [1] Scientists have warned that TFA is a threat to 'planetary boundaries'. [2]



PAN Europe has repeatedly urged the Commission to ban all PFAS pesticides, yet no comprehensive action has been taken. In response, PAN Europe has now filed a formal request for internal review. This obliges the Commission to respond and enables PAN Europe to take the case to the EU Court if it fails to act. This step is unprecedented, as such reviews are usually used to challenge specific decisions. However, under the Aarhus Regulation they can also be used to contest a failure to take legally required action.

TFA has been shown to cause developmental toxicity in animal studies, including eye and skeletal malformations in rabbit offspring [3]. EU Pesticide Regulation prohibits approval of substances if they, or their toxic metabolites, lead to levels in groundwater exceeding the legal threshold of 0.1 μ g/L. Yet, monitoring data show that TFA already exceeds this threshold in many regions. [4] Continuing to allow PFAS based pesticides will inevitably lead to further contamination beyond legal levels.

Read More

PAN Europe, 24-07-25

https://www.pan-europe.info/press-releases/2025/07/pan-europedemands-eu-commission-act-pfas-pesticides

INTERNATIONAL

Why PETA US Is Changing Its No-Testing List Requirements

2025-08-07

If you've ever bought cosmetics, bath products, makeup, or personal care items, you will have seen the Beauty Without Bunnies logo. Borne of a pioneering campaign launched by PETA US in the 1980s, Beauty Without Bunnies is a cruelty-free programme designed to provide consumers with information on companies that do and don't test on animals. The list of certified companies has grown immensely over the years, from fewer than a dozen to a searchable online global database of more than 6,300 companies.

In the decades since its inception, companies from as far as the UK, Australia, and Europe have joined the programme. Now, due to testing requirements in the EU, companies that sell in some countries will no longer be eligible to be listed as cruelty-free.

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The Conflict Between Chemicals and Cosmetics Regulations

The issue lies in the differing objectives of the EU's Cosmetics Regulation and the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), the EU's large-scale testing programme for industrial chemicals.

Cosmetics ingredient manufacturers are subject to numerous regulatory requirements, including REACH. While the Cosmetics Regulation aims to ensure the safety of products and ingredients by relying on human-relevant, non-animal tests, REACH mandates a prescribed list of test data, often requiring tests on animals.

This discrepancy has led to animal testing on cosmetic ingredients to comply with REACH, undermining the animal-test-free status of these products and creating a loophole that PETA has been fighting to close

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PETAUK, 07-08-25

https://www.peta.org.uk/blog/beauty-without-bunnies-changes/



Rolling Action Plan (RAP) for UK REACH 2025, 2026 and 2027

2025-08

- 1. In accordance with Article 44 of UK REACH and the criteria outlined in the "Approach to substance evaluation in UK REACH", the UK rolling action plan (RAP) is updated as shown in table 1.
 - Our approach to substance selection seeks to complement rather than replicate evaluation work that has been or will be performed by other regulatory regimes (such as via EU REACH) and avoid unnecessary duplication of work where testing is indicated as the outcome of evaluation.
 - The selection of substances for inclusion in the RAP is based on the hazard profile of substances and their exposure potential in GB, including consideration of the quantities supplied. We consider information from the following sources to identify priorities: the GB specific registration data, where available, within the UK database (Comply with UK REACH)
- UK REACH processes (such as dossier evaluation)
- Other intelligence such as the Environment Agency's Prioritisation and Early Warning System (PEWS) and horizon scanning of other regulatory regimes, both domestic (e.g., GB CLP) and international (e.g., EU REACH and positions on chemicals adopted by other countries)

 Substances that are registered under UK REACH can be prioritised for evaluation where a potential concern has been identified (such as where there are grounds for considering that a substance constitutes a risk to human health or the environment). An evaluation will determine if a conclusion on the concern can be drawn from the available data. If a conclusion cannot be drawn, we can as the Agency for UK REACH, request that registrants provide additional information. In such cases, deadlines will be set by which the information shall be provided. A substance will only be included in the RAP where a request for further information from the UK registrants may help to clarify the concern.

Using the sources referred to in paragraph 3, along with the criteria referred to in paragraph 1, the Agency has not identified any priorities to take forward for formal substance evaluation under UK REACH in 2025. However, we will continue to consider the information available to us to define future priorities.

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REACH Update

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Read More

UK REACH

https://www.hse.gov.uk/reach/reports/rap/rap2527.htm

Janet's Corner

AUG. 15, 2025

100

Who am I?

2025-08-15

I am the eighth element on the periodic table. I'm a nonmetal and a crucial component of the air you breathe, making up about 21% of Earth's atmosphere. I'm highly reactive and support combustion, meaning things burn much more readily in my presence. You need me to live, and I'm often found in compounds with silicon in the Earth's crust.

(Send in your answers and get a surprise Chemwatch merch from us for free)

I am the eighth element on the periodic table.

Silver

2025-08-15

CHEMWATCH

Hazard Alert

Silver is a chemical element with symbol Ag and atomic number 47. The metal occurs naturally in its pure, free form (native silver), as an alloy with gold and other metals, and in minerals such as argentite and chlorargyrite. Most silver is produced as a by-product of copper, gold, lead, and zinc refining. [1]

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Pure silver is nearly white, lustrous, soft, very ductile, malleable, it is an excellent conductor of heat and electricity. It is not a chemically active metal, but it is attacked by nitric acid (forming the nitrate) and by hot concentrated sulfuric acid. It has the highest electrical conductivity of all metals, but its greater cost has prevented it from being widely used for electrical purposes. Silver does not oxidise in air but reacts with the hydrogen sulfide present in the air, forming silver sulfide (tarnish). This is why silver objects need regular cleaning. Silver is stable in water. [1,2]

USES [2,3]

Silver is used to make jewellery, silverware, electronic equipment, and dental fillings. It is also used to make photographs, in brazing alloys and solders, to disinfect drinking water and water in swimming pools, and as an antibacterial agent. Silver has also been used in lozenges and chewing gum to help people stop smoking.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Exposure Sources

- Breathing low levels in air.
- Swallowing it in food or drinking water.
- Carrying out activities such as jewellery making, soldering, and photography.
- Using anti-smoking lozenges or other medicines containing it.

Routes of Exposure

Silver's wide variety of uses allows exposure through various routes of entry into the body. Ingestion is the primary route of entry for silver compounds and colloidal silver proteins. Inhalation of dusts or fumes containing silver occurs primarily in occupational settings. Skin contact occurs in occupational settings, from the application of burn creams and from contact with jewellery. Silver can also gain entry into the body

Hazard Alert

through the use of acupuncture needles, catheters, dental amalgams, or accidental puncture wounds.

HEALTH EFFECTS [4]

Acute Health Effects

- Exposure to high levels of silver for a long period of time may result in a condition called arygria, a blue-grey discoloration of the skin and other body tissues. Argyria is a permanent effect, but it appears to be a cosmetic problem that may not be otherwise harmful to health.
- Lower-level exposures to silver may also cause silver to be deposited in the skin and other parts of the body; however, this is not known to be harmful.
- Eye contact: may cause severe corneal injury if liquid comes in contact with the eyes.
- Skin contact: may cause skin irritation. Repeated and prolonged contact with skin may cause allergic dermatitis.
- Inhalation hazards: exposure to high concentrations of vapours may cause dizziness, breathing difficulty, headaches or respiratory irritation. Extremely high concentrations may cause drowsiness, staggering, confusion, unconsciousness, coma or death.
- Liquid or vapour may be irritating to skin, eyes, throat, or lungs.
 Intentional misuse by deliberately concentrating and inhaling the contents of this product can be harmful or fatal.
- Ingestion hazards: moderately toxic. May cause stomach discomfort, nausea, vomiting, diarrhoea, and narcosis.
- Aspiration of material into lungs if swallowed or if vomiting occurs can cause chemical pneumonitis, which can be fatal.
- Animal studies have shown that swallowing silver results in the deposit
 of silver in the skin. One study in mice found that the animals exposed
 to silver in drinking water were less active than unexposed animals.
- No studies are available on whether silver affects reproduction or causes developmental problems in people.
- No studies are available on whether silver may cause cancer in people.
- The only available animal studies showed both positive and negative results when silver was implanted under the skin.
- The EPA has determined that silver is not classifiable as to human carcinogenicity.

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SAFETY

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First Aid Measures [5]

- Eye Contact: Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.
- Skin Contact: After contact with skin, wash immediately with
 plenty of water. Gently and thoroughly wash the contaminated skin
 with running water and non-abrasive soap. Be particularly careful
 to clean folds, crevices, creases and groin. Cover the irritated skin
 with an emollient. If irritation persists, seek medical attention. Wash
 contaminated clothing before reusing.
- Serious Skin Contact: Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.
- **Inhalation:** Allow the victim to rest in a well ventilated area. Seek immediate medical attention.
- Ingestion: Do not induce vomiting. Examine the lips and mouth to
 ascertain whether the tissues are damaged, a possible indication that
 the toxic material was ingested; the absence of such signs, however,
 is not conclusive. Loosen tight clothing such as a collar, tie, belt or
 waistband. If the victim is not breathing, perform mouth-to-mouth
 resuscitation. Seek immediate medical attention.

Workplace Controls & Practices [4]

- Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits.
- If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protective Equipment [5]

The following personal protective equipment is recommended when handling silver:

- Splash goggles;
- · Lab coat.

Personal Protection in Case of a Large Spill:

- Splash goggles;
- Full suit;

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- Boots;
- Gloves.
- Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

REGULATION

United States

Exposure Limit	Limit Values	HE Codes	Health Factors and Target Organs
OSHA Permissible Exposure Limit (PEL) - General Industry See <u>29 CFR</u> <u>1910.1000 Table</u> <u>Z-1</u>	0.01 mg/m³ TWA	HE3	Argyria
OSHA PEL - Construction Industry See <u>29 CFR</u> <u>1926.55 Appendix</u> <u>A</u>	0.01 mg/m³ TWA	HE3	Argyria
OSHA PEL - Shipyard Employment See 29 CFR 1915.1000 Table Z-Shipyards	0.01 mg/m³ TWA	HE3	Argyria
National Institute for Occupational Safety and Health (NIOSH) Recommended Exposure Limit (REL)	0.01 mg/m³ TWA	HE3	Argyria
		HE4	Eye and skin burns
		HE14	Eye and skin irritation

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Exposure Limit	Limit Values	HE Codes	Health Factors and Target Organs
American Conference of Governmental Industrial Hygienists (ACGIH) Threshold Limit Value (TLV) (2001)	Metal dust: 0.1 mg/m³ TWA Soluble compounds: 0.01 mg/m³ TWA	HE3	Argyria
CAL/OSHA PELs	Metal: 0.01 mg/m³ TWA Soluble compounds: 0.01 mg/m³ TWA		

References

- 1. https://en.wikipedia.org/wiki/Silver
- 2. http://www.lenntech.com/periodic/elements/ag.htm
- 3. http://www.atsdr.cdc.gov/toxfaqs/tf.asp?id=538&tid=97
- 4. http://annhyg.oxfordjournals.org/content/49/7/575.full
- 5. http://www.sciencelab.com/msds.php?msdsld=9927253
- 6. http://www.safeworkaustralia.gov.au/sites/SWA/about/Publications/Documents/772/Workplace-exposure-standards-airborne-contaminants.pdf

Gossip

A new type of vaccine is needle-free and doubles as dental floss

2025-08-09

In a recent experiment that sounds more sci-fi than science class, researchers have successfully developed a novel vaccine platform that uses ordinary dental floss embedded with tiny dissolvable microneedles. The study, published in Nature Biomedical Engineering, showcases how everyday materials can be reimagined to offer adaptable and accessible vaccine solutions.

Researchers at North Carolina State University and the University of North Carolina at Chapel Hill have developed a microneedle-thread platform designed to deliver vaccine antigens through oral mucosal tissue. In preclinical trials, they investigated whether this approach could induce both local and systemic immune responses – a strategy intended to enhance protection against pathogens that enter through the respiratory tract.

This new method targets the junctional epithelium, the "leaky" tissue where gums meet teeth. On any given day, this permeable region serves as an immunological checkpoint, allowing immune cells to surveil for bacteria accumulating along the gumline. Intrigued by its natural permeability, researchers asked a deceptively simple question: could this oral gateway be repurposed to deliver vaccines?

To put their idea to the test, the team turned to the lab, where they conducted controlled experiments in mice to assess delivery through the gingival sulcus – a permeable, densely vascularized tissue with direct access to immune surveillance. Instead of syringes, they used a strand of floss: biodegradable threads embedded with dissolvable microneedles designed to deliver antigens directly into the tissue (imagine that on your resume: mouse flosser intern).

The results were striking. Mice that received vaccines via floss developed strong immune responses across multiple arms of immunity: mucosal antibodies, systemic antibodies, and T cells. These responses were achieved using a variety of vaccine formats, including protein antigens, inactivated virus, nanoparticles, and mRNA. In one trial, all mice vaccinated against influenza using the floss-based method survived a normally lethal viral challenge, while the unvaccinated mice did not.

What makes this unconventional vaccination site so effective comes down to its biology. Unlike skin, which acts as a tight physical barrier, the junctional epithelium is naturally porous. CHEMWATCH

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Gossip

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"This is a unique gateway," explained Harvinder Singh Gill, corresponding author of the study and professor of nanomedicine at North Carolina State University. "Mucosal surfaces are a common entry point for respiratory pathogens like influenza and COVID. Delivering a vaccine here allows us to generate immune responses not only in the bloodstream, but also right where the pathogen tries to enter."

This dual-action response is pivotal. Traditional injected vaccines typically stimulate systemic immunity alone. But when delivered at mucosal sites, vaccines can also produce local antibodies, such as IgA, which coat mucosal membranes in the nose, throat, and lungs; creating a first line of defense.

To explore whether this method could translate to humans, the researchers conducted a pilot study using floss picks impregnated with dye in place of the vaccine. Volunteers then used the floss picks to work the dye into their gums at the gingival sulcus. In about 60% of participants, the dye was successfully deposited – a promising sign that human tissue may be similarly receptive to this oral delivery route.

That said, the technique wouldn't apply to infants and toddlers who lack teeth, and researchers note that its performance in people with gum disease or oral infections remains an open question.

If further research confirms safety and efficacy in humans, floss-based vaccines might one day serve as a supplemental tool, targeting respiratory viruses at their point of entry. While further testing is needed, the study serves as a reminder that medical innovation doesn't always require high-tech solutions, sometimes it just takes repurposing a common tool.

This study was published in the journal Nature: Biomedical Engineering.

Source: North Carolina State University and Science News

New Atlas, 9 August 2025

https://newatlas.com

Concrete Reinvented: AI Simulates 4 Billion Atoms To Build Better Materials

2025-08-03

Imagine a future where buildings don't just stand the test of time—they actively fight climate change.

Toward Smart, Sustainable Concrete

Picture a future where the concrete used in buildings and bridges not only resists aging and extreme conditions, such as intense wildfire heat, but also repairs itself or absorbs carbon dioxide from the air.

Scientists at the USC Viterbi School of Engineering have now introduced a groundbreaking artificial intelligence model capable of simulating billions of atoms at once. This advancement unlocks a new era in material design, enabling discoveries at a scale previously thought impossible.

Climate change is rapidly intensifying. Droughts, melting glaciers, and increasingly destructive storms and wildfires are becoming more frequent and severe. A key factor driving global warming is the steady release of carbon dioxide into the atmosphere.

From Wildfires to Innovation

After witnessing the devastating January wildfires in Los Angeles, USC Viterbi professor Aiichiro Nakano (who specializes in computer science, physics, astronomy, and computational biology) began rethinking how science could help. He contacted longtime research collaborator Kenlchi Nomura, a fellow USC Viterbi professor with expertise in chemical engineering and materials science. The two have worked together for over two decades.

Their conversation led to the creation of Allegro-FM, an advanced Alpowered simulation platform. In their theoretical research, the model revealed something remarkable: it may be possible to reabsorb the carbon dioxide released during concrete production by embedding it back into the same material.

"You can just put the CO2 inside the concrete, and then that makes a carbon-neutral concrete," Nakano said.

CO2 Sequestration, Reimagined

Nakano and Nomura, along with Priya Vashishta, a USC Viterbi professor of chemical engineering and materials science, and Rajiv Kalia, a USC professor of physics and astronomy, have been doing research on what they call "CO2 sequestration," or the process of recapturing carbon dioxide and storing it, a challenging process.

By simulating billions of atoms simultaneously, Allegro-FM can test different concrete chemistries virtually before expensive real-world experiments. This could accelerate the development of concrete that acts

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as a carbon sink rather than just a carbon source — concrete production currently accounts for about 8% of global CO2 emissions.

The breakthrough lies in the model's scalability. While existing molecular simulation methods are limited to systems with thousands or millions of atoms, Allegro-FM demonstrated 97.5% efficiency when simulating over four billion atoms on the Aurora supercomputer at Argonne National Laboratory.

This represents computational capabilities roughly 1,000 times larger than conventional approaches.

Predicting Across the Periodic Table

The model also covers 89 chemical elements and can predict molecular behavior for applications ranging from cement chemistry to carbon storage.

"Concrete is also a very complex material. It consists of many elements and different phases and interfaces. So, traditionally, we didn't have a way to simulate phenomena involving concrete material. But now we can use this Allegro-FM to simulate mechanical properties [and] structural properties," Nomura said.

Concrete is a fire-resistant material, making it an ideal building choice in the wake of the January wildfires. But concrete production is also a huge emitter of carbon dioxide, a particularly concerning environmental problem in a city like Los Angeles. In their simulations, Allegro-FM has been shown to be carbon neutral, making it a better choice than other concrete.

Echoes of Ancient Engineering

This breakthrough doesn't only solve one problem. Modern concrete only lasts about 100 years on average, whereas ancient Roman concrete has lasted for over 2,000 years. But the recapture of CO2 can help this as well.

"If you put in the CO2, the so-called 'carbonate layer,' it becomes more robust," Nakano said.

In other words, Allegro-FM can simulate a carbon-neutral concrete that could also last much longer than the 100 years concrete typically lasts nowadays. Now it's just a matter of building it.



Behind the Scenes

The professors led the development of Allegro-FM with an appreciation for how AI has been an accelerator of their complex work. Normally, to simulate the behavior of atoms, the professors would need a precise series of mathematical formulas — or, as Nomura called them, "profound, deep quantum mechanics phenomena."

But the last two years have changed the way the two research.

"Now, because of this machine-learning AI breakthrough, instead of deriving all these quantum mechanics from scratch, researchers are taking [the] approach of generating a training set and then letting the machine learning model run," Nomura said. This makes the professors' process much faster as well as more efficient in its technology use.

A Unified Atomic Model

Allegro-FM can accurately predict "interaction functions" between atoms — in other words, how atoms react and interact with each other. Normally, these interaction functions would require lots of individual simulations.

But this new model changes that. Originally, there were different equations for individual elements within the periodic table, with several unique functions for these elements. With the help of Al and machine-learning, though, we can now potentially simulate these interaction functions with nearly the entire periodic table at the same time, without the requirement for separate formulas.

"The traditional approach is to simulate a certain set of materials. So, you can simulate, let's say, silica glass, but you cannot simulate [that] with, let's say, a drug molecule," Nomura said.

Efficiency and Quantum-Level Accuracy

This new system is also a lot more efficient on the technology side, with Al models making lots of precise calculations that used to be done by a large supercomputer, simplifying tasks and freeing up that supercomputer's resources for more advanced research.

"[The AI can] achieve quantum mechanical accuracy with much, much smaller computing resources," Nakano said.

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The Road Ahead

Nomura and Nakano say their work is far from over.

"We will certainly continue this concrete study research, making more complex geometries and surfaces," Nomura said.

This research was published recently in The Journal of Physical Chemistry Letters and was featured as the journal's cover image.

Sci Tech Daily, 3 August 2025

https://scitechdaily.com

Cheap virgin plastic limits recycling potential

2025-08-13

Global plastic treaty negotiations risk being derailed by minority opposed to production caps

This week, government negotiators are meeting in Switzerland to try and agree the final details of a global treaty to end plastic pollution, closely watched by lobbyists from across industry and environmental groups.

So far, negotiations have been slowed by a staunch minority coalition of countries whose economies rely heavily on plastics and petrochemicals. They are pushing for the treaty to focus primarily on improving collection and recycling of plastic waste – to prevent it ending up in the environment – without including commitments to reduce production of virgin plastic materials, or to restrict use of certain chemicals within plastic production that increase the hazard posed by plastic during and after its use.

Groups representing the plastics and associated chemicals industries have lobbied hard for a similar focus on waste management and recycling, and strongly resisted efforts to formalise any kind of cap on new plastic production.

As it stands, initiatives to increase levels of plastic recycling have so far had relatively little impact. Collecting, cleaning, separating and processing material for recycling – particularly in ways that yield high-quality materials for food contact or other demanding applications – is expensive, and those costs are relatively fixed. Favourable oil prices and expanding production capacity in Asia and the US mean that virgin plastic is significantly cheaper than recycled material in many cases.

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The EU has introduced broad plastic and packaging waste regulations

to promote recycling and reduce non-recycled plastic waste. The UK has implemented taxes intended to penalise businesses if their plastic packaging incorporates less than 30% recycled materials.

While this may be achievable in some applications, domestic supplies of suitable recycled materials are limited and expensive compared to virgin plastic. Several UK recycling facilities aiming to produce such materials are facing closure – within the last week, Biffa has said it will close a plant in Sunderland and Viridor will decommission its site in Rochester, Kent, having also stopped recycling at Avonmouth.

Large volumes of UK plastic waste are exported cheaply for processing abroad, but there is little clarity on what proportion of that waste is actually recycled. Likewise, many businesses import materials that purport to include recycled content, but are cheaper than verified UK recyclates. But with relatively little oversight and enforcement, there are suggestions that significant portions of such materials do not meet the criteria to be classed as recycled, and yet are still dodging the UK's plastic tax.

But if we are ever to reach a more circular plastic economy, there has to be consistent and economic supply and demand for recycled materials. By necessity, that means virgin materials must become more expensive – either by taxation, limiting production or both. As long as virgin plastic is cheap and abundant, recyclates will struggle to compete.

Chemistry World, 13 August 2025

https://chemistryworld.com

You're inhaling 68,000 bits of microplastic at home every single day

2025-07-31

Research out of the University of Toulouse, France, has revealed that we're probably harming our lungs a lot more than we knew. Every day, we're inhaling teeny tiny bits of plastic that are smaller than a speck of dust without even leaving the house – and the findings show the amount is 100 times greater than previously estimated.

That's from a study led by researcher Nadiia Yakovenko, who measured fine microplastic particles seven times thinner than a strand of human hair, suspended in the air in both homes and cars (including Yakovenko's CHEMWATCH

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own apartment) a couple of years ago. Yakovenko's paper on the research appeared in PLOS this week.

We've known about the presence of microplastics for a couple of decades now, and they've been polluting our oceans, our food, and our water for much longer than that. As Yakovenko explained in an interview, these miniscule fragments "can enter deep into our respiratory system and potentially cause inflammation or irritation. Microplastics carry toxic additives, such as bisphenol A, or phthalates, which can reach our bloodstream. While research is still ongoing, there is concern that long-term exposure to microplastics and their additives may contribute to respiratory problems, disrupt endocrine function and increase risk for neurodevelopmental disorders, reproductive birth defects, infertility, cardiovascular disease, and cancers."

Our general understanding of microplastics has led us to believe they're mostly concentrated in polluted oceans and industrial areas, but this study highlights how we're basically surrounded by these particles even in places we think of as safe and clean. Previous efforts to study air quality have only ever identified particles, ranging from 20 to 200 micrometers in diameter, which are on the larger side and are less likely to penetrate the lungs. than particles of 10 micrometers across or less.

To arrive at an accurate scale of the amount of microplastics we're exposed to in our homes and cars, the researchers used an analytical technology called Raman Spectroscopy to study tiny particles with the help of lasers, along with a microscope and free software to count the number of objects in an image. This method allowed the team to quantify even small microplastics down to one micrometer.

What the researchers found was alarming: adults inhale about 3,200 larger microplastic particles per day in the range of 10 to 300 micrometers across, and 68,000 tinier particles of 1 to 10 micrometers per day. The team notes this is 100 times more than previous estimates of the amount of small-diameter particles.

So how do all these microplastics find a way into our homes and vehicles? They basically break off from slowly degrading plastic objects like frequently used household items, carpeting, and fabrics. And most cars typically have a range of plastic-based materials on the inside (like the dashboard and seats) that are worn down from day-to-day use, and the heat and solar irradiance from the sun. And all this is in addition to the microplastics we already know we're already exposing ourselves to. A

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recent study showed that a packaged bottle of water was found to contain

This is worrying, because it shows that we've previously underestimated – and may continue to do so – how much microplastic we're unknowingly allowing into our environments and our bodies. We also don't yet know the full extent of the harm this can cause.

But studies like Yakovenko's can inform the choices we make in the materials we use, the measures we put in place to negate the harmful effects of microplastics, and the health recommendations and standards we enforce to create safe indoor environments. The team plans to apply its approach to study air quality in different indoor settings for a more comprehensive understanding of the pervasiveness of microplastics in the air around us.

Sources: PLOS, EurekAlert

240,000 fragments of plastic.

New Atlas, 31 July 2025

https://newatlas.com

Chemists synthesize a new allotrope of carbon

2025-08-14

In a new study led by Oxford University's Department of Chemistry, chemists have demonstrated the synthesis of a cyclocarbon that is stable enough for spectroscopic characterization in solution at room temperature. The study is published in the journal Science.

The synthesis of a new type of molecular carbon allotrope that can be studied under normal laboratory conditions is a rare achievement. The only previous example was the synthesis of fullerenes in 1990.

In the new study, the molecule cyclo[48]carbon was synthesized as a catenane, i.e. with the C48 ring threaded through three other macrocycles. These threaded macrocycles increase the stability of C48 by preventing access to the protected cyclocarbon.

Previously, molecular rings consisting purely of carbon atoms have only been studied in the gas phase or at very low temperatures (4 to 10 K). Now, the team have synthesized a cyclocarbon that is stable in solution at 20°C (half-life 92 hours). This has been achieved by using threaded macrocycles, choosing a large cyclocarbon with a low level of strain, and developing

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mild reaction conditions for the unmasking step in the reaction (where a precursor molecule is transformed into the final product).

The cyclocarbon catenane was characterized by mass spectrometry, NMR, UV-visible and Raman spectroscopy. The observation of a single intense 13C NMR resonance for all 48 sp1 carbon atoms indicates that all of the carbons are in equivalent environments, which provides strong evidence for the cyclocarbon catenane structure.

Lead author Dr. Yueze Gao (Department of Chemistry, University of Oxford) said, "Achieving stable cyclocarbons in a vial at ambient conditions is a fundamental step. This will make it easier to study their reactivity and properties under normal laboratory conditions."

Study senior author, Professor Harry Andersen (Department of Chemistry, University of Oxford), said, "This achievement marks the culmination of a long endeavor to synthesize cyclocarbon catenanes, based on the hope that they might be stable enough to study at room temperature.

"The original grant proposal was written in 2016, based on preliminary results from 2012–2015. It is satisfying to have reached this point, because there were many times when the goal seemed unrealistic and unachievable. This work would not have been possible without the outstanding facilities for NMR spectroscopy in the Department of Chemistry at Oxford."

Phys Org, 14 August 2025

https://phys.org

The "Love Hormone" Is Also the "Friendship Hormone"

2025-08-12

A new UC Berkeley study shows that the so-called love hormone, oxytocin, is also critical for the formation of friendships.

Oxytocin is released in the brain during sex, childbirth, breastfeeding and social interactions and contributes to feelings of attachment, closeness and trust. Never mind that it's also associated with aggression; the hormone is commonly referred to as the "cuddle" or "happy" hormone, and people are encouraged to boost their oxytocin levels for better well-being by touching friends and loved ones, listening to music and exercising.

But recent studies involving the prairie vole have called this love association into question. They've shown that oxytocin, which in the brain

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acts as a neuromodulator, is not essential for long-term mate bonding, or "social monogamy," or for parenting behavior, though without it, voles take

longer to form such bonds.

Scientists focus on prairie voles because, like humans, they form stable and selective relationships. While most studies focus on mate bonds, the Beery lab at UC Berkeley is particularly interested in selective peer relationships, analogous to human friendships. Such studies could shed light on human psychiatric conditions, such as autism and schizophrenia, that interfere with a person's ability to form or maintain social bonds.

"Prairie voles are special because they allow us to get at the neurobiology of friendship and how it's similar to and different from other types of relationships," said Annaliese Beery, a UC Berkeley associate professor of integrative biology and neuroscience and senior author of the study.

Beery and integrative biology graduate student Alexis Black, one of two first authors of the study, found that prairie voles that lack oxytocin receptors take longer than normal voles to form peer relationships. Prairie voles that are close friends typically huddle side by side, groom and even sit on one another.

"Oxytocin seems to be particularly important in the early formation phase of relationships and especially in the selectivity of those relationships: 'I prefer you to this stranger,' for example," Beery said. "The animals that didn't have intact oxytocin signaling took longer to form relationships. And then when we challenged those relationships by making new groups, they lost track of their original partners right away."

The voles, genetically modified in the UC San Francisco laboratory of collaborator and co-author Dr. Devanand Manoli, also lacked the social rewards that normally come from selective attachments — they didn't work very hard to snuggle up with their friends and were less avoidant of and less aggressive towards strangers.

"In other words, oxytocin is playing a crucial role not so much in how social they are, but more in who they are social with, their selectivity," she said.

Lacking oxytocin receptors also changed the regulation of oxytocin availability and release in the brain, which the group documented using a novel oxytocin nanosensor in collaboration with postdoctoral fellow Natsumi Komatsu and Markita Landry, a UC Berkeley professor of chemical and biomolecular engineering.

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"That helped us understand the feedback consequences of lacking this receptor, and how oxytocin signaling was altered in the brain," said Beery.

The study was published Aug. 8 in the journal Current Biology.

What social voles tell us about social humans

Beery has long been interested in social relationships in rodents, focusing primarily on the animals' seldom-studied peer or friendship relationships. While voles are her main focus, she believes studying similar behaviors across multiple species is key to determining what's species-specific versus generalizable across species.

To complement her laboratory research, she has conducted field studies comparing social behavior and oxytocin receptor distribution in the brain within and across species in a group of South American rodents and North American Belding's ground squirrels, which vary in whether or not they live in groups. She also recently began field tests of multiple vole species — there are about 50 worldwide — to compare their social behavior.

She suspects that in rodents such as voles, and perhaps in other mammals, the formation of peer relationships may have preceded the evolution of monogamous mating relationships.

"While most rodents prefer to interact with unfamiliar individuals, it turns out that the majority of vole species we've tested in our early trials form peer-partner preferences, which is what we call these selective friendships. So there seems to be this widespread tendency to bond," Beery said. "But only a couple of those species are also monogamous. Someday, I hope to be able to tell you, 'Do selective peer relationships precede the development of monogamy? Is that why monogamy has evolved so many times in this genus?' I think this familiarity preference is deeply rooted."

Beery was a co-author of a 2023 study led by Manoli that threw into question the association of oxytocin with sex and parenting. That study showed that prairie voles unable to respond to oxytocin exhibit the same monogamous mating, attachment and parenting behaviors as regular voles. Those voles had been genetically engineered to have no cellular receptors for oxytocin, and were the same voles used in the current study.

But while oxytocin isn't essential for eventual bond formation, additional studies by the same group published in 2024 showed that these receptor-deficient (or "null mutant") prairie voles took about twice as long as normal voles to establish a relationship with a potential mate.

Interested in how the lack of an oxytocin receptor affects voles' friendship bonds, as opposed to mating bonds, Beery and Black conducted three

sets of experiments. In one, they tested how long it took for voles to establish a preference for a partner. Whereas normal voles take about 24 hours of close proximity to form a relationship that makes them choose that partner over a stranger, oxytocin receptor-deficient voles showed no preference in that amount of time, and took up to a week to establish a peer preference.

"Wild-type animals form this incredibly robust preference within one day of co-housing, but the null mutants have no sign of a relationship after 24 hours. After a week, they mostly get there, and the lifetime partners look no different from each other," Beery said. "Our conclusion from that experiment is that oxytocin isn't required to have a relationship, but it's really important in those early phases of a relationship to facilitate it happening quickly and efficiently."

They then put long-term pair-bonded voles in a party-like, mixed-group situation: an enclosure with other voles and many rooms connected by tubes. In such a situation, normal voles would hang out with known friends until they eventually started to socialize with strangers.

"They can all separate, they can all come together, or they can hang out in any combinations that they want," she said. "The wild-type animals keep track of who they know. It's like if I went to a party with a friend, I would stand near that friend for the first part of the party and then I might start to mingle. The voles that lack oxytocin receptors just mixed. It was as if they didn't even have a partner in there with them."

In the third experiment, they tested the strength of both peer and mate bonding by having the voles press levers to get access to either a friend/ mate or a stranger.

"Female wild-type voles typically press more to get their partner than to get a stranger, in both peer and mate relationships. The oxytocin receptor deficient mutants also press more to get to their mating partner, but not for peer relationships," Beery said. "That makes sense at some level because we think mate relationships are more rewarding than peer relationships, or at least they depend more on reward-signaling pathways."

Lack of oxytocin signaling thus not only delays the formation of relationships, but also creates deficits in long-term peer relationships.

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On the flip side, voles lacking oxytocin receptors were also less aggressive toward strangers and less avoidant of them.

"You can see contributions of oxytocin signaling to both sides of selectivity," Beery said. "On the prosocial side, it's involved in wanting to be with a known friend or peer, while on the antisocial side, it's aiding in rejecting an unfamiliar animal. We've seen effects of oxytocin on both affiliation and aggression in our other studies in prairie voles, and it parallels human findings on a role of oxytocin in in-group/out-group dynamics."

Oxytocin nanosensors

The researchers used a new oxytocin sensor developed in Landry's UC Berkeley lab to determine whether lack of an oxytocin receptor caused increases or decreases in oxytocin release. If oxytocin release increased in these voles, it could potentially interact with a receptor for a similar neuropeptide that is also involved in formation of social relationships, compensating for the absence of oxytocin receptors.

Landry, an associate professor in the departments of chemical and biomolecular engineering, neuroscience, and molecular and cell biology and a co-corresponding author of the paper, created these sensors from carbon nanotubes joined with specific single-stranded DNA sequences selected because they latch onto the oxytocin molecule and fluoresce. Komatsu and Landry found no excess of oxytocin in the voles' brains. In fact, oxytocin was being released in lower amounts from fewer sites in the nucleus accumbens, a key brain region for social reward across species.

Technology Networks, 12 August 2025

https://technologynetworks.com

Coffee fortified with iron—new microparticles can be added to food and beverages to fight malnutrition

2025-08-13

Around the world, about 2 billion people suffer from iron deficiency, which can lead to anemia, impaired brain development in children, and increased infant mortality.

To combat that problem, MIT researchers have come up with a new way to fortify foods and beverages with iron, using small crystalline particles. These particles, known as metal-organic frameworks, could be sprinkled

on food, added to staple foods such as bread, or incorporated into drinks

"We're creating a solution that can be seamlessly added to staple foods across different regions," says Ana Jaklenec, a principal investigator at MIT's Koch Institute for Integrative Cancer Research.

"What's considered a staple in Senegal isn't the same as in India or the U.S., so our goal was to develop something that doesn't react with the food itself. That way, we don't have to reformulate for every context—it can be incorporated into a wide range of foods and beverages without compromise."

The particles designed in this study can also carry iodine, another critical nutrient. The particles could also be adapted to carry important minerals such as zinc, calcium, or magnesium.

"We are very excited about this new approach and what we believe is a novel application of metal-organic frameworks to potentially advance nutrition, particularly in the developing world," says Robert Langer, the David H. Koch Institute Professor at MIT and a member of the Koch Institute.

Jaklenec and Langer are the senior authors of the study, which appears in the journal Matter. MIT postdoc Xin Yang and Linzixuan (Rhoda) Zhang, Ph.D. are the lead authors of the paper.

Iron stabilization

like coffee and tea.

Food fortification can be a successful way to combat nutrient deficiencies, but this approach is often challenging because many nutrients are fragile and break down during storage or cooking. When iron is added to foods, it can react with other molecules in the food, giving the food a metallic taste.

In previous work, Jaklenec's lab has shown that encapsulating nutrients in polymers can protect them from breaking down or reacting with other molecules. In a small clinical trial, the researchers found that women who ate bread fortified with encapsulated iron were able to absorb the iron from the food.

However, one drawback to this approach is that the polymer adds a lot of bulk to the material, limiting the amount of iron or other nutrients that end up in the food.

"Encapsulating iron in polymers significantly improves its stability and reactivity, making it easier to add to food," Jaklenec says. "But to be

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effective, it requires a substantial amount of polymer. That limits how much iron you can deliver in a typical serving, making it difficult to meet daily nutritional targets through fortified foods alone."

To overcome that challenge, Yang came up with a new idea: Instead of encapsulating iron in a polymer, they could use iron itself as a building block for a crystalline particle known as a metal-organic framework, or MOF (pronounced "moff").

MOFs consist of metal atoms joined by organic molecules called ligands to create a rigid, cage-like structure. Depending on the combination of metals and ligands chosen, they can be used for a wide variety of applications.

"We thought maybe we could synthesize a metal-organic framework with food-grade ligands and food-grade micronutrients," Yang says.

"Metal-organic frameworks have very high porosity, so they can load a lot of cargo. That's why we thought we could leverage this platform to make a new metal-organic framework that could be used in the food industry."

In this case, the researchers designed a MOF consisting of iron bound to a ligand called fumaric acid, which is often used as a food additive to enhance flavor or help preserve food.

This structure prevents iron from reacting with polyphenols—compounds commonly found in foods such as whole grains and nuts, as well as coffee and tea. When iron does react with those compounds, it forms a metal polyphenol complex that cannot be absorbed by the body.

The MOFs' structure also allows them to remain stable until they reach an acidic environment, such as the stomach, where they break down and release their iron payload.

Double-fortified salts

The researchers also decided to include iodine in their MOF particle, which they call NuMOF. lodized salt has been very successful at preventing iodine deficiency, and many efforts are now underway to create "double-fortified salts" that would also contain iron.

Delivering these nutrients together has proven difficult because iron and iodine can react with each other, making each one less likely to be absorbed by the body. In this study, the MIT team showed that once they formed their iron-containing MOF particles, they could load them with iodine, in a way that the iron and iodine do not react with each other.

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In tests of the particles' stability, the researchers found that the NuMOFs could withstand long-term storage, high heat and humidity, and boiling

Throughout these tests, the particles maintained their structure. When the researchers then fed the particles to mice, they found that both iron and iodine became available in the bloodstream within several hours of the NuMOF consumption.

The researchers are now working on launching a company that is developing coffee and other beverages fortified with iron and iodine. They also hope to continue working toward a double-fortified salt that could be consumed on its own or incorporated into staple food products.

Phys Org, 13 August 2025

https://phys.org

By learning to harness light like nature, we're launching a new era of green chemistry

2025-08-11

water.

Photosynthesis is nature's way of turning sunlight into chemical energy.

Plants use a green pigment called chlorophyll to absorb sunlight, using this solar energy to convert carbon dioxide from the air and water from the soil into glucose, which they use as a food source. This process also produces oxygen, which is released into the atmosphere.

This transformation, however, does not happen in a single step. Instead, plants absorb four photons (particles of light) in a carefully choreographed sequence, gradually accumulating the energy required to split water molecules and release oxygen.

This multi-photon process is a remarkably elegant solution to the challenge of capturing and storing solar energy.

For decades, we chemists have looked to photosynthesis for inspiration, seeking ways to harness visible light to drive important chemical transformations.

Yet a major challenge has been that most synthetic light-absorbing chemicals—known as photocatalysts—can only absorb one photon at a time. So they don't produce enough energy to power complex reactions.

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As a result, many energy-demanding chemical processes, like building intricate pharmaceuticals or advanced materials, have remained beyond the reach of being powered by visible light alone.

Mimicking nature's multi-photon mastery

In the Polyzos research group at the School of Chemistry, we have developed a new class of photocatalysts that, like plants, can absorb energy from multiple photons.

This breakthrough allows us to harness light energy more effectively, driving challenging and energy-demanding chemical reactions.

We have applied this technology to generate carbanions—negatively charged carbon atoms that serve as crucial building blocks in the creation, or synthesis, of carbon- and hydrogen-rich chemicals known as organic chemicals.

Carbanions are vital in making drugs, polymers and many other important materials. However, traditional methods to produce carbanions often require lots of energy and dangerous reagents, and generate significant chemical waste, posing environmental and safety challenges.

These reagents are most commonly organolithium reagents or Grignard reagents that require extremely cold temperatures to control their reactivity.

Our new method offers a greener, safer alternative.

By using visible light and renewable starting materials, and a photocatalyst system that mimics the energy-accumulating multiple photon steps of photosynthesis, the technology generates carbanions under mild, environmentally friendly conditions.

Unlocking the hidden potential of alkenes

Alkenes—simple molecules with strong, carbon-carbon double bonds—are among the most abundant and versatile building blocks in chemistry.

Yet, turning them into highly reactive carbanions has been a longstanding challenge.

Using our multi-photon photocatalytic system, we transform alkenes into carbanions and then rapidly convert these into complex molecules.



This approach is a significant departure from classical methods. Instead of relying on toxic metals or other harsh reagents, the reaction proceeds

From lab-scale to industrial-scale

Beyond the scientific novelty of designing this process, our method has practical impact.

We've used it to synthesize important drug molecules, including antihistamines, in a single step using simple, cheap and commonly available "commodity chemicals"—amines and alkenes.

under gentle conditions, is scalable, and generates less waste.

And importantly, the reaction scales well in commercial-scale continuous flow reactors, highlighting its potential for industrial applications.

Toward a sustainable, light-driven future

Our discovery reframes how chemists approach alkenes, showing they can serve as sources of highly reactive carbanions accessed through visible light under mild conditions.

The strategy aligns with nature's own principles of efficiency and sustainability, promising new routes for constructing complex organic molecules without reliance on heavy metals or harsh reagents.

Looking ahead, the team plans to expand this light-driven chemistry to include more diverse carbon–carbon bond-forming reactions and combine it with enzyme catalysis.

Enzymes, nature's precise molecular machines, offer unmatched selectivity and could, together with our photocatalysts, enable the synthesis of complex three-dimensional molecules crucial for discovering new medicines.

By learning from the subtle mastery of photosynthesis, our research group is forging a new paradigm for chemical manufacturing—one where sunlight powers sustainable and elegant solutions for the molecules that shape our world.

By using light to break alkenes into carbanions, we can then add different chemical groups stepwise in a controlled way—building complex molecules like amino acids and pharmaceuticals with greater efficiency.

Phys Org, 11 August 2025

https://phys.org

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AUG. 15, 2025

Catalyst can efficiently reduce NO across a wide temperature range

2025-08-13

Nitrogen oxides (NOx), a major contributor to air pollution, are emitted from a variety of fuel combustion sources—including industrial smokestacks, vehicles, and ships. The emission temperatures of NOx vary significantly depending on the type of fuel used and operating conditions of the equipment. In light of these changes, researchers have developed a catalyst capable of consistently and efficiently removing NOx across a wide temperature spectrum.

Led by Professor Seungho Cho from the Department of Materials Science and Engineering at UNIST, in collaboration with Dr. Hong-Dae Kim at the Korea Institute of Industrial Technology (KITECH), the research team developed a novel denitrification catalyst effective between 240°C and 400°C.

This innovation promises to significantly improve the stability and efficiency of NOx reduction in diverse real-world environments. The study is published in the journal Applied Catalysis B: Environment and Energy.

NOx released into the atmosphere are known to contribute to severe environmental issues, including fine dust formation, ozone pollution, and acid rain. While Selective Catalytic Reduction (SCR) systems are widely used to convert NOx into harmless nitrogen (N2), conventional vanadium-tungsten catalysts typically operate optimally only around 350°C. This narrow temperature window often results in performance degradation under fluctuating field conditions, limiting their effectiveness.

In contrast, the new catalyst demonstrates an impressive 93.6% removal efficiency at 240°C and maintains more than 97% conversion efficiency at higher temperatures. Compared to existing commercial SCR catalysts, which achieve approximately 62.4% efficiency at 240°C, this advancement represents a substantial leap forward.

In addition, the catalyst converts more than 97% of NOx into nitrogen, with minimal formation of byproducts such as nitrous oxide (N2O), a potent greenhouse gas. The catalyst also exhibits enhanced longevity, promising more durable and cost-effective operation.

The exceptional performance of this catalyst is primarily attributed to the strategic incorporation of a small amount of hexagonal boron nitride (h-BN). This material plays a crucial role in maintaining vanadium ions

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in an active state and protecting the catalyst surface from fouling by contaminants such as sulfates and moisture—factors that typically shorten

To facilitate industrial application, the research team also validated the performance of the catalyst in a monolithic form. While powdered catalysts offer superior reactivity, their practical use is often hindered by issues such as dust generation and pressure loss. The monolith structure developed by the team effectively handles high gas flow conditions—processing several tens of micrograms of NO per second at 20 L/min—making it suitable for real-world deployment.

Professor Cho remarked, "The broad operational temperature range of our catalyst enables stable and efficient removal of NOx from various emission sources, including factories, vehicles, and ships. We anticipate that reducing the reliance on toxic and expensive vanadium will enhance both safety and economic viability in industrial settings."

Phys Org, 13 August 2025

https://phys.org

catalyst lifespan.

Leaf it out! Chemical engineers develop bioplastic that breaks down in soil

2025-08-11

US CHEMICAL engineers inspired by leaves have created a form of bioplastic packaging that degrades in the environment in ambient conditions.

Plastic packaging is a staple of modern life – it helps keep food fresh for longer and is lighter than many alternatives, reducing transport costs. Yet, too much of this single-use packaging is lost as litter to the environment, where plastic bottles and wrappers fragment into microplastics that end up polluting the environment and our bodies.

There are alternatives that can biodegrade without producing persistent microplastics such as the bioplastic polylactic acid (PLA). However, it won't break down in the soil or the sea where packaging pollution is prevalent, requiring industrial composting conditions instead.

Now researchers at Washington University in St Louis, US, inspired by the cellulose-rich cell walls of plants, have added cellulose nanofibres to create a form of PLA that breaks down in soil in five weeks.

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"We created this multilayer structure where cellulose is in the middle and the bioplastics are on two sides," said Joshua Yuan, professor of energy, environmental and chemical engineering at the university.

Publishing their results in Nature Communications, the team said the technique makes the resulting film highly transparent and water stable, and achieves high gas barrier properties to improve food shelf life and reduce waste.

"On top of all of this, the [composite's] underlying cellulose structure gives it a higher tensile strength than even petrochemical plastics like polyethylene and polypropylene," says study author Puneet Dhatt.

The team is now looking for funding to help develop the technology for industrial use. While concerned the US lags behind European and Asian research institutions working on similar technologies, they believe they can compete by tapping into the country's vast farming sector to supply the corn and starch feedstocks needed for bioplastic building blocks like lactic acid.

"The US is particularly strong in agriculture," Yuan said. "We can provide the feedstock for bioplastic production at a lower price compared to other parts of the world.

"The United States has a waste problem, and circular reuse could go a long way to turning that waste into useful materials. If we can ramp up our bioplastic supply chain, it would create jobs and new markets."

The Chemical Engineer, 11 August 2025

https://thechemicalengineer.com



Antifungal Drug Candidates Discovered in University Greenhouse

2025-08-12

A research team at McMaster University has discovered a new drug class that could someday lead to breakthrough treatments for dangerous fungal infections.

The new molecules, dubbed coniotins, were isolated from a plant-dwelling fungus called Coniochaeta hoffmannii — the samples of which were collected from the McMaster greenhouse, located on the university's campus.

Detailed recently in the journal Nature Communications, the discovery responds to a critical need for new antifungal medicines.

"There is a huge, growing clinical need for new drugs that target fungal infections," says Gerry Wright, a professor of biochemistry and biomedical sciences at McMaster and principal investigator on the new study. "Unlike antibiotics, of which there are dozens of different classes approved for use in clinics, there are really only three classes of antifungals on the market right now."

The reason for such a limited arsenal, Wright says, is two-fold.

First, although disease-causing fungi are microscopic like bacteria and viruses, they're actually more closely related to humans than they are to other microbes — "so things that kill fungi tend to kill us too," he says. This makes finding antifungals that are safe for human consumption a real challenge.

And then there's the historical lack of urgency. Wright says that most fungi cannot withstand our internal body temperature, and usually die off before they can cause serious infection. It's why fungal infections typically occur on us instead of in us — think athlete's foot, for example. Because our bodies can generally handle these pathogens naturally, Wright says there's been little incentive for pharmaceutical companies to invest in antifungal R&D — until recently.

"Discovery remains a challenge today, but the level of urgency has changed dramatically over the past 15 years or so," he says. "In 2009, a novel fungal pathogen called Candida auris emerged all over the world, and this fungus thrives at higher temperatures — and it can be extremely drug-resistant, too."

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C. auris is particularly problematic for individuals with compromised immune systems, like cancer patients undergoing chemotherapy. It can infect the lungs, the bloodstream, and the nervous system, and can be fatal. For these reasons, C. auris sits atop the World Health Organization's list of priority fungal pathogens.

It's a good thing then that the Wright Lab's new molecule exhibits potent activity against C. auris.

Indeed, the research team showed that coniotins not only attack C. auris and several other fungal pathogens, but do so without harming human cells.

The new molecules function unlike any other antifungal on the market. Where most target proteins and membranes, coniotins instead bind to the fungal cell wall.

Wright, a member of the Michael G. DeGroote Institute for Infectious Disease Research at McMaster, likens the cell wall to the candy coating on an M&M — a protective shell that provides structural integrity for what's inside. Disturbing this structure, as coniotins do, fundamentally changes how well the organism can survive.

Xufei Chen, a postdoctoral fellow in Wright's lab and first-author on the new paper, identified the new drug class through a process called prefractionation, which allows scientists to tease specific molecules out from complex chemical mixtures.

"Since the golden age of antibiotic discovery, progress has slowed, due primarily to the frequent rediscovery of known compounds," she says. "To address this, we implemented a prefractionation screening approach to target overlooked or masked metabolites. By integrating mass spectrometry, metabolomics, and computational analysis, I was able to discover this previously hidden molecule."

Using this same process, Wright's lab recently discovered a new class of antibiotics. They have also used prefractionation to identify several other new drug candidates, which remain under study.

"What's really amazing is that we've only screened about five percent of the chemical library that we've built here at McMaster," Wright says. "We have an immense, largely unexplored chemical space at our fingertips, and a cost-effective way to reduce the rediscovery of known compounds. Who knows what else is in there?"



Wright's team is eager to move coniotins along the development pathway. The next steps, he says, include producing it at scale through

fermentation, and formulating the new drug class so that it may eventually be suitable intravenous (IV) delivery.

Technology Networks, 12 August 2025

https://technologynetworks.com

Nanoflowers: The new frontier in healing brain cells & treating disease

2025-08-08

Metallic nanoflowers may be the next frontier in brain health, reducing oxidative stress, protecting mitochondria, and even extending lifespan in lab models. A new study shows they hold "incredible potential" as neuroprotective agents.

Nanoparticles have been used for some time now to deliver targeted treatment in the form of drugs, genes, or other therapeutic agents. Lately, though, another unique type of nanomaterial has entered the scene and is making waves: the nanoflower.

Looking just like their name suggests, researchers from Texas A&M University have used these flower-shaped nanoparticles to improve and protect brain cell health via their effect on mitochondria, the energy-producing machinery of cells.

"These nanoflowers look beautiful under a microscope, but what they do inside the cell is even more impressive," said the study's corresponding author, Dmitry Kurouski, associate professor in biochemistry and biophysics at Texas A&M's College of Agriculture and Life Sciences. "By improving the health of brain cells, they help address one of the key drivers of neurodegenerative diseases that have long resisted therapeutic breakthroughs."

Dysfunction in mitochondria is seen in a wide spectrum of pathologies, including neurodegenerative diseases like Parkinson's, Alzheimer's, and amyotrophic lateral sclerosis (ALS). Common causes of mitochondrial dysfunction include genetic mutation, reactive oxygen species (ROS), neuroinflammation, epigenetic changes, and environmental factors. This dysfunction then results in a buildup of toxic proteins, such as tau and amyloid-beta, associated with neurodegenerative disorders. For this

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reason, many therapies focus on restoring healthy function to these tiny but important organelles.

The benefit that nanoflowers offer is that their distinct shape – multiple "petals" radiating from a central core – provides a large surface-to-volume ratio, meaning that their outer surface area is large compared to their internal volume. This, arguably, makes nanoflowers more useful than regular nanoparticles for functions like drug delivery and catalysis, or increasing the rate of a chemical reaction by adding a catalyst.

In the present study, the researchers experimented with two novel types of metallic nanoflowers, made from molybdenum disulfide (MoS2) and molybdenum diselenide (MoSe2). They first used the nanoflowers on cells in the lab, studying how they affected neurons and astrocytes, mitochondrial function and oxidative stress (measured by ROS).

They found that both MoS2 and MoSe2 nanoflowers were absorbed by neurons and astrocytes, the specialized, star-shaped central nervous system cells that provide energy and support to neurons, among other important functions. Significant increases in cell proliferation were observed in the first 24 hours after treatment, especially with MoS2 in neurons, where there was up to a 93% increase.

Both nanoflowers substantially reduced ROS levels, with MoSe2 showing stronger effects. The MoSe2 nanoflowers reduced ROS in neurons by up to 80% at higher concentrations. Astrocytes also showed a dose-dependent ROS reduction. Why are ROS bad? ROS are byproducts of cellular metabolism that normally help regulate essential processes like cell survival and death. But when their levels spike, they can damage cells and trigger inflammation.

The researchers also saw that mitochondrial damage fell significantly in all cell types. MoSe2 reduced signs of mitochondrial damage in neurons by up to 99%, suggesting a strong protective effect. While MoS2 also had strong protective effects, they were slightly less pronounced. Both nanoflowers increased levels of proteins linked to mitochondrial health, and gene expression tests showed an upregulation of the pathway known to promote mitochondrial repair and protect against stress.

"Even in healthy cells, some oxidative stress is expected," Kurouski said. "But the nanoflowers seem to fine-tune the performance of mitochondria, ultimately bringing the levels of their toxic byproducts down to almost nothing. If we can protect or restore mitochondrial health, then we're not just treating symptoms – we're addressing the root cause of the damage."

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After experimenting with individual cells, the researchers moved on to test the nanoflowers in an animal model, to see how they affected lifespan in Caenorhabditis elegans, a type of microscopic worm commonly used in biomedical research. Compared to controls, MoSe2 extended the worms' lifespan by up to six days. It might not sound like much, but C. elegans typically has a lifespan of 18 days, so that's a one-third extension. MoS2 had milder effects but still slightly increased lifespan.

Of course, the usual limitations apply. Most of the study was conducted on cultured cells, which may not fully reflect the complexity of living organisms. And while C. elegans is a powerful research tool, its results may not directly translate to humans. Long-term safety and efficacy of the nanoflowers remain unknown. Very high doses of MoSe2 slightly impaired cell viability, suggesting a need for careful dosing.

These metallic nanoflowers have huge potential as neuroprotective materials capable of treating conditions like stroke, Alzheimer's and Parkinson's diseases. And more research is needed before these therapies move from the lab to the clinic.

"We think this could become a new class of therapeutics," said Kurouski.

"We want to make sure it's safe, effective and has a clear mechanism of action. But based on what we've seen so far, there's incredible potential in nanoflowers."

The study was published in the Journal of Biological Chemistry.

New Atlas, 8 August 2025

https://newatlas.com

Creating safe medicinal molecules with sustainable electrochemistry

2025-08-14

Cornell chemists have developed a way to use electrochemistry, a sustainable technique, to make chiral molecules, which occur in mirrored pairs, like human hands. Common in pharmaceuticals, chiral molecules are important to get right to be effective and safe.

"Many drug molecules are chiral—like our hands, they look similar, but one could be very effective in treating a disease while the other could be inactive or even a poison," said Song Lin, the Howard Milstein Faculty Fellow/Tisch University Professor of chemistry and chemical biology in the

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College of Arts and Sciences (A&S). "A lot of times, making only one of the two mirror image molecules is important in medicinal chemistry."

In some medicines, such as the pain reliever ibuprofen, one side of a chiral molecule is active and effective while the other (called its enantiomer) is present but benign, Lin said. In many other drugs, the active side is mirrored by a toxic enantiomer that must be eliminated, making chiral molecule synthesis an important objective in organic chemistry. Work on asymmetric catalysis—using chiral catalysts in a solution to induce handedness—earned Nobel Prizes in 2001 and 2021.

In "Dynamic Kinetic Resolution of Phosphines with Chiral Supporting Electrolytes," published in Nature, Lin, the corresponding author, and collaborators describe how they use electrochemistry to selectively synthesize chiral compounds using the reaction's electrolytes to introduce a chiral environment, a completely new strategy for inducing chirality in electrochemistry.

Although it has clear environmental benefits, electrochemistry, an expertise of the Lin Lab, is rarely used to create chiral molecules, Lin said, because of challenges where the solid electrode, made of metal or carbon, meets the liquid solution. The Cornell researchers overcame this problem by introducing a chiral shape to the reaction through electrolytes, usually a background element.

"Supporting electrolytes are salts added to experiments just to make sure the solution is conducting," Lin said. "They do not usually play explicit roles in the reaction. But in this work, we use electrolytes to interact with electrochemically generated molecules through simple electrostatic interactions, so that only one of the two mirror image products, the desired enantiomer, is formed."

Because the electrolyte is always there at the interface, Lin said, this technique can theoretically be generally applied to many different types of electrochemical reactions, including making drug molecules.

Chiral molecules are common in medicines because chirality is common in nature, from spiraling vines and shells to amino acids and various proteins, to the human body's protein receptors, the site of drug interaction.

"Humans are made of chiral molecules," Lin said. "Because your protein receptors are chiral, they're going to interact with chiral molecules differently."



The researchers collaborated with a lab at Brown University to observe the reaction on the molecular level using molecular dynamics simulation, an advanced computational technique.

"It is well known that the ions in the supporting electrolyte (e.g. salt), which you dissolve in the solution, become even more concentrated near the electrode surface with the opposite charge," said Yue Qi, the Joan Wernig Sorensen Professor of Engineering at Brown University. "So now you have an even higher concentration of the chiral inducer near the electrode surface, which is going to make the electrochemical reaction more effective."

This collaboration was facilitated through the National Science Foundation Center for Synthetic Organic Electrochemistry. The collaborators plan to examine the mechanism in more detail to understand exactly how it works. They also want to explore what other types of molecules they can make using chiral supporting electrolyte.

"I think this technology could, in the future, be used in industry, but going from academic discovery to industry application always takes a long time," Lin said. "It's important that NSF supports fundamental research. It allows us to discover something that might not be immediately useful but could play a big role in the long-term."

Phys Org, 14 August 2025

https://phys.org

New adhesive is so sticky it can glue a rubber duck to a seaside rock

2025-08-13

New water-resistant hydrogels, designed with the help of machine learning, are more adhesive than any comparable materials found in nature. The hydrogels were developed with the aid of an algorithm trained on the adhesives produced by natural organisms, such as geckos and mussels. The researchers that created them suggest that the new substances could have applications in areas such as surgery, marine farming and deep-sea exploration.

Soft, gelatinous adhesives are difficult to design because the very properties that make adhesives strong also tend to make them brittle. Elastomeric polymer hydrogels are the best examples available, but these tend not to be very water resistant as their hydrated bonding networks

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are easily disrupted if water penetrates them. However, the natural world contains thousands of examples of water-resistant adhesive hydrogels in marine animals, bacteria, fungi and viruses.

In the new research, soft matter expert Jian Ping Gong at Hokkaido University in Japan and colleagues elsewhere in Japan and China mined a dataset of 24,707 natural adhesive protein sequences found in a biotechnology database hosted by the US National Institutes of Health. The researchers then synthesised 180 candidates using a free-radical random copolymerisation process and tested their adhesive strength. The strongest candidate was made from amino acid chains derived from a protein produced by Escherichia bacteria.

The researchers then studied features present in the most promising hydrogels and used iterative machine learning to develop a new set of candidates stronger and more stable than any found in nature. 'Our approach aims to build a systematic, data-driven, and generalisable framework, going beyond individual bio-mimic motifs to statistically capture broader sequence logic,' explains Hailong Fan, then at Hokkaido University, now at Shenzhen University in The team ultimately arrived at three hydrogels, one of which was around 7 times as powerful the Escherichia adhesive and could stick a rubber duck to a seaside rock, withstanding salt water and waves. Another could resist high water pressure to seal a burst pipe. The researchers showed that all three were biocompatible by implanting them in mice. 'We are customising the hydrogel for use in medical adhesives, marine repairs, and soft robotics,' says Fan.

Materials scientist Ting Xu at University of California, Berkeley in the US is impressed by the materials' properties. However, she believes that the importance of machine learning in their development should not be overstated, as she doubts that the researchers would have succeeded without Gong's predictive skills. 'Jian Ping is the goddess of hydrogel,' she says. 'She has decades of experience, she just has the knowledge to be able to pick the right monomers, pick the right regions, and couple that with experimental high throughput and machine learning. I wouldn't say the modelling here is particularly exceptional, I would say it's a very good coupling of human intelligence with artificial intelligence.'China.

Chemistry World, 13 August 2025

https://chemistryworld.com



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Scientists finally solve the mystery of what triggers lightning

2025-08-01

In the study published on July 28 in the Journal of Geophysical Research, the authors described how they determined strong electric fields in thunderclouds accelerate electrons that crash into molecules like nitrogen and oxygen, producing X-rays and initiating a deluge of additional electrons and high-energy photons -- the perfect storm from which lightning bolts are born.

"Our findings provide the first precise, quantitative explanation for how lightning initiates in nature," Pasko said. "It connects the dots between X-rays, electric fields and the physics of electron avalanches."

The team used mathematical modeling to confirm and explain field observations of photoelectric phenomena in Earth's atmosphere -- when relativistic energy electrons, which are seeded by cosmic rays entering the atmosphere from outer space, multiply in thunderstorm electric fields and emit brief high-energy photon bursts. This phenomenon, known as a terrestrial gamma-ray flash, comprises the invisible, naturally occurring bursts of X-rays and accompanying radio emissions.

"By simulating conditions with our model that replicated the conditions observed in the field, we offered a complete explanation for the X-rays and radio emissions that are present within thunderclouds," Pasko said. "We demonstrated how electrons, accelerated by strong electric fields in thunderclouds, produce X-rays as they collide with air molecules like nitrogen and oxygen, and create an avalanche of electrons that produce high-energy photons that initiate lightning."

Zaid Pervez, a doctoral student in electrical engineering, used the model to match field observations -- collected by other research groups using ground-based sensors, satellites and high-altitude spy planes -- to the conditions in the simulated thunderclouds.

"We explained how photoelectric events occur, what conditions need to be in thunderclouds to initiate the cascade of electrons, and what is causing the wide variety of radio signals that we observe in clouds all prior to a lightning strike," Pervez said. "To confirm our explanation on lightning initiation, I compared our results to previous modeling, observation studies and my own work on a type of lightning called compact intercloud discharges, which usually occur in small, localized regions in thunderclouds."

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Published by Pasko and his collaborators in 2023, the model, Photoelectric Feedback Discharge, simulates physical conditions in which a lightning bolt is likely to originate. The equations used to create the model are available in the paper for other researchers to use in their own work.

In addition to uncovering lightning initiation, the researchers explained why terrestrial gamma-ray flashes are often produced without flashes of light and radio bursts, which are familiar signatures of lightning during stormy weather.

"In our modeling, the high-energy X-rays produced by relativistic electron avalanches generate new seed electrons driven by the photoelectric effect in air, rapidly amplifying these avalanches," Pasko said. "In addition to being produced in very compact volumes, this runaway chain reaction can occur with highly variable strength, often leading to detectable levels of X-rays, while accompanied by very weak optical and radio emissions. This explains why these gamma-ray flashes can emerge from source regions that appear optically dim and radio silent."

In addition to Pasko and Pervez, the co-authors include Sebastien Celestin, professor of physics at the University of Orléans, France; Anne Bourdon, director of research at École Polytechnique, France; Reza Janalizadeh, ionosphere scientist at NASA Goddard Space Flight Center and former postdoctoral scholar under Pasko at Penn State; Jaroslav Jansky, assistant professor of electrical engineering and communication at Brno University of Technology, Czech Republic; and Pierre Gourbin, postdoctoral scholar of astrophysics and atmospheric physics at the Technical University of Denmark.

The U.S. National Science Foundation, the Centre National d'Etudes Spatiales (CNES), the Institut Universitaire de France and the Ministry of Defense of the Czech Republic supported this research.

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Chemistry LLM developed for faster drug discovery 2025-08-14

Southwest Research Institute scientists and engineers have developed a custom large language model (LLM) to accelerate drug design and discovery.

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A multidisciplinary team developed the Generative Approaches for Molecular Encodings (GAMES) LLM to generate Simplified Molecular Input Line Entry System (SMILES) strings. SMILES is an industry standard system that represents the structure of molecules using a short series of text characters to facilitate storage, retrieval and modeling. Researchers trained GAMES to understand and generate valid new SMILES combinations.

"This project demonstrates a systematic way to build databases and networks of molecules for AI processing and comparison using only language," said Institute Scientist Dr. Jonathan Bohmann, lead developer of SwRI's Rhodium molecular docking software designed to virtually screen drug compounds.

Rhodium software uses descriptors along with graphical processing to visualize the chemical properties of compounds. Incorporating GAMES into the Rhodium workflow offers a faster generalized approach to drug discovery and design.

"Using LLMs, we can directly apply machine learning and AI to molecules via SMILES strings, because they appear as readable text characters and don't require translation into abstract representations," Bohmann said.

SwRI trained the GAMES model with classes of carbon-based molecules and other reference compounds to validate and fine-tune the SMILES strings it generated.

"This project showcases the power of training LLMs in highly technical scientific domains to focus on specific tasks," said SwRI Lead Computer Scientist Michael Hartnett. "In this case, we are working in the drug discovery domain, and our fine-tuning is focused on unlocking the most relevant knowledge."

GAMES combines LoRA (Low-Rank Adaptation) and QLoRA (Quantized LoRA) techniques to efficiently fine tune LLMs, reducing the hardware and energy needed to run Rhodium models. The team hopes to apply this approach to other applications and domains across the Institute.

"Using LLMs to generate accurate SMILES could transform the drug discovery process, especially when trained using specific datasets," said SwRI Research Scientist Daniel Hinojosa. "The fine-tuned techniques significantly improved performance, increasing the number of valid SMILES while reducing invalid outputs. Structured datasets and specific training techniques were key to this accomplishment."

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Researchers hope GAMES will offer a powerful framework for ranking compounds found in chemical libraries based on drug-likeness, a shorthand term for a combination of properties that make it most likely to be approved as a safe drug. Additionally, they plan to explore chemical landscapes systematically through testing. Hinojosa and Bohmann plan to pursue additional internal funding to advance the next phase of the project.

"While we're in early stages of development, the results are already having a direct impact on ongoing research programs at SwRI," Bohmann said.

Phys Org, 14 August 2025

https://phys.org

Bye-Bye Teflon? This Slick New Material Could Change Cookware Forever

2025-08-11

Engineers have crafted a new non-stick coating that could finally give Teflon some competition—without the dangerous "forever chemicals" that have raised health alarms.

By bonding silicone-based bristles with the tiniest PFAS molecule possible, the team created a surface that resists both water and grease as effectively as traditional coatings.

Safer Non-Stick Alternative Emerges

Researchers at the University of Toronto's Faculty of Applied Science & Engineering have created a new type of material that could provide a safer option for the non-stick coatings widely used in cookware and other everyday products.

This innovation repels both water and grease as effectively as many standard non-stick surfaces, but contains much smaller amounts of perand polyfluoroalkyl substances (PFAS). PFAS are a group of chemicals linked to environmental and health concerns.

"The research community has been trying to develop safer alternatives to PFAS for a long time," says Professor Kevin Golovin (MIE), who heads the Durable Repellent Engineered Advanced Materials (DREAM) Laboratory at U of T Engineering.



"The challenge is that while it's easy to create a substance that will repel water, it's hard to make one that will also repel oil and grease to the same degree. Scientists had hit an upper limit to the performance of these alternative materials."

The Science Behind Teflon and PFAS

First introduced in the late 1930s, Teflon (polytetrafluoroethylene or PTFE) became famous for its ability to keep water, oil, and grease from sticking. Teflon is part of the larger PFAS family.

PFAS molecules are made of carbon atoms bonded to multiple fluorine atoms. These carbon-fluorine bonds are extremely stable, which is what gives PFAS their strong non-stick properties.

That same chemical stability also makes PFAS resistant to natural breakdown processes. This persistence in the environment has earned them the nickname "forever chemicals."

Health Concerns and Ubiquity of PFAS

In addition to their persistence, PFAS are known to accumulate in biological tissues, and their concentrations can become amplified as they travel up the food chain.

Various studies have linked exposure to high levels of PFAS to certain types of cancer, birth defects, and other health problems, with the longer chain PFAS generally considered more harmful than the shorter ones.

Despite the risks, the lack of alternatives means that PFAS remain ubiquitous in consumer products: they are widely used not only in cookware, but also in rain-resistant fabrics, food packaging, and even in makeup.

Searching for a Safer Substitute

"The material we've been working with as an alternative to PFAS is called polydimethylsiloxane or PDMS," says Golovin.

"PDMS is often sold under the name silicone, and depending on how it's formulated, it can be very biocompatible — in fact it's often used in devices that are meant to be implanted into the body. But until now, we couldn't get PDMS to perform quite as well as PFAS."

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To overcome this problem, MIE PhD student Samuel Au developed a new chemistry technique that the team is calling nanoscale fletching. The technique is described in a paper published in Nature Communications.

Mimicking Feathered Arrows at the Nanoscale

"Unlike typical silicone, we bond short chains of PDMS to a base material — you can think of them like bristles on a brush," says Au.

"To improve their ability to repel oil, we have now added in the shortest possible PFAS molecule, consisting of a single carbon with three fluorines on it. We were able to bond about seven of those to the end of each PDMS bristle.

"If you were able to shrink down to the nanometre scale, it would look a bit like the feathers that you see around the back end of an arrow, where it notches to the bow. That's called fletching, so this is nanoscale fletching."

Matching PFAS Performance with Minimal Risk

Au and the team coated their new material on a piece of fabric, then placed drops of various oils on it to see how well it could repel them. On a scale developed by the American Association of Textile Chemists and Colorists, the new coating achieved a grade of 6, placing it on par with many standard PFAS-based coatings.

"While we did use a PFAS molecule in this process, it is the shortest possible one and therefore does not bioaccumulate," says Golovin.

"What we've seen in the literature, and even in the regulations, is that it's the longest-chain PFAS that are getting banned first, with the shorter ones considered much less harmful. Our hybrid material provides the same performance as what had been achieved with long-chain PFAS, but with greatly reduced risk."

Toward a PFAS-Free Future

Golovin says that the team is open to collaborating with manufacturers of non-stick coatings who might wish to scale up and commercialize the process. In the meantime, they will continue working on even more alternatives.

"The holy grail of this field would be a substance that outperforms Teflon, but with no PFAS at all," says Golovin.



"We're not quite there yet, but this is an important step in the right

Sci Tech Daily, 11 August 2025

https://scitechdaily.com

Ocean carbon capture raises concerns over marine stress, say UK scientists

2025-08-14

direction."

CAPTURING CO2 directly from seawater could negatively impact marine organisms and put them under stress, according to research from the University of Exeter and Plymouth Marine Laboratory.

The study is part of the researchers' joint SeaCURE project, which uses electrodialysis to extract inorganic carbon from seawater for storage, before returning the treated water back into the ocean.

Earlier this year, the SeaCURE project launched its first pilot plant for Direct Ocean Carbon Capture and Storage (DOCCS) at the Sea Life Centre in Weymouth, UK. The plant can process 3,000 L of seawater per minute and remove around 100 t/y of CO2.

The new study raises concerns about scaling the technology to commercial levels, citing a lack of research into its potential impact on marine ecosystems.

Guy Hooper, the lead author of the study, said: "Our ongoing work shows that DOCCS technology is potentially a very powerful tool, but further investigation on the biological effects is now urgently needed in order to understand when and where they might occur and how they can be mitigated."

Stressful waters

In the DOCCS process, seawater is acidified to release CO2 that is then captured and stored. The treated seawater is then neutralised with alkaline chemicals and returned to the sea.

The study identified several potential impacts of DOCCS-treated seawater on marine life, including reduced availability of dissolved inorganic carbon, which plankton and seaweeds require for photosynthesis, and shellfish and crustaceans need for shell formation. The elevated pH of

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treated seawater may also place physiological stress on certain marine organisms.

Hooper explained: "It's clear from our lab-based experiments that returning treated decarbonised and high pH seawater to the ocean, without sufficient dilution, could place stress on certain marine organisms."

Further research

The SeaCURE team has identified further areas of investigation, including lab studies on how specific marine organisms respond to DOCCS discharge conditions, and the long-term impacts of DOCCS on marine food webs.

Paul Halloran, another co-author of the study, said: "Understanding potential environmental risks is crucial not only for protecting marine ecosystems but also for supporting licensing applications, developing mitigation strategies, and ensuring public acceptance of these technologies."

The team is now conducting environmental impact studies and engaging with the public and other marine users to understand expectations around marine CO2 removal research.

The Chemical Engineer, 14 August 2025

https://thechemicalengineer.com

Bioelectrosynthesis platform enables switch-like, precision control of cell signaling

2025-08-13

Cells use various signaling molecules to regulate the nervous, immune, and vascular systems. Among these, nitric oxide (NO) and ammonia (NH₃) play important roles, but their chemical instability and gaseous nature make them difficult to generate or control externally.

A KAIST research team has developed a platform that generates specific signaling molecules in situ from a single precursor under an applied electrical signal, enabling switch-like, precise spatiotemporal control of cellular responses. This approach could provide a foundation for future medical technologies such as electroceuticals, electrogenetics, and personalized cell therapies.



The research team led by Professor Jimin Park from the Department of Chemical and Biomolecular Engineering, in collaboration with Professor Jihan Kim's group, has developed a bioelectrosynthesis platform capable of producing either nitric oxide or ammonia on demand using only an electrical signal. The platform allows control over the timing, spatial range, and duration of cell responses.

The findings are published in Angewandte Chemie.

Inspired by enzymes involved in nitrite reduction, the researchers implemented an electrochemical strategy that selectively produces nitric oxide or ammonia from a single precursor, nitrite (NO2). By changing the catalyst, the team generated ammonia or nitric oxide from nitrite using a copper-molybdenum-sulfur catalyst (Cu2MoS4) and an iron-incorporated catalyst (FeCuMS4), respectively.

Through electrochemical measurements and computer simulations, the team revealed that Fe sites in the FeCuMoS4 catalyst bind nitric oxide intermediates more strongly, shifting product selectivity toward nitric oxide. Under the same electrical conditions, the Fe-containing catalyst preferentially produces nitric oxide, whereas the Cu2MoS4 catalyst favors ammonia production.

The research team demonstrated biological functionality by using the platform to activate ion channels in human cells. Specifically, electrochemically produced nitric oxide activated TRPV1 channels (responsive to heat and chemical stimuli), while electrochemically produced ammonia induced intracellular alkalinization and activated OTOP1 proton channels. By tuning the applied voltage and electrolysis duration, the team modulated the onset time, spatial extent, and termination of cellular responses, which effectively turned cellular signaling on and off like a switch.

Professor Park said, "This work is significant because it enables precise cellular control by selectively producing signaling molecules with electricity. We believe it has strong potential for applications in electroceutical technologies targeting the nervous system or metabolic disorders."

Phys Org, 13 August 2025

https://phys.org



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Concrete Reinvented: Al Simulates 4 Billion Atoms To Build Better Materials

2025-08-03

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Imagine a future where buildings don't just stand the test of time—they actively fight climate change.

Toward Smart, Sustainable Concrete

Picture a future where the concrete used in buildings and bridges not only resists aging and extreme conditions, such as intense wildfire heat, but also repairs itself or absorbs carbon dioxide from the air.

Scientists at the USC Viterbi School of Engineering have now introduced a groundbreaking artificial intelligence model capable of simulating billions of atoms at once. This advancement unlocks a new era in material design, enabling discoveries at a scale previously thought impossible.

Climate change is rapidly intensifying. Droughts, melting glaciers, and increasingly destructive storms and wildfires are becoming more frequent and severe. A key factor driving global warming is the steady release of carbon dioxide into the atmosphere.

From Wildfires to Innovation

After witnessing the devastating January wildfires in Los Angeles, USC Viterbi professor Aiichiro Nakano (who specializes in computer science, physics, astronomy, and computational biology) began rethinking how science could help. He contacted longtime research collaborator Kenlchi Nomura, a fellow USC Viterbi professor with expertise in chemical engineering and materials science. The two have worked together for over two decades.

Their conversation led to the creation of Allegro-FM, an advanced Alpowered simulation platform. In their theoretical research, the model revealed something remarkable: it may be possible to reabsorb the carbon dioxide released during concrete production by embedding it back into the same material.

"You can just put the CO2 inside the concrete, and then that makes a carbon-neutral concrete," Nakano said.

CO2 Sequestration, Reimagined

Nakano and Nomura, along with Priya Vashishta, a USC Viterbi professor of chemical engineering and materials science, and Rajiv Kalia, a USC

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professor of physics and astronomy, have been doing research on what

they call "CO2 sequestration," or the process of recapturing carbon dioxide and storing it, a challenging process.

By simulating billions of atoms simultaneously, Allegro-FM can test different concrete chemistries virtually before expensive real-world experiments. This could accelerate the development of concrete that acts as a carbon sink rather than just a carbon source — concrete production currently accounts for about 8% of global CO2 emissions.

The breakthrough lies in the model's scalability. While existing molecular simulation methods are limited to systems with thousands or millions of atoms, Allegro-FM demonstrated 97.5% efficiency when simulating over four billion atoms on the Aurora supercomputer at Argonne National Laboratory.

This represents computational capabilities roughly 1,000 times larger than conventional approaches.

Predicting Across the Periodic Table

The model also covers 89 chemical elements and can predict molecular behavior for applications ranging from cement chemistry to carbon storage.

"Concrete is also a very complex material. It consists of many elements and different phases and interfaces. So, traditionally, we didn't have a way to simulate phenomena involving concrete material. But now we can use this Allegro-FM to simulate mechanical properties [and] structural properties," Nomura said.

Concrete is a fire-resistant material, making it an ideal building choice in the wake of the January wildfires. But concrete production is also a huge emitter of carbon dioxide, a particularly concerning environmental problem in a city like Los Angeles. In their simulations, Allegro-FM has been shown to be carbon neutral, making it a better choice than other concrete.

Echoes of Ancient Engineering

This breakthrough doesn't only solve one problem. Modern concrete only lasts about 100 years on average, whereas ancient Roman concrete has lasted for over 2,000 years. But the recapture of CO2 can help this as well.

"If you put in the CO2, the so-called 'carbonate layer,' it becomes more robust," Nakano said.

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In other words, Allegro-FM can simulate a carbon-neutral concrete that could also last much longer than the 100 years concrete typically lasts nowadays. Now it's just a matter of building it.

Behind the Scenes

The professors led the development of Allegro-FM with an appreciation for how AI has been an accelerator of their complex work. Normally, to simulate the behavior of atoms, the professors would need a precise series of mathematical formulas — or, as Nomura called them, "profound, deep quantum mechanics phenomena."

But the last two years have changed the way the two research.

"Now, because of this machine-learning AI breakthrough, instead of deriving all these quantum mechanics from scratch, researchers are taking [the] approach of generating a training set and then letting the machine learning model run," Nomura said. This makes the professors' process much faster as well as more efficient in its technology use.

A Unified Atomic Model

Allegro-FM can accurately predict "interaction functions" between atoms — in other words, how atoms react and interact with each other. Normally, these interaction functions would require lots of individual simulations.

But this new model changes that. Originally, there were different equations for individual elements within the periodic table, with several unique functions for these elements. With the help of Al and machine-learning, though, we can now potentially simulate these interaction functions with nearly the entire periodic table at the same time, without the requirement for separate formulas.

"The traditional approach is to simulate a certain set of materials. So, you can simulate, let's say, silica glass, but you cannot simulate [that] with, let's say, a drug molecule," Nomura said.

Efficiency and Quantum-Level Accuracy

This new system is also a lot more efficient on the technology side, with Al models making lots of precise calculations that used to be done by a large supercomputer, simplifying tasks and freeing up that supercomputer's resources for more advanced research.



"[The AI can] achieve quantum mechanical accuracy with much, much smaller computing resources," Nakano said.

The Road Ahead

Nomura and Nakano say their work is far from over.

"We will certainly continue this concrete study research, making more complex geometries and surfaces," Nomura said.

This research was published recently in The Journal of Physical Chemistry Letters and was featured as the journal's cover image.

Sci Tech Daily, 3 August 2025

https://scitechdaily.com

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Technical Notes

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Insights into the disinfection byproduct bromochloroacetamide-induced cardiotoxicity of zebrafish embryo-larvae: A multiomics approach and comparison of biomarker responsiveness

<u>The Trojan horse effect of nanoplastics exacerbates methylmercury-induced neurotoxicity during zebrafish development</u>

<u>Unraveling profiles of organic ultraviolet filters in coastal waters of the East</u> <u>China Marginal Seas</u>

ENVIRONMENTAL RESEARCH

<u>Development and application of an LC-MS/MS method for urinary DNA</u> adduct profiling in residents of environmentally vulnerable areas

<u>Environmental fibrotic hypersensitivity pneumonitis: A case report in a coal mine worker</u>

PHARMACEUTICAL/TOXICOLOGY

PFOA exposure promotes prostate cancer progression by enhancing autophagy through m6A modification of MAPK15 mRNA

Effect of combined high iodine-fluorine water exposure on the occurrence of dental fluorosis in school-age children: a cross-sectional study from rural Jiangsu, China

OCCUPATIONAL

<u>Hexavalent Chromium Exposure Induces Immune Dysregulation and Lung Tissue Neutrophil Extracellular Traps Formation</u>

Gestational exposure to micro and nanoplastics differentially impactscardiac development and function in male and female rats throughout the lifespan

Ex vivo exposure to p,p'-DDE decreases human macrophage polarization to the M1 phenotype