CHEMWATCH

Bulletin Board

Contents

MAY. 09, 2025

(click on page numbers for links)

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HAZARD ALERT

GOSSIP

CURIOSITIES

TECHNICAL NOTES

CHEMWATCH
Bulletin Board
Contents
MAY. 09, 2025

ASIA PACIFIC

Will China's rare earth export rules spur production elsewhere?

2025-04-22

New rules requiring firms in China to get a license before exporting some rare earth elements are bolstering plans to establish rare earth processing in other countries. The US and European Union are eager to support these projects, but new producers still face a difficult path forward.

Rare earth elements are used to manufacture powerful magnets for electric motors, wind turbines, missiles, and many other products. A number of mines around the world, including one in California, yield ores that contain a mixture of rare earth elements. But nearly all the rare earths in those ores are processed in China at facilities that separate them and convert them into metals.

China announced the licensing rules for seven elements—mainly heavy rare earths like dysprosium and terbium that are crucial for high-performance magnets—shortly after the US imposed high tariffs on Chinese products.

David Merriman, who covers rare earth elements for the minerals research firm Project Blue, says the licensing requirements are causing rare earths to pile up at China's ports. He expects the backlog to clear as companies get their paperwork in order, but the regulatory changes are also a warning that China can clamp down more tightly in the future.

For example, China limited the amount of gallium and germanium that companies could export in 2023 and then escalated this limit to an outright ban on exports to the US the following year after the US prohibited the sale of advanced chip-manufacturing equipment to China. Similarly, in 2010, China significantly restricted exports of rare earths, sending prices skyward.

Aware of the economic and military importance of rare earths, policymakers in the US and Europe have been encouraging domestic production. President Donald J. Trump signed an executive order in March aimed at speeding up permitting for US mining projects. Also in March, the European Union identified dozens of mineral projects it plans to

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 09, 2025

support, including rare earth–processing facilities in France, Poland, and Sweden.

Read More

c&en, 22-04-25

https://cen.acs.org/materials/inorganic-chemistry/Chinas-rare-earth-export-rules/103/web/2025/04?sc=250430_news_eng_cennews_cen_NonMember

Agricultural chemical products and approved labels

2025-04-29

Pursuant to the Agricultural and Veterinary Chemicals Code scheduled to the Agricultural and Veterinary Chemicals Code Act 1994, the APVMA hereby gives notice that it has registered or varied the relevant particulars or conditions of the registration in respect of the following products and has approved the label or varied the relevant particulars or conditions of the approval in respect of the containers for the chemical product, with effect from the dates shown.

Table 1: Agricultural products based on existing active constituents

Application no.	144809
Product name	Yates Lawn Weed Killer Bindii & Clover Buffalo Lawn
Active constituents	15 g/L bromoxynil as the N-octanoyl ester, 15 g/L MCPA as the ethyl hexyl ester
Applicant name	Duluxgroup (Australia) Pty Ltd
Applicant ACN	000 049 427
Date of registration	7 April 2025
Product registration no.	95148
Label approval no.	95148/144809
Description of the application and its purpose, including the intended use of the chemical product	Registration of a 15 g/L bromoxynil present as the N-octanoyl ester and 15 g/L MCPA present as the ethyl hexyl ester 'hose-on' formulation product for use on buffalo and other common lawn types for the control of broad leaf weeds

Application no.	144765
Product name	Keyrole Insecticide
Active constituent	500 g/kg clothianidin
Applicant name	Shandong Rainbow International Co Ltd
Applicant ACN	N/A
Date of registration	9 April 2025
Product registration no.	95130
Label approval no.	95130/144765
Description of the application and its purpose, including the intended use of the chemical product	Registration of a water dispersible granule (WG) formulation containing 500 g/kg clothianidin for the control of mealybug, woolly aphid and codling moth in apples and pears; mealybug in grapes; Queensland and mediterranean fruit fly in table grapes, persimmon and pome fruit; and the control of african black beetle in turf

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APVMA Gazette No 9, Tuesday 29 April 2025

https://www.apvma.gov.au/news-and-publications/publications/gazette/gazette-9-29-april-25

Veterinary chemical products and approved labels

2025-04-29

Pursuant to the Agricultural and Veterinary Chemicals Code scheduled to the Agricultural and Veterinary Chemicals Code Act 1994, the APVMA hereby gives notice that it has registered or varied the relevant particulars or conditions of the registration in respect of the following products and has approved the label or varied the relevant particulars or conditions of the approval in respect of the containers for the chemical product, with effect from the dates shown.

Table 3: Veterinary products based on existing active constituents

Application no.	145793
Product name	Defend Extra Spray-on Sheep Blowfly Treatment
Active constituent	65 g/L dicyclanil

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 09, 2025

Application no.	145793
Applicant name	Nutrien Ag Solutions Limited
Applicant ACN	008 743 217
Date of registration	9 April 2025
Product registration no.	95482
Label approval no.	95482/145793
Description of the application and its purpose, including the intended use of the chemical product	Registration of a 65 g/L dicycanil emulsion product for the protection of sheep, either off-shears or with any length wool, against fly strike (caused by dicyclanil-susceptible strains of blowflies (*Lucilia cuprina*)) for up to 29 weeks; and for the protection of mulesing and marking wounds on sheep against fly strike (caused by dicyclanil-susceptible strains of blowflies (*Lucilia cuprina)*) during the wound healing process

Application no.	145884
Product name	Owtbac Eprishield Pour-On for Beef and Dairy Cattle
Active constituent	5 mg/mL eprinomectin
Applicant name	Jiangsu Univopharm Co Ltd
Applicant ACN	N/A
Date of registration	9 April 2025
Product registration no.	95501
Label approval no.	95501/145884
Description of the application and its purpose, including the intended use of the chemical product	Registration of a 5 mg/mL Eprinomectin solution for the treatment and control of internal and external parasites of beef and dairy cattle and internal parasites of deer

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APVMA Gazette No 9, Tuesday 29 April 2025

https://www.apvma.gov.au/news-and-publications/publications/gazette/gazette-9-29-april-25

Approved active constituents

2025-04-29

Pursuant to the Agricultural and Veterinary Chemicals Code scheduled to the Agricultural and Veterinary Chemicals Code Act 1994, the APVMA hereby gives notice that it has approved or varied the relevant particulars or conditions of the approval of the following active constituents, with effect from the dates shown.

Table 5: Approved active constituents

Application no.	143875
Active constituent	Metalaxyl-M
Applicant name	Jiangsu Baoling Chemical Co., Ltd
Applicant ACN	N/A
Date of approval	8 April 2025
Approval no.	94857
Description of the application and its purpose, including the intended use of the active constituent	Approval of the active constituent metalaxyl-M for use in agricultural chemical products

Application no.	145231
Active constituent	Haloxyfop-p-methyl
Applicant name	Sinochem International Australia Pty. Ltd.
Applicant ACN	160 164 616
Date of approval	8 April 2025
Approval no.	95306
Description of the application and its purpose, including the intended use of the active constituent	Approval of the active constituent haloxyfop-p-methyl for use in agricultural chemical products

Application no.	139792
Active constituent	Vatinoxan hydrochloride
Applicant name	Dechra Regulatory B.V.
Applicant ACN	N/A

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 09, 2025

Application no.	139792
Date of approval	9 April 2025
Approval no.	93588
Description of the application and its purpose, including the intended use of the active constituent	Approval of the active constituent vatinoxan hydrochloride for use in veterinary chemical products

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APVMA Gazette No 9, Tuesday 29 April 2025

https://www.apvma.gov.au/news-and-publications/publications/gazette/gazette-9-29-april-25

AMERICA

156 Million Americans At Risk: Air Pollution Hits Dangerous Levels!

202504-27

A new American Lung Association report warns that 156 million Americans are breathing unhealthy air, with pollution worsening due to climate change and wildfires. Cities like Bakersfield face the highest risks.

Breathing in the air across nearly half of the United States may be putting residents' health at serious risk, according to a new report from the American Lung Association. The group's annual "State of the Air" study reveals that 156 million people are living in areas where the air quality is considered unhealthy.

Analyzing data from 2021 to 2023, the report found a troubling trend: air pollution is not improving, but actually getting worse. Compared to the previous report, an additional 25 million people are now breathing unhealthy levels of pollution — the highest number recorded in the past decade.

Climate Change Driving Air Quality Decline

Since the passage of the Clean Air Act in 1970, the country has seen significant improvements in air quality. However, recent years have shown signs of reversal. Laura Kate Bender, assistant vice president at the American Lung Association, told CBS News that climate change is partly to blame. "Climate change is making conditions like wildfires and extreme

heat—which drive ozone pollution—worse for much of the country," Bender explained.

Read More

TNN, 27-04-25

https://www.timesnownews.com/health/156-million-americans-at-risk-air-pollution-hits-dangerous-levels-article-151507619

EPA Provides Technical Support for Companies Submitting New Chemical Data

2025-04-25

On April 25, 2025, the U.S. Environmental Protection Agency (EPA) announced the availability of new resources intended to help companies with the requirements described in EPA's December 2024 final rule governing the review of new chemicals under the Toxic Substances Control Act (TSCA). According to EPA, the new materials "provide companies with clear instructions on how to include required data elements in the current system used for new chemical submissions while the agency works to update that system." EPA's final rule clarifies the level of detail for the data elements that submitters are required to provide with new chemical notices whenever that information is known to or reasonably ascertainable by the submitter. EPA states that "[a] s noted in the preamble to the final rule, enhancements to the Central Data Exchange (CDX) for submitting the data elements were not finalized concurrently with the amendments."

Read More

B&C, 25-04-25

https://www.lawbc.com/epa-provides-technical-support-for-companies-submitting-new-chemical-data/

"I'm Interested in a Revolution" -- RFK, Jr. Outlines His FDA Priorities in the Regulation of Food Ingredients and Food Packaging

2025-04-29

Health and Human Services Secretary Robert F. Kennedy, Jr. recently addressed a diverse group of stakeholders at the "Chemicals of Concern Policy Summit," stressing the need for industry, regulators, and public

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 09, 2025

advocacy groups—aka non-governmental organizations (NGOs)—to work together to reduce exposures to toxic chemicals, to which Secretary Kennedy attributes, at least in part, to the rise of chronic disease in the United States, particularly in children.

"Microplastics and chemicals from food production, assembly lines and packaging not only end up in our food, they also contaminate our soil, our water, our oceans, and from there, they re-enter the food supply," he said. (His presentation can be found here.)

Secretary Kennedy followed his talk as a participant in a panel discussion with scientists from NGOs and academia to discuss actionable policy pathways to achieve his stated goal of addressing what he referred to as "a meteoric rise in chronic disease." The panel focused on ways to minimize exposure to perceived harmful substances in food and food packaging.

Read More

The National Law Review, 29-04-25

https://natlawreview.com/article/im-interested-revolution-rfk-jr-outlines-his-fda-priorities-regulation-food

EPA Releases Strategy to Better Protect Endangered Species from Insecticides Using Commonsense Practices, Provides Flexibilities to States and Growers

2025-04-29

Today, U.S. Environmental Protection Agency (EPA) released its final Insecticide Strategy that identifies practical protections for federally endangered and threatened species from the use of insecticides, while providing flexibility for pesticide users and growers. The Strategy identifies mitigations aimed at protecting more than 900 species listed by the U.S. Fish and Wildlife Service (FWS) that EPA considers when it registers a new insecticide or reevaluates an existing one.

"Today's action is another example of how protecting our environment and safeguarding our economy can go hand in hand," said EPA Administrator Lee Zeldin. "We have found commonsense ways to keep endangered species safe that won't place unneeded burden on the growers who rely on these tools for their livelihood, and which are necessary to ensure a safe and plentiful food supply. We are committed to ensuring the agriculture community has the tools they need to protect our country, especially our food supply, from pests and diseases."

"American agriculture demonstrates that production and stewardship go hand in hand," said U.S. Secretary of Agriculture Brooke Rollins. "Thank you to Administrator Zeldin for working towards unleashing regulatory burdens for American farmers & ranchers with the release of this final insecticide strategy today. This strategy provides much needed improvements that will undoubtedly better protect U.S. homegrown crops from pests and diseases. We look forward to continued partnership with EPA to ensure our growers continue to have the crop protection tools and flexibility needed to feed, fuel, and clothe our nation and the world."

Read More

US EPA, 29-04-25

https://www.epa.gov/endangered-species/strategy-protect-endangered-species-insecticides

Canada Ranks Top 10 for Air Quality in New OECD Study

2025-04-24

A recent analysis by the Fraser Institute ranks Canada 8th out of 31 high-income OECD nations for air quality performance, signaling effective long-term environmental governance. The report, Air Quality in Canada and the OECD, presents a data-driven view of how well developed countries are managing the health impacts of air pollution. Authored by researchers Annika Segelhorst and Elmira Aliakbari, the study uses a broad set of metrics that go beyond simple pollutant concentration.

Canada scored 84 out of 100 in the latest air quality rankings—well above the average of 71 for other developed countries. The country stood out in particular for keeping fine particle pollution (PM2.5) at very low levels. On average, Canadians are exposed to just 6.5 micrograms per cubic meter, which is lower than both Canada's own air quality standard and the World Health Organization's target.

Almost 98% of Canadians live in areas where air pollution from fine particles stays within safe health limits. When it comes to the impact of

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 09, 2025

this kind of pollution on people's health, Canada ranks 5th best among its peers, showing that cleaner air is making a real difference.

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E+E Leader, 24-04-25

https://www.environmentenergyleader.com/stories/canada-ranks-top-10-for-air-quality-in-new-oecd-study,73590

EUROPE

EU mobility Updated rules for safer roads, less air pollution and digital vehicle documents

2025-04-28

For better road safety and air quality across the EU, the Commission is proposing a comprehensive overhaul of the EU's road safety and vehicle registration rules.

The new rules will take into account the growing presence of electric vehicles and adapt to emerging technologies. They will introduce enhanced inspections, including periodic technical inspections for electric vehicles and advanced driver-assistance systems, annual inspections for older cars and vans, and advanced emission testing methods to detect high-emitting vehicles to reduce fine particles pollution. Additionally, the Commission proposes to introduce digital vehicle registration and periodic testing certificates, simplify cross-border data sharing, and protect citizens against fraudulent activities such as odometer tampering. Also, periodic technical inspections will be made easier for those temporarily residing in another EU country.

The proposed changes reflect the EU's commitment to safe and sustainable mobility while ensuring the free movement of people and goods. Between 2026 and 2050, it is estimated that these proposals will save around 7,000 lives and prevent around 65,000 serious injuries.

For this purpose, the Commission is proposing to revise three directives: on periodic technical inspection (PTI) of vehicles, vehicle registration documents, and the roadside inspection (RSI) of commercial vehicles.

Read More

EU Reporter, 28-04-25

https://www.eureporter.co/environment/sustainable-urban-mobility/2025/04/28/updated-rules-for-safer-roads-less-air-pollution-and-digital-vehicle-documents/

INTERNATIONAL

World Day for Safety and Health at Work: Why it matters and how it began

2025-05-28

Imagine a world where every worker, no matter where they are, returns home safely at the end of the day. That is the goal behind the World Day for Safety and Health at Work, celebrated each year on April 28. In 2025, the day once again reminds businesses, workers, and governments why protecting health and ensuring safety at work is more important than ever. Here's a look at how the day began and why it continues to matter.

What is safety and health at work?

A safe and healthy working environment, referred to as occupational safety and health (OSH), is defined by the International Labour Organization (ILO) as the discipline concerned with preventing work-related injuries and diseases, and with protecting and promoting workers' health.

History of World Day for Safety and Health at Work

The World Day for Safety and Health at Work was first initiated by the ILO in 2003. It was launched as part of a global strategy to promote the prevention of occupational accidents and diseases. The day draws inspiration from the long-standing tradition of workers' remembrance, particularly in countries like Canada and the United States, where April 28 is also recognised as Workers' Memorial Day to honour workers who have lost their lives at work.

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 09, 2025

The idea was to establish an official platform to raise awareness and stimulate dialogue about the critical need for safe and healthy working conditions across all industries and sectors.

Read More

Business Standard, 28-05-25

https://www.business-standard.com/health/world-day-safety-health-at-work-2025-ilo-ai-digitalisation-theme-125042800154_1.html

To Whales, Our Plastic Debris Sounds Like Dinner

2025-04-23

We've likely all seen videos of how dark the deep ocean is.

Think of the scenes of deep-water submersibles exploring shipwrecks like the Titanic. It's pitch-black, and the spotlights on the vessels barely penetrate the darkness to illuminate the wreck.

That's because light's brightness in the ocean decreases with depth. The National Ocean Service reports that while minimal light may be detected as deep as 1,000 meters (3,280 feet), there's rarely any significant light beyond 200 meters (656 feet).

And that's a huge problem if you're a deep-diving whale looking for food. It's impossible to see your next meal.

Scientists assume seals and toothed whales are washing up dead with stomachs full of plastic because they mistake it for food. Sadly, plastic bags and film can look like squid or jellyfish with wavy tentacles, especially if there's not a lot of light.

That doesn't explain, however, why deep-diving whales that use echolocation, like sperm whales and beaked whales, are ingesting plastic. So, marine scientists from Duke University, NC State, UNC-Chapel Hill and the National Oceanic and Atmospheric Administration compared the way sound bounces off plastic floating underwater to the prey that whales usually eat, namely squid and squid beaks.

Their study found that plastic bags "sound" a lot like dinner to a whale.

Read More

PBS North Carolina, 23-04-25

https://www.pbsnc.org/blogs/science/deep-diving-whales-mistake-plastic-for-prey/

UN chemicals negotiators to debate potential global chlorpyrifos ban

2025-04-28

International chemicals negotiators began a biennial meeting today in Geneva, Switzerland, to decide how the global community should deal with certain toxic chemicals, including pesticides and some used in plastics. The Conference of the Parties (COP) to the Basel, Rotterdam, and Stockholm conventions—United Nations treaties related to chemicals management—will focus on potential global bans of three persistent organic pollutants (POPS)—chlorpyrifos, medium-chain chlorinated paraffins, and long-chain perfluorocarboxylic acids (LC-PFCAs), among other topics.

"Chemicals are an integral part of the modern world," Jacqueline Alvarez, chief of the chemicals and health branch at the United Nations Environment Programme (UNEP), said in a statement. "But too often, exposure to harmful chemicals through food, consumer products, and the environment can have severe consequences for people and the planet."

Although each treaty is a separate entity, together they try to mitigate chemical harm to human health and the environment. The Stockholm Convention governs POPs, while the Rotterdam Convention deals with chemicals management, and the Basel Convention guides rules on international import and export of hazardous waste, including chemicals waste.

In October 2024, the Stockholm Convention POP scientific review committee recommended that chlorpyrifos, medium-chain chlorinated paraffins, and long-chain perfluorocarboxylic acids (LC-PFCAs) no longer be used. Chlorpyrifos is an organophosphate pesticide that's already banned in some countries but allowed for critical uses on 11 food and feed crops in the US. Medium-chain chlorinated paraffins are mixtures of chlorinated alkanes between 14 and 17 atoms long and are used as flame retardants and plasticizers. The health effects of LC-PFCAs are much

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 09, 2025

like those of their per- and polyfluoroalkyl substances (PFAS) cousins and include developmental effects, neurotoxicity, and altered thyroid function, according to the POP scientific review committee. LC-PFCAs are often generated in the manufacture and incineration of PFAS.

Read More

c&en, 28-04-25

https://cen.acs.org/environment/pollution/UN-chemicals-negotiators-debate-potential/103/web/2025/04?sc=250430_news_eng_cennews_cen_NonMember

ECHA proposes restrictions on chromium(VI) substances to protect health

2025-04-29

The European Chemicals Agency brings forward a proposal for an EU-wide restriction on certain hexavalent chromium, Cr(VI), substances. The aim is to reduce the harmful effects of these carcinogenic chemicals for both workers and the public.

Helsinki, 29 April 2025 – At the request of the European Commission, ECHA has assessed the risks posed by certain Cr(VI) substances to workers and the public as well as the socio-economic impacts of potential restrictions.

The Agency concluded that an EU-wide restriction is justified as Cr(VI) substances are among the most potent workplace carcinogens and pose a serious risk to workers' health. People living near industrial sites that release these substances into the environment are also at risk of lung and intestinal cancers.

ECHA proposes to introduce a ban on Cr(VI) substances, except in the following use categories when they meet defined limits for worker exposure and environmental emissions:

1. Formulation of mixtures
2. Electroplating on plastic substrate
3. Electroplating on metal substrate
4. Use of primers and other slurries
5. Other surface treatment
6. Functional additives/process aids

Such a restriction could replace the current authorisation requirements under REACH, ensuring that the risks associated with Cr(VI) substances are effectively controlled once they are no longer subject to REACH authorisation. Additionally, barium chromate is included in the scope of the restriction to avoid regrettable substitution.

The restriction could prevent up to 17 tonnes of Cr(VI) from being released into the environment and avoid up to 195 cancer cases each year. Over 20 years, the total monetised benefits are estimated to be €331 million or €1.07 billion, depending on the restriction option chosen. The total cost to European society is estimated at either €314 million or €3.23 billion. These costs include investments in measures to reduce environmental releases and worker exposure, cost of closures and relocations, and replacing Cr(VI) substances with safer alternatives.

CHEMWATCH
Bulletin Board
REACH Update
MAY. 09, 2025

All stakeholders have the opportunity to provide information backed by robust evidence during a six-month consultation, which is expected to start on 18 June 2025. ECHA is planning to organise an online information session to explain the restriction process and help stakeholders take part in the consultation.

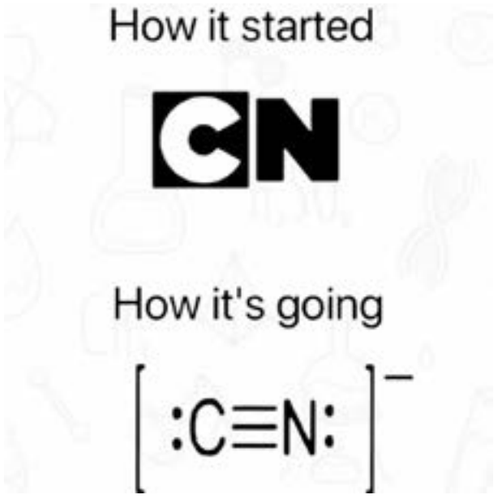
Read More

ECHA, 29-04-25

https://echa.europa.eu/-/echa-proposes-restrictions-on-chromium-vi-substances-to-protect-health#msdynttrid=x5e-T1ChEBuJAhjMpavJ91FJkAWC1ss0Qn-MAVCTZnU

How It Started

2025-05-09



https://au.pinterest.com/pin/1084312047788799570/?e_t=31488b14247c4b438d3501b05caf6f35&utm_campaign=hfdigestpins&utm_content=1084312047788799570&utm_medium=2004&utm_source=31&utm_term=1

CHEMWATCH
Bulletin Board

Toluene diisocyanate

2025-05-09

USES [2,3]

TDI is used primarily to manufacture flexible polyurethane foams for use in furniture, bedding, and automotive and airline seats. Other, smaller uses are for polyurethane elastomers (for automobile bumper covers, industrial rollers, sport soles and boots, and mechanical goods) and coatings (for automotive refinishing, wood finishes, and high-performance anti-corrosion coatings). Toluene diisocyanate–based rigid polyurethane foam is used in household refrigerators and for residential sheathing or commercial roofing in board or laminate form. "Pour-in-place" or "spray-in" rigid foam is used as insulation for truck trailers, railroad freight cars, and cargo containers. Polyurethane-modified alkyds contain approximately 6% to 7% isocyanate, mostly toluene diisocyanates, and are used as coating materials, such as floor finishes, wood finishes, and paints. Moisture-curing coatings are used as wood and concrete sealants and floor finishes. Aircraft, truck, and passenger-car coatings often are composed of toluene diisocyanate prepolymer systems. Castable urethane elastomers are used in applications requiring strength, flexibility, and shock absorption, and are resistant to oil, solvents, and ultraviolet radiation. They are used in adhesive and sealant compounds and in automobile parts, shoe soles, rollerskate wheels, pond liners, and blood bags. They are also used in oil fields and mines. Certain elastomer products are produced from the pure 2,4 isomer rather than the 80:20 mixture.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Exposure Sources

- Industry sources: Industrial emissions to air (especially companies producing the materials listed above) or spills.
- Diffuse sources: Emission to air (by outgassing) from products containing TDI.
- Natural sources: There are no known or expected natural sources of TDI emissions.
- Transport sources: No significant mobile emission sources.
- Consumer products: Polyurethane coatings, cement sealers, polyurethane mastic sealants, and polyurethane cushions and pads.

Toluene diisocyanate (TDI) is an organic compound with the formula CH3C6H3(NCO)2. Two of the six possible isomers are commercially important: 2,4-TDI (CAS: 584-84-9) and 2,6-TDI (CAS: 91-08-7). They are combustible when exposed to heat or flame and darken when exposed to sunlight (IARC 1999, HSDB 2009). [1,2]

Very low emissions of TDI have been infrequently detected from cushions.

Routes of Exposure

The main routes of exposure to TDI are inhalation, ingestion, skin and/or eye contact.

HEALTH EFFECTS [4]

Acute Health Effects

Acute exposure to high levels of 2,4-toluene diisocyanate in humans, via inhalation, results in severe irritation of the skin, eyes, and nose, and causes nausea and vomiting. Acute animal tests in rats have shown 2,4-toluene diisocyanate to have moderate to extreme acute toxicity from inhalation exposure and low acute toxicity from oral exposure.

Carcinogenicity

Information is not adequate to determine the carcinogenic effects of 2,4-toluene diisocyanate in humans. Three epidemiology studies did not find an increased occurrence of cancer among exposed workers. Animal studies have reported significantly increased incidences of tumours of the pancreas, liver, and mammary glands from exposure to 2,4-toluene diisocyanate via gavage. Animal studies, via inhalation, did not report an increased incidence of tumours. A study by the National Toxicology Program (NTP) on a mixture of toluene 2,4- and 2,6-diisocyanate administered by gavage showed an increase in tumours of subcutaneous tissues in male and female rats, the pancreas in male rats, mammary gland and liver in female rats, and liver and circulatory system in female mice. EPA has not classified 2,4-toluene diisocyanate for carcinogenicity. IARC has classified 2,4-toluene diisocyanate as a Group 2B, possible human carcinogen.

Other Effects

Chronic inhalation exposure to 2,4-toluene diisocyanate in workers has caused significant decreases in lung function, an asthma-like reaction characterised by wheezing, dyspnea, and bronchial constriction. Animal studies have reported irritation of respiratory tissues, bronchopneumonia, and weight loss from chronic exposure to 2,4-toluene diisocyanate. EPA has not established a Reference Concentration (RfC) or a Reference Dose (RfD) for 2,4-toluene diisocyanate. However, EPA has established an RfC

CHEMWATCH
Bulletin Board
Hazard Alert
MAY. 09, 2025

of 0.00007 milligrams per cubic metre (mg/m3) for the mixture of toluene 2,4- and 2,6-diisocyanate based on respiratory effects in humans.

SAFETY

First Aid Measures [5]

- Eye contact: In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Use lukewarm water if possible. Use fingers to ensure that eyelids are separated and that the eye is being irrigated. Then remove contact lenses, if easily removable, and continue eye irrigation for not less than 15 minutes. Get medical attention.
- Skin contact: Immediately remove contaminated clothing and shoes. Wash off with soap and water. Use lukewarm water if possible. Wash contaminated clothing before re-use. For severe exposures, immediately get under safety shower and begin rinsing. Get medical attention if irritation develops.
- Inhalation: Move to an area free from further exposure. Get medical attention immediately. Administer oxygen or artificial respiration as needed. Asthmatic symptoms may develop and may be immediate or delayed up to several hours. Extreme asthmatic reactions can be life threatening.
- Ingestion: Do NOT induce vomiting. Wash mouth out with water. Do not give anything by mouth to an unconscious person. Get medical attention.
- Notes to physician: Eyes: Stain for evidence of corneal injury. If cornea is burned, instil antibiotic/steroid preparation as needed. Workplace vapours could produce reversible corneal epithelial oedema impairing vision. Skin: This compound is a skin sensitiser. Treat symptomatically as for contact dermatitis or thermal burn. Ingestion: Treat symptomatically. There is no specific antidote. Inducing vomiting is contraindicated because of the irritating nature of the compound. Inhalation: Treatment is essentially symptomatic. An individual having a dermal or pulmonary sensitisation reaction to this material should be removed from further exposure to any diisocyanate.

Workplace Controls & Practices [4]

Local exhaust should be used to maintain levels below the threshold values whenever diisocyanate is handled, processed, or spray-applied. At normal room temperatures (70 F) TDI levels quickly exceed the TLV or PEL

unless properly ventilated. Standard reference sources regarding industrial ventilation should be consulted for guidance about adequate ventilation. To ensure that published exposure limits have not been exceeded, monitoring for airborne diisocyanate should become part of the overall employee exposure characterisation program.

Personal Protective Equipment [5]

- Respiratory protection: At normal room temperatures, airborne TDI can exceed limits; therefore, in inadequately ventilated environments, respiratory protection must be worn. The type of respiratory protection selected must comply with the requirements set forth in OSHA's Respiratory Protection Standard (29 CFR1910.134). The type of respiratory protection available includes (1) an atmosphere-supplying respirator such as a self-contained breathing apparatus (SCBA) or a supplied air respirator (SAR) in the positive pressure or continuous flow mode, or (2) an air-purifying respirator (APR). If an APR is selected then (a) the cartridge must be equipped with an end-of-service life indicator (ESLI) certified by NIOSH, or (b) a change out schedule, based on objective information or data that will ensure that the cartridges are changed out before the end of their service life, must be developed and implemented. Furthermore, if an APR is selected, the airborne diisocyanate concentration must be no greater than 10 times the TLV or PEL. An organic vapour (OV) cartridge is recommended for APR use.
- Hand protection: Gloves should be worn. Nitrile rubber showed excellent resistance. Butyl rubber, neoprene, and PVC are also effective.
- Eye protection: When directly handling liquid product, eye protection is required. Examples of eye protection include a chemical safety goggle, or chemical safety goggle in combination with a full-face shield when there is a greater risk of splash.
- Skin and body protection: Avoid all skin contact. Depending on the conditions of use, cover as much of the exposed skin area as possible with appropriate clothing to prevent skin contact.

CHEMWATCH
Bulletin Board
Hazard Alert
MAY. 09, 2025

REGULATION

United States

Exposure Limit	Limit Values	HE Codes	Health Factors and Target Organs
OSHA Permissible Exposure Limit (PEL) - General Industry See 29 CFR 1910.1000 Table Z-1	0.02 ppm (0.14 mg/m^3) Ceiling	HE9	Allergic sensitisation of respiratory tract; asthma
OSHA PEL - Construction Industry See 29 CFR 1926.55 Appendix A	0.02 ppm (0.14 mg/m^3) Ceiling	HE9	Allergic sensitisation of respiratory tract; asthma
OSHA PEL - Shipyard Employment See 29 CFR 1915.1000 Table Z-Shipyards	0.02 ppm (0.14 mg/m^3) Ceiling	HE9	Allergic sensitisation of respiratory tract; asthma
National Institute for Occupational Safety and Health (NIOSH) Recommended Exposure Limit (REL) See Appendix A	Lowest Feasible Concentration Ca	HE2	Carcinogenicity (pancreas, liver, skin, mammary glands, and circulatory system)
American Conference of Governmental Industrial Hygienists (ACGIH) Threshold Limit Value (TLV) (2004)*	0.005 ppm (0.036 mg/m^3) TWA 0.02 ppm (0.14 mg/m^3) STEL A4; SEN	HE9	Allergic sensitisation of respiratory tract; asthma
		HE11	Bronchitis, pneumonitis, pulmonary oedema
		HE14	Eye, mucous membrane, and respiratory irritation

Exposure Limit	Limit Values	HE Codes	Health Factors and Target Organs
CAL/OSHA PELs	0.005 ppm (0.04 mg/m^3) TWA 0.02 ppm Ceiling 0.02 ppm (0.15 mg/m^3) STEL	HE9	Allergic sensitisation of respiratory tract; asthma
		HE11	Bronchitis, pneumonitis, pulmonary oedema
		HE14	Eye, mucous membrane, and respiratory irritation

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CHEMWATCH
Bulletin Board

Iron-generated rust binds and removes selenium, offering safer water treatment options

2025-05-08

Selenium is a critical element, particularly for the thyroid and immune system, but too little or too much can be harmful to both humans and wildlife. A team of researchers at Washington University in St. Louis has made strides in removing selenium contamination from water, which could ensure safe treatment of water from agricultural ponds, mining discharge or power plant wastewater to meet federal maximum levels.

Daniel Giammar, the Walter E. Browne Professor of Environmental Engineering and director of the university's Center for the Environment, and his lab used iron electrocoagulation to remove selenium from water in different experiments. Results of the research were recently published in Environmental Science & Technology and ACS ES&T Engineering.

Removing selenium from water is challenging because it's so water soluble, Giammar said. Iron electrocoagulation is up to the challenge by generating iron-containing solids with large surface areas. During coagulation, selenium then chemically binds to those surfaces. It can also be chemically transformed into a type of selenium that will bind more strongly.

In one study, published in Environmental Science & Technology, graduate student Xicheng He in Giammar's Aquatic Chemistry Laboratory removed selenium from water using iron electrocoagulation in a flow-through reactor, built by research partner WaterTectonics, to generate different forms of rust.

"We apply a current to the iron reactor, which forces it to corrode faster than it normally would and generate rust," Giammar said. "Iron can generate green rust before red rust, and the green rust is incredibly reactive. This reacts with selenium to pull selenium out of the water into these iron-containing particles, which we then remove with a filter."

This process removed more than 98% of selenium by flowing through the iron reactor for 11 seconds then settling for an hour, where it remained tightly bound in solids that would be considered nonhazardous.

In another study, published in ACS ES&T Engineering, graduate student Yihang Yuan studied 15 different combinations of water chemistry and the different effects of the electrochemical operating conditions on selenium removal in batch reactors.

By running experiments in well-mixed and continuously monitored beakers of selenium-containing solution, Yuan developed a reaction-based model to predict electrocoagulation performance to remove selenium with varying conditions of oxygen and pH.

"We showed that this works in relatively simple compositions because we really wanted to isolate the effects of pH and dissolved oxygen," Giammar said. "We see that it works in the lab, and we can make it relevant to the real world."

Going forward, Giammar's lab is looking beyond selenium.

"Now that we have the reactor and the protocols, we are looking at some other contaminants and natural organic matter, both where we control the compositions and with some real water samples," he said. "We didn't invent the reactor technology, but we showed WaterTectonics that it could work in different cases than what they might have thought about."

Phys Org, 8 May 2025

https://phys.org

Temporary Menstrual Cycle Shifts After Flu and COVID-19 Vaccines

2025-04-29

Vaccine research covers many outcomes, but menstrual health isn't usually one of them.

A new study conducted by researchers from Oregon Health & Science University investigates whether seasonal influenza vaccines, alone or given alongside a COVID-19 vaccine, cause changes in menstrual cycle length. The findings point to small, temporary shifts, but no long-term effects were observed.

The study was published in JAMA Network Open.

Menstrual health matters in vaccine research

Despite menstruation being a regular part of life for many, clinical trials have rarely considered how vaccines might affect menstrual cycles. With the rollout of COVID-19 vaccines, this gap gained renewed urgency. As people began sharing personal experiences of cycle changes, such as delays or heavier bleeding, questions about possible links between

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

vaccination and menstruation became more widespread. These concerns, whether grounded in data or not, contributed to vaccine hesitancy.

This isn't an isolated issue. A similar situation unfolded in Japan following reports of menstrual disturbances after the human papillomavirus vaccine. Public concern led to a dramatic fall in vaccine uptake, with lasting effects on health outcomes.

"Misinformation and the dearth of data to confirm or refute the vaccine experience can decrease acceptability and uptake of a vaccine," said the authors.

Previous studies have found a small, short-lived increase in menstrual cycle length after COVID-19 vaccination. But whether other vaccines, like the widely recommended seasonal influenza vaccine, might have similar effects, hasn't been well studied.

"While the COVID-19 pandemic brought many challenges, it did highlight the lack of evidence on this important patient-oriented outcome," the authors commented.

Technology Networks, 29 April 2025

https://technologynetworks.com

Bacterium salvaged from compost could reduce side effects of chemotherapy drugs

2025-05-08

New research led by the University of Sydney has revealed the potential of engineered proteins to more precisely deliver drugs within the body.

The proof-of-concept research could potentially pave the way to developing more accurate delivery of cytotoxic drugs. Commonly used in chemotherapy, they work by killing cells and can cause significant side effects if not delivered to the exact site of the disease they are targeting.

Led by Dr. Taylor Szyszka and Associate Professor Yu Heng Lau from the University's School of Chemistry, a team of researchers has developed protein cages that have been able to package a commonly used chemotherapy drug.

Their findings are published in Angewandte Chemie International Edition.

Known by most as a source of nutrition, proteins are essential to our existence in many ways. There are 42 million proteins in every human

cell and each protein comprises varying configurations of 20 different amino acids. The characteristics of those amino acids determine a protein's characteristics and function.

"Nearly everything that happens in a cell, from building its protective membranes to producing energy, requires a protein," said Dr. Szyszka.

Dr. Szyszka and her team research and develop protein cages, groups of identical proteins bound together to form a spherical shell. They focus on encapsulins—a sub-group of protein cages—which are highly stable, able to protect their cargo from outside attackers and also prevent its escape.

The encapsulin underpinning this research was first identified, through separate findings by US researchers, in bacteria found in a compost heap in 2019. Dr. Szyszka's team re-engineered the newly discovered encapsulin by fusing it to another protein. This prevented the encapsulin from assembling before the drug was added; had that occurred, the encapsulin would have been unable to hold or transport drugs.

The researchers then loaded their turbocharged encapsulin with doxorubicin, a chemotherapy drug, and successfully triggered its assembly in vitro, outside a living organism.

"Doxorubicin is a fluorescent drug and the fluorescent signal we detected after loading demonstrated the drug was successfully packaged during our triggered encapsulin assembly," said Dr. Szyszka.

"This is a first. Until now, it hasn't been possible for encapsulins to efficiently load drugs. Previously, this could happen only by pulling encapsulins apart, loading them with a drug and then reassembling them, a messy process which compromises the encapsulin's stability."

The findings mark the very preliminary stages of harnessing encapsulins as a new, precise, drug delivery mechanism. The next stage in this research is to continue protein engineering the encapsulin so it can gravitate to its target.

"It's now all about engineering the shell's exterior so the encapsulin we developed can target specific cells," said Dr. Szyszka. "If it holds a drug designed to treat liver disease, for instance, we want the encapsulin to find its way to liver cells.

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

"We've built the car, now we need to learn how to drive it."

Phys Org, 8 May 2025

https://phys.org

New discovery shows how molecules can mute heat like music

2025-05-07

Imagine you are playing the guitar -- each pluck of a string creates a sound wave that vibrates and interacts with other waves.

Now shrink that idea down to a small single molecule, and instead of sound waves, picture vibrations that carry heat.

A team of engineers and materials scientists in the Paul M. Rady Department of Mechanical Engineering at CU Boulder has recently discovered that these tiny thermal vibrations, otherwise known as phonons, can interfere with each other just like musical notes -- either amplifying or canceling each other, depending on how a molecule is "strung" together.

Phonon interference is something that's never been measured or observed at room temperature on a molecular scale. But this group has developed a new technique that has the power to display these tiny, vibrational secrets.

The breakthrough study was led by Assistant Professor Longji Cui and his team in the Cui Research Group. Their work, funded by the National Science Foundation in collaboration with researchers from Spain (Instituto de Ciencia de Materiales de Madrid, Universidad Autónoma de Madrid), Italy (Istituto di Chimica dei Composti Organometallici) and the CU Boulder Department of Chemistry, was recently published in the journal Nature Materials.

The group says their findings will help researchers around the world gain a better understanding of the physical behaviors of phonons, the dominant energy carriers in all insulating materials. They believe one day, this discovery can revolutionize how heat dissipation is managed in future electronics and materials.

"Interference is a fundamental phenomenon," said Cui, who is also affiliated with the Materials Science and Engineering Program and the Center for Experiments on Quantum Materials. "If you have the capability

to understand interference of heat flow at the smallest level, you can create devices that have never been possible before."

The world's strongest set of ears

Cui says molecular phononics, or the study of phonons in a molecule, has been around for quite some time as a primarily theoretical discussion. But you need some pretty strong ears to "listen" to these molecular melodies and vibrations first-hand, and that technology just simply hasn't existed.

That is, until Cui and his team stepped in.

The group designed a thermal sensor smaller than a grain of sand or even a sawdust particle. This little probe is special: it features a record-breaking resolution that allows them to grab a molecule and measure phonon vibration at the smallest level possible.

Using these specially designed miniature thermal sensors, the team studied heat flow through single molecular junctions and found that certain molecular pathways can cause destructive interference -- the clashing of phonon vibrations to reduce heat flow.

Sai Yelishala, a PhD student in Cui's lab and lead author of the study, said this research using their novel scanning thermal probe represents the first observation of destructive phonon interference at room temperature.

In other words, the team has unlocked the ability to manage heat flow at the scale where all materials are born: a molecule.

"Let's say you have two waves of water in the ocean that are moving towards each other. The waves will eventually crash into each other and create a disturbance in between," Yelishala said. "That is called destructive interference and that is what we observed in this experiment. Understanding this phenomenon can help us suppress the transport of heat and enhance the performance of materials on an extremely small and unprecedented scale."

Tiny molecules, vast potential

Developing the world's strongest set of ears to measure and document never-before-seen phonon behavior is one thing. But just what exactly are these tiny vibrations capable of?

"This is only the beginning for molecular phononics," said Yelishala. "New-age materials and electronics have a long list of concerns when it comes to heat dissipation. Our research will help us study the chemistry, physical

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

behavior and heat management in molecules so that we can address these concerns."

Take an organic material, like a polymer, as an example. Its low thermal conductivity and susceptibility to temperature changes often poses great risks, such as overheating and degradation.

Maybe one day, with the help of phonon interference research, scientists and engineers can develop a new molecular design. One that turns a polymer into a metal-like material that can harness constructive phonon vibrations to enhance thermal transport.

The technique can even play a large role in areas like thermoelectricity, otherwise known as the use of heat to generate electricity. Reducing heat flow and suppressing thermal transport in this discipline can enhance the efficiency of thermoelectric devices and pave the way for clean energy usage.

The group says this study is just the tip of the iceberg for them, too. Their next projects and collaborations with CU Boulder chemists will expand on this phenomenon and use this novel technique to explore other phononic characteristics on a molecular scale.

"Phonons travel virtually in all materials," Yelishala said. "Therefore we can guide advancements in any natural and artificially made materials at the smallest possible level using our ultra-sensitive probes."

Science Daily, 7 May 2025

https://sciencedaily.com

New device instantly detects dangerous street drugs, offering hope for harm reduction

2025-05-07

A portable device that can instantly detect dangerous street drugs at extremely low concentrations has been developed at the University of Bath in the UK.

The device, which is being trialed by drug-checking services in the UK, Norway and New Zealand, can identify substances such as benzodiazepines and synthetic opioids that are difficult to detect with existing mobile technologies and are major contributors to drug overdoses globally.

The device, which is similar to an ultraviolet spectrometer, will allow drugs to be tested cheaply and at volume. Its on-the-spot analysis reveals both the contents of a substance and the concentration of each ingredient. The technology is described in Analytical Chemistry.

Biochemist Professor Chris Pudney—who leads the team that developed the technology from the Department of Life Sciences at Bath—says the potential life-saving benefits of this invention are considerable. By using the device to reveal the precise composition of an illicit substance, the risks associated with taking unknown or adulterated drugs can be reduced significantly.

Professor Pudney envisions the new machine being deployed in areas where illicit drugs are commonly used, such as at clubs and festivals, as well as in services that provide support and treatment for dependent-drug users.

Testing times

Detecting substances at low concentrations is more challenging than identifying larger quantities of highly pure substances. The equipment currently available for this task often requires extensive training and can only be operated by chemists.

By contrast, the device invented by Professor Pudney can be operated by a non-expert, yielding results with the simple press of a button, and can detect drugs at extremely low concentrations. This allows it to determine the potency of a formulation and identify any contamination with undeclared substances.

Many 'red flag' substances, including synthetic opioids such as nitazenes and fentanyl, are toxic even in minute quantities, and being able to detect them is critical to saving lives.

Professor Pudney said, "Whatever we're doing at the moment to prevent deaths from drug misuse isn't working, so we need a new kind of service that can be where it's needed—cheaply, easily and anywhere.

"Our device would support community harm reduction. Telling people not to take drugs doesn't work, so different strategies are needed. By letting people know exactly what's in a drug and how strong it is, we can empower them to make safer decisions about whether or not to take it, or to use it in a safer way."

Drug adulteration

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

Globally, there is a growing problem of people unknowingly taking street drugs that have been mixed with undeclared substances. For instance, illicit pills containing benzodiazepines (which can produce feelings of euphoria, relaxation and calmness in the user) can be contaminated with synthetic opioids, turning them into ultrapotent mixtures that dramatically increase the risk of adverse effects and fatal overdoses.

The rise of potent synthetic drugs has made the landscape of drug use particularly dangerous, essentially presenting people who believe they are taking a known dosage of a known drug with a 'Russian roulette' of risk.

Professor Pudney said, "Now, more than ever, there are serious health risks associated with taking all drugs. People may think they have bought something relatively unharmful—perhaps a substance they know well—but the drug they have may in fact be contaminated with a far more dangerous and more addictive substance that could endanger their lives.

"This is why drug checking is so important and so needed. We need simple, instant detection that anyone in a drug and alcohol service can use to support their clients."

Deaths in England and Wales from drug poisoning have increased year on year, rising from 4,359 in 2018 to 4,907 in 2023 (these figures include both illicit drug use and prescription drug misuse).

Local and international trials

The new technology—currently a prototype—is being trialed by drug services both in the UK and internationally.

- **Devon & Cornwall Police, UK**

A device acquired by Devon & Cornwall Police (UK) in June 2024 has allowed the force to fast-track suspicious substances linked to near-fatal and fatal overdoses. This lets them provide real-time drug warnings to drug treatment services in the area, rather than waiting for several months for results from forensic drug-detection service providers.

Nick Burnett, drug expert witness for Devon & Cornwall Police, said, "A prime example of this was testing of some oxycodone tablets in 2024 following a death. The tablets were found to contain a nitazene. We were able to put out a drug warning within 36 hours of that death occurring."

He added that the technology had improved the police's working relationship with its drug treatment services, especially in relation to information sharing and, where necessary, the issuing of drug warnings.

- **The Loop, UK**

Unlike in New Zealand, drug checking services in the UK require a Home Office license for the possession of controlled drugs to operate legally. To date, The Loop Drug Checking Service is the only community-based drug-checking service in the UK that has been granted a license. It has been operating in Bristol since 2024, and uses, alongside other analytical technologies, Professor Pudney's device.

Katy Porter, CEO of The Loop said, "We have been pleased to work alongside the team at the University of Bath to explore the use and potential of the device in drug checking services and for the purpose of reducing drug-related harms. We share the concerns regarding the changing drug market in the UK and are working together to ensure drug checking is accessible and available to more people."

- **Drug-checking service, New Zealand**

For two weeks last year, hundreds of drug samples were tested in New Zealand using Professor Pudney's new device as part of an initiative involving the country's three front-line drug-checking services: the Needle Exchange Program, the New Zealand Drug Foundation and KnowYourStuffNZ. New Zealand is one of few countries in the world where drug-checking services are explicitly legal.

KnowYourStuffNZ deputy manager Dr. Jez Weston said, "The spectrometers that we use are currently the best tech for mobile drug analysis, but science moves ever on. The University of Bath's new technology could help us help our clients with better and faster analysis of their samples."

- **Drug-checking service, Norway**

The device is also being trialed by the Association for Safer Drug Policies (ASDP) in Norway. Norway is another country that operates community-based drug checking.

Dagfinn Hessen Paust, chief scientific officer at the ASDP—a leading advocate for harm prevention and evidence-based drug policies in Norway and the Nordics, said, "We use a number of different technologies to check drugs, mostly using infrared spectrometry, which is great for most use cases but not for testing benzodiazepines and very potent, very dangerous opioids.

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

"These substances—unlike, say, MDMA—are found in very low concentrations in the tablets people consume and cannot be picked up by established devices.

"The new device from Bath is helping us fill this gap—it's very exciting for us to be trialing this new technology."

Shining light

The new technology from Bath works through a combination of fluorescence and reflectance spectroscopies.

Fluorescence is a technique that involves shining light on a substance and measuring the light that the substance emits in response. Different substances emit light in unique ways, which makes it possible to identify them.

Reflectance Spectroscopy is a technique that measures the light bouncing off a substance. The way light is reflected provides information about the substance's properties.

The device is trained using a deep-learning algorithm, meaning it is exposed to a library of Nanoparticle Spectroscopy (NPS) light patterns from which it learns to make accurate identifications.

Professor Pudney said, "Our aim is for this device to support drug-checking services, as a means to decrease the harm caused by drugs across different groups. The landscape of drug use is changing rapidly and we hope this tool can fill some of the gaps that are emerging."

phys Org, 7 May 2025

https://phys.org

Cement-like building material doubles up as an electrolyte in rechargeable battery

2025-05-08

Researchers in France and Spain have developed a cement-like material from a geopolymer and shown how it can simultaneously serve as a solid electrolyte in a rechargeable electrochemical energy storage system. 'This is more than a battery', says Vadim Kovrugin, who led the work at the University of Bordeaux and the University of the Basque Country. 'It is a new material concept, where infrastructure does not merely stand still but can actively contribute to the energy ecosystem.'

Previous research into construction materials with integrated energy storage has focused on storing waste heat energy in Portland cement. Storing energy electrochemically, rather than thermally is much more efficient, so a few studies have explored using traditional cement or concrete mixtures as battery components.

The issue with cement, however, is that producing it generates significant carbon dioxide emissions. Kovrugin's team has therefore been investigating the electrochemical properties of more sustainable building binders.

Here they used a synthetic aluminosilicate called metakaolin that's made by heating the clay mineral kaolinite. Metakaolin has high mechanical strength and durability, as well as good ionic conductivity. Mixing metakaolin with an activation solution formed a paste into which the team embedded zinc and manganese dioxide electrodes to create a battery with a classic probe-style configuration.

In previous studies into cement-based batteries, the alkaline conditions of such materials can see them react with zinc to form calcium zincate. The mildly acidic metakaolin electrolyte in Kovrugin's team's battery, however, allows zinc to remain in its ionic form. This makes the system rechargeable via a reversible plating and stripping process.

'The use of metakaolin-based geopolymers as a solid electrolyte for energy storage is a great advancement, and it is exciting to see the dual functionality of this material in energy storage and construction. As we transition to renewable energy, the need for efficient and integrated energy storage solutions becomes more urgent, making this research particularly timely,' remarks Damian Stefaniuk, from the Massachusetts Institute of Technology in the US, who was part of a team that created a supercapacitor out of cement in 2023.

Durability is a key challenge when incorporating batteries into permanent structures and Stefaniuk explains 'one of the functions – energy storage – may degrade much sooner due to the chemical reactions present in batteries'.

Hydrogen evolution is a well-known stumbling-block in zinc battery development and in the metakaolin-based system it generates hexahydrated zinc sulfate. This side product could compromise the interface between the negative electrode and electrolyte, and lead to cracks in the geopolymer material. The team therefore suggests that using a modular design, where battery components are structured in accessible

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

layers or compartments, could make this less of an issue by allowing components to be maintained or replaced without compromising the structural integrity of any construction.

Another key consideration in the geopolymer material's durability is its hydration and drying behaviour. There was heavy water loss in the batteries after 40 days of curing, by which time the electrochemical stability had decreased. This implies hydration levels are important for maintaining sufficient conductivity. However, increasing the water content could potentially affect the material's mechanical integrity. The geopolymer formulation and curing processes will need to be optimised, but further work on this could help to make the material more suitable for real structures.

Despite the challenges involved in embedding energy storage functionality into structural materials, Kovrugin notes that 'with each step forward, we move closer to a future where walls and bridges are not just passive structures, but active elements capable of storing energy and monitoring their own health – for example, by detecting the appearance of cracks or other signs of structural degradation.'

Chemistry World, 8 May 2025

https://chemistryworld.com

Chatbot opens computational chemistry to nonexperts

2025-04-07

Advanced computational software is streamlining quantum chemistry research by automating many of the processes of running molecular simulations. The complicated design of these software packages, however, often limits their use to theoretical chemists trained in specialized computing techniques.

A new web platform developed at Emory University overcomes this limitation with a user-friendly chatbot.

The chatbot guides nonexperts through a multistep process for setting up molecular simulations and visualizing molecules in solution. It enables any chemist -- including undergraduate chemistry majors -- to configure and execute complex quantum mechanical simulations through chatting.

The free, publicly available platform -- known as AutoSolvateWeb -- operates primarily on cloud infrastructure, further expanding access to sophisticated computational research tools.

The journal Chemical Science published a proof-of-concept for AutoSolvateWeb, which marks a significant step forward in the integration of AI into education and scientific research.

AutoSolvateWeb is geared to set up simulations for a particular chemical to be dissolved (a solute) and a substance to dissolve it in (a solvent), resulting in a solution (a solvate).

The simulations are delivered in the form of 3D movies.

"It's a bit like a microscope, giving you an atomic-level view of molecules interacting in a solution," says Fang Liu, Emory assistant professor of chemistry, who led the development of AutoSolvateWeb.

The broad accessibility of AutoSolvateWeb makes it a valuable tool to create large, high-quality datasets addressing the behaviors of molecules in solution. Such datasets provide a foundation to apply machine-learning techniques to drive innovations in everything from renewable energy to human health.

"Our goal is to help speed up scientific discovery," says Fangning Ren, co-author of the Chemical Science paper and an Emory PhD student of chemistry.

Rohit Gadde, a former Emory research specialist, is first author of the paper. Additional co-authors include Lechen Dong, Emory graduate student of chemistry; Yao Wang, Emory assistant professor of chemistry; Sreelaya Devaguptam, a former Emory visiting scholar; and Rajat Mittal, a former graduate research assistant at Clemson University.

Automating complex tasks

A theoretical chemist, Liu leads a team specializing in computational chemistry, including modeling and deciphering molecular properties and reactions in the solution phase.

Before running a quantum chemistry program for a molecule in solution it's necessary to determine the geometry of the solute molecule and the location and orientation of the surrounding solvent molecules through molecular simulation. The process of setting up and running these simulations is complicated and time consuming, limiting how often researchers can perform such calculations.

In 2022, the Liu group developed a way to automate many of these calculations with a system it dubbed AutoSolvate. That system reduced the lines of code that a computational chemist needs to enter into a

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

supercomputer to run a simulation from hundreds of lines to just a few lines.

In addition to the command-line interface geared toward more experienced theoretical chemists, AutoSolvate included an intuitive graphical interface suitable for graduate students learning to run simulations.

AutoSolvateWeb builds on this foundation.

Expanding access

By operating primarily on cloud infrastructure, AutoSolvateWeb overcomes hardware configuration challenges, further flattening the learning curve for sophisticated computational research. The chatbot communicates via natural language rather than computer code on the front end, while AutoSolvateWeb automates the software processes on the backend.

"Chemists can spend less time learning to write computer code so they can focus more of their efforts on specific problems that they want to solve," Liu explains. "We also want to enable students to run simulations by themselves so that they can understand the dynamics of molecules in solution more fully."

Rather than a large language model (LLM) chatbot, like ChatGPT, the AutoSolvateWeb chatbot is primarily rules-based. It doesn't converse like a real human over a range of subjects but is geared to specific tasks, similar to chatbots used for customer services like online banking.

The chatbot prompts a user to type in the name of a molecule of interest, such as caffeine, then select a solvent to dissolve the caffeine in, such as water. The system taps data from PubChem -- the world's largest collection of The chatbot guides the user step-by-step through the cloud environment, seamlessly integrating multiple open-source software programs needed for the workflow. Once all the proper parameters are calculated through the automated process, AutoSolvateWeb submits the results to a National Science Foundation supercommuter to create the simulation.

The supercommuter returns a trajectory file. The user can download this file and use open-source software to turn the file into a 3D movie of their requested simulation.

Seeing is believing -- and understanding

AutoSolvateWeb is poised to enhance how chemistry is taught.

"As computers become more and more powerful, they become more important to scientific research," Ren says. "Undergraduate chemistry students need to get familiar with computer simulations so they can keep pace with advances in how research is done."

He cites solvatochromism, a technique to analyze the makeup of chemicals in a liquid, as an example of the power of computer simulations for education.

Undergraduate students typically learn about solvatochromism in lab experiments by dissolving a solute known as Riechart's dye in different solvents. The solution turns blue, red, green or yellow depending on how the solute molecules absorb light.

The simplest explanation for this phenomenon is that the color variations are due to variations in the polarity of a solvent. Changes in polarity stabilize the ground state of a molecule differently, which in turn affects a molecule's absorption peak along the wavelength of light.

What's trickier to explain are exceptions to this rule. Sometimes solvents of similar polarities produce different colors because of the way hydrogen bonds formed between the solute and the solvent.

"To fully understand how hydrogen bonding plays a special role in this situation the students need to run a computer simulation," Liu says. "Seeing is believing. You need to look directly at the structure in motion so that you can understand things at the microscopic scale."

Such detailed visualizations help students learn to think critically, she says, so they can go beyond memorizing concepts in textbooks to making and analyzing their own discoveries.

"In science we don't want to just understand what is happening," Ren adds. "We want to know why it is happening."

Small molecules, big data

Liu and her colleagues are now working to expand the range of chemical systems that AutoSolvateWeb can simulate, going beyond limitations such as single organic molecules as the solute. They are also enhancing the platform's ability to not only generate data but to store and freely exchange that data across the chemistry community in an open-source format.

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

The researchers hope that their pioneering work to democratize computational chemistry research will inspire similar initiatives across the natural sciences. Their ultimate goal, Ren explains, is to help connect AI across various domains of basic science, boosting the power of interdisciplinary research.

Science Daily, 7 May 2025

https://sciencedaily.com

The ozone layer shields life on Earth. We'll soon lose a key way to monitor its health

2025-04-04

Humankind will soon lose a great deal of vigilance over the ozone layer, which shields life on Earth from harmful solar radiation.

The impending loss of NASA's Aura and the Canadian Space Agency's SCISAT satellites threatens scientists' ability to closely monitor compounds that destroy ozone and alter stratospheric circulation. With no planned missions to replace either satellite, a data desert in the stratosphere appears imminent, researchers warn in the March Bulletin of the American Meteorological Society.

"We've been thinking about this for years," says atmospheric scientist David Fahey of the National Oceanic and Atmospheric Administration in Boulder, Colo., who was not involved in the assessment. "These satellites, as of today, will go dark in the absence of a torchbearer into the future."

The satellites will sunset while the ozone layer's recovery has unpredictably stalled over the midlatitude Northern Hemisphere. And experts warn that increasing amounts of space debris from dying satellites could unleash more ozone-depleting substances. What's more, scientists will lose their ability to watch for harmful impacts to the ozone layer from wildfires and stratospheric aerosol injections aimed at countering climate warming.

To be clear, other instruments will continue monitoring the ozone layer itself. What will be lost is the ability to thoroughly scan the stratosphere for substances that can damage the ozone layer. "It's like taking MRI and CAT scanning away and going back to just X-rays," says coauthor Ross Salawitch, an atmospheric scientist at the University of Maryland in College Park. "We will know what is happening to the ozone. What we'll lack is why."

SCISAT took to the skies in 2003, followed the next year by Aura. Ever since, these satellites have advanced scientists' understanding of the stratosphere and ozone layer. But by mid-2026, Aura's solar panels will be unable to power its operations. And although SCISAT could theoretically remain in orbit until around 2035 — if no crucial hardware failures or funding issues arise — the spacecraft is already 18 years beyond its intended lifetime.

Once the satellites go dark, scientists will lose access to daily global measurements of ozone-destroying gases. These include halogenated gases such as hydrogen chloride and chlorine monoxide, as well as nitrogen oxides.

The origins of most of these gases can be traced to chemicals and materials manufactured by humans. Many of these source substances are regulated by the Montreal Protocol, an international agreement enacted in 1989 to phase out ozone-depleting substances. But without observations from both satellites, it will be more difficult to track how these substances are harming the ozone layer, Fahey says. "We're going to lose that vigilance factor."

What's more, data from SCISAT and Aura revealed how smoke from the 2019–2020 Australian wildfires damaged the ozone layer, an impact that was unanticipated at the time. "We're just at the beginning of trying to understand how that happens," says atmospheric chemist Lyatt Jaeglé of the University of Washington in Seattle.

As blazes are expected to become more intense and frequent due to climate change, some researchers have proposed that wildfire emissions could have increasingly significant effects on stratospheric ozone. And large-scale injections of stratospheric aerosols — a proposed technique to mitigate climate warming by reflecting sunlight back into space — could have effects similar to a volcanic winter. That means the aerosols could potentially damage the ozone layer over large portions of the globe. The loss of the ability to monitor these impacts is a major concern, Salawitch, Fahey and Jaeglé agree.

Two potential successor missions are being considered by NASA and the European Space Agency.

One is the Changing-Atmosphere Infra-Red Tomography Explorer, or CAIRT, a concept the ESA is weighing for its next Earth Explorer mission. The satellite would provide global observations of ozone, water vapor,

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

aerosols and ozone-damaging compounds. A decision will be announced later this year, with plans to launch the selected mission around 2032.

Meanwhile, NASA is considering the Stratosphere Troposphere Response using Infrared Vertically-resolved light Explorer or STRIVE. This satellite would wield Aura's monitoring capabilities and then some, providing enhanced resolution and greater coverage, says Jaeglé, who is lead investigator of the mission's science team. A decision could be made later this year, with a potential launch in 2030 or 2032.

"If either one of these goes forward, then that's obviously good news," Salawitch says. "We'd like to continue to be diagnosing the patient."

Science News, 4 April 2025

https://sciencenews.com

Scientists Finally Confirm "Crazy" Vitamin B1 Theory From 1958

2025-05-06

Chemists have confirmed a 67-year-old theory about vitamin B1 by stabilizing a highly reactive molecule in water, a breakthrough that was long considered impossible. This discovery not only resolves a long-standing biochemical question but also paves the way for more sustainable and efficient methods of producing pharmaceuticals.

The molecule involved is a carbene, a form of carbon atom with only six valence electrons instead of the usual eight. This electron deficiency makes carbenes extremely unstable and reactive, especially in water, where they typically break down almost immediately. However, for decades, scientists have suspected that vitamin B1, or thiamine, might form a carbene-like intermediate during essential reactions in the body.

Confirming Breslow's 1958 hypothesis

Now, for the first time, researchers have successfully created a stable carbene in water. They were able to isolate it, seal it in a container, and observe it remaining intact for several months. This achievement is detailed in a new paper published in Science Advances.

"This is the first time anyone has been able to observe a stable carbene in water," said Vincent Lavallo, a professor of chemistry at UC Riverside and corresponding author of the paper. "People thought this was a crazy idea. But it turns out, Breslow was right."

The reference is to Ronald Breslow, a Columbia University chemist who proposed in 1958 that vitamin B1 could convert into a carbene to drive biochemical transformations in the body. Breslow's idea was compelling, but carbenes were so unstable, especially in water, that no one could prove they actually existed in a biological setting.

Shielding the carbene for stability

Lavallo's team succeeded by wrapping the carbene in what he calls "a suit of armor," a molecule they synthesized in the laboratory that shields the reactive center from water and other molecules. The resulting structure is stable enough to be studied with nuclear magnetic resonance spectroscopy and x-ray crystallography, providing conclusive evidence that carbenes like this can exist in water.

"We were making these reactive molecules to explore their chemistry, not chasing a historical theory," said first author Varun Raviprolu, who completed the research as a graduate student at UCR and is now a postdoctoral researcher at UCLA. "But it turns out our work ended up confirming exactly what Breslow proposed all those years ago."

Toward greener pharmaceutical chemistry

Beyond confirming a biochemical hypothesis, the discovery has practical implications. Carbenes are often used as "ligands," or support structures, in metal-based catalysts — the chemical workhorses used to produce pharmaceuticals, fuels, and other materials. Most of these processes rely on toxic organic solvents. The researchers' method of stabilizing carbenes in water could help make those reactions cleaner, less expensive, and safer.

"Water is the ideal solvent — it's abundant, non-toxic, and environmentally friendly," Raviprolu said. "If we can get these powerful catalysts to work in water, that's a big step toward greener chemistry."

Mimicking cell chemistry in the lab

Knowing that such reactive intermediate molecules can be generated and survive in water also brings scientists one step closer to mimicking the kind of chemistry that happens naturally in cells, which are mostly made of water.

"There are other reactive intermediates we've never been able to isolate, just like this one," Lavallo said. "Using protective strategies like ours, we may finally be able to see them and learn from them."

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

For Lavallo, who has spent two decades designing carbenes, the moment is both professional and personal.

"Just 30 years ago, people thought these molecules couldn't even be made," he said. "Now we can bottle them in water. What Breslow said all those years ago — he was right."

For Raviprolu, the discovery serves as a reminder to persevere in scientific research and discovery.

"Something that seems impossible today might be possible tomorrow, if we continue to invest in science," he said.

Sci Tech Daily, 6 May 2025

https://scitechdaily.com

Alloy design model offers faster, more accurate predictions by factoring in material defects

2025-05-07

Humans began creating alloys about 5,000 years ago by combining copper and tin to produce bronze. Since then, alloy design has advanced dramatically, says Moneesh Upmanyu, professor of mechanical and industrial engineering at Northeastern University.

"Now, it's definitely a science [and] less of an art because we have the periodic table and we know the properties of all these elements that we are mixing together," he says.

The Journal of Applied Physics recently selected Upmanyu's new research paper on alloy design as an Editor's Pick.

The paper introduces a new computational model that offers strategies for alloy design of real materials in seconds. Compared to traditional lab experiments and AI-based approaches, the model offers greater speed, cost efficiency and accuracy.

The work was conducted in collaboration with Changjian Wang, a former Northeastern graduate student.

Previous computational tools—including those based on machine learning and artificial intelligence—often failed to account for a critical factor, Upmanyu says, real-life crystalline materials, such as metals and ceramics, contain defects.

In materials science, defects are irregularities or imperfections in a crystal's atomic structure. While they may sound like flaws, defects are often intentionally introduced to enhance properties such as strength, conductivity and corrosion resistance.

The new model takes into account an important class of material defects (grain boundaries) and the tendency of the mixed solutes to gather—or segregate—around the structural imperfections during alloy formation.

"You are dealing with these defective materials by default, and all these alloy design techniques ignore this," Upmanyu says. "They just can't factor that in because it's a very complex system with all these defects in place."

One well-known example of such material defect that has been studied extensively over the past century, Upmanyu says, is a dislocation. It occurs when an entire atomic plane is missing from a crystal's structure. Despite this imperfection, dislocations allow for plastic deformation of a material without breaking by letting the defect move through the crystal lattice.

When alloys are formed by mixing with solutes, or dissolved substances, the dislocations act as preferred locations for the solutes. The solutes attach to dislocation threads like a swarm of bees, making it harder for dislocations to move. By engineering these defects and behaviors of solutes in alloys, Upmanyu says, humans can make stronger, cost-effective materials.

His research focuses on another key defect: grain boundaries. These occur in polycrystalline materials—such as copper—at the interfaces where differently oriented crystal grains meet. Unlike dislocations, these defects run along surfaces within the material.

"For a crystal small enough to hold between your fingers, conventional alloys with micron-sized grains have a grain boundary area as large as a basketball court," Upmanyu says.

That is a vast area for solutes to attach to, he says, which affects the entire mixing strategy when alloys are being made as well as their mechanical, electrical and magnetic properties.

Material engineers often manipulate these boundaries to control, for example, the direction of electricity conduction, by orienting the grains in the crystals along one direction.

"The motion of grain boundaries with the solutes is completely ignored in current general alloying theory," Upmanyu says.

CHEMWATCH
Bulletin Board
Gossip
MAY. 09, 2025

His model examines how solutes affect that motion.

"If I look under a microscope at finite temperature (non-zero absolute temperature that affects the energy state of a system), these grain boundaries and these defects are not static, they are dancing around, they are moving," Upmanyu says. "And we exploit these fluctuations of the grain boundaries with solute segregated to them."

The model tracks how much and when solute segregates, and how it impacts the motion of grain boundaries.

"Which is a first step toward understanding how the properties of the material are modified by these solutes at the grain boundaries," he says.

The paper focuses on steel, an alloy of iron and carbon. However, Upmanyu notes the model applies broadly—not just to metals but also to ceramics like metal oxides.

"We feel it's general enough because it's based on fluctuations of interfaces and grain boundaries. All these interfaces fluctuate at finite temperature," he says. "There is always segregation of solutes. It's universal."

To reflect this broader scope, the researchers use the term "interface" rather than "grain boundary" to include non-crystalline materials.

The model realistically simulates how solutes interact with both defects and each other.

"If I take a snapshot of what we actually have simulated and use it as an input to actually extract the alloy properties, it's identical to what you see in an experiment," Upmanyu says.

The model works with two or more base materials and can be extended to predict thermal, electrical and magnetic properties of resulting alloys.

Another advantage: it delivers accurate predictions using very short simulation times.

"We're looking at a computational investigation of this fluctuation over nanoseconds," Upmanyu says. "You're taking a very brief snapshot of how this thing fluctuates, and coming up with the modified behavior based on that."

Phys Org, 7 may 2025

https://phys.org

Common Plastic Chemical Linked to Heart Disease Deaths

2025-04-29

Daily exposure to certain chemicals used to make plastic household items could be linked to the more than 356,000 global deaths from heart disease that occurred in 2018 alone, a new analysis of population surveys shows.

Although the chemicals, called phthalates, are in widespread use globally, the Middle East, South Asia, East Asia and the Pacific bore a much larger share of the death toll than others – about three-fourths of the total.

For decades, experts have connected health problems to exposure to certain phthalates found in cosmetics, detergents, solvents, plastic pipes, bug repellants and other products. These chemicals break down into microscopic particles and are ingested and studies have linked such exposure to an increased risk of conditions ranging from obesity and diabetes to fertility issues and cancer.

Led by researchers at NYU Langone Health, the current study focused on a kind of phthalate called di-2-ethylhexyl phthalate (DEHP), which is used to make food containers, medical equipment, and other plastic items softer and more flexible. Exposure has been shown in other studies to prompt an overactive immune response (inflammation) in the heart's arteries, which over time is associated with increased risk of heart attack or stroke. In their new analysis, the authors estimated that DEHP exposure contributed to 356,238 deaths, or more than 13 percent of all global mortality from heart disease in 2018 among men and women ages 55 through 64.

"By highlighting the connection between phthalates and a leading cause of death across the world, our findings add to the vast body of evidence that these chemicals present a tremendous danger to human health," said study lead author Sara Hyman, BS, an associate research scientist at NYU Grossman School of Medicine.

In a past study from 2021, the research team tied phthalates to more than 50,000 premature deaths each year, mostly from heart disease, among older Americans. Their latest investigation is believed to be the first global estimate to date of cardiovascular mortality—or indeed any health outcome—resulting from exposure to the chemicals, said Hyman, who is also a graduate student at NYU School of Global Public Health.

A report on the findings was published online April 29 in the journal Lancet eBioMedicine.

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

For the research, the team used health and environmental data from dozens of population surveys to estimate DEHP exposure across 200 countries and territories. The information included urine samples containing chemical breakdown products left by the plastic additive. Mortality data was obtained from the Institute for Health Metrics and Evaluation, a research group in the United States that collects medical information worldwide to identify trends in public health.

Among the key findings, the study showed that losses in the combined region of East Asia and the Middle East and the combined region of East Asia and the Pacific accounted, respectively, for about 42 percent and 32 percent of the mortality from heart disease linked to DEHP. Specifically, India had the highest death count, at 103,587 deaths, followed by China and Indonesia. The larger heart death risks in these populations held true even after the researchers adjusted their statistical analysis to take into account population size within the studied age group.

A possible explanation, the authors say, is that these countries face higher rates of exposure to the chemicals, possibly because they are undergoing a boom in plastic production but with fewer manufacturing restrictions than other regions.

"There is a clear disparity in which parts of the world bear the brunt of heightened heart risks from phthalates," said study senior author Leonardo Trasande, MD, MPP. "Our results underscore the urgent need for global regulations to reduce exposure to these toxins, especially in areas most affected by rapid industrialization and plastic consumption," added Dr. Trasande, the Jim G. Hendrick, MD, Professor of Pediatrics at NYU Grossman School of Medicine.

Dr. Trasande, who is also a professor in the Department of Population Health, cautions that the analysis was not designed to establish that DEHP directly or alone caused heart disease and that higher death risks did not take into account other types of phthalates. Nor did it include mortality among those in other age groups. As a result, the overall death toll from heart disease connected to these chemicals is likely much higher, he says.

Dr. Trasande says that the researchers next plan to track how reductions in phthalate exposure may, over time, affect global mortality rates, as well as to expand the study to other health concerns posed by the chemicals, such as preterm birth. Dr. Trasande also serves as director of NYU Grossman School of Medicine's Division of Environmental Pediatrics and the Center for the Investigation of Environmental Hazards.

Funding for the study was provided by National Institutes of Health grant P2CES033423. Further study funding was provided by Beyond Petrochemicals.

Dr. Trasande has received support for travel or meetings from the Endocrine Society, the World Health Organization, the United Nations Environment Programme, Japan's Environment and Health Ministries, and the American Academy of Pediatrics. He has also received royalties and licenses from Houghton Mifflin Harcourt, Audible, Paidós, and Kobunsha, and has served in leadership or fiduciary roles at Beautycounter, Ahimsa, Grassroots Environmental Education, and Footprint. None of these activities were related to the current study. The terms and conditions of all of these relationships are being managed by NYU Langone Health.

In addition to Hyman and Dr. Trasande, other NYU Langone researchers involved in the study are Jonathan Acevedo, MPH and Chiara Giannarelli, MD, PhD.

Technology Networks, 29 April 2025

https://technologynetworks.com

Single hair-like electrode outperforms traditional 21-lead EEG

2025-05-05

Researchers have developed a 3D-printable electrode that looks like a single strand of human hair and measures brain activity more reliably than the current method used to diagnose things like epilepsy and sleep disorders.

When you imagine someone having an electroencephalogram (EEG) to diagnose a condition such as epilepsy, for example, you probably picture them with a head covered in electrodes. That's because the standard EEG typically uses 21 of them, affixed to the scalp in strategic positions to capture activity from various brain regions.

However, a team of researchers from Pennsylvania State University (Penn State) has ushered in the future of EEG, developing a single electrode that looks just like a strand of hair and is more reliable than the standard, multi-electrode version.

"This electrode allows for more consistent and reliable monitoring of EEG signals and can be worn without being noticeable, which enhances both functionality and patient comfort," said Tao Zhou, a professor of

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

engineering science and mechanics at Penn State and the study's co-corresponding author.

Used to record the brain's electrical activity, an EEG is important for diagnosing and monitoring neurological conditions such as epilepsy, seizures, sleep disorders, and brain damage. The rigidity of the electrodes used in current EEGs means that even slight movement introduces noise and artifacts into the recording and limits the ability of patients to move freely. Commonly, "wet electrodes" are used, which require the application of conductive gel to maintain proper contact with the scalp. That approach is messy (think gel in the hair), and because the gel tends to dry out over time, it must be reapplied to maintain signal quality.

"This will change the impedance – or interface – between the electrodes and the scalp and it can affect the brain signal that's recorded," Zhou said. "We also don't always apply the electrodes in the exact same position either because we're human. But if you change the position, even a little bit, the brain signals you're monitoring can be different."

With these downsides in mind, Penn State researchers developed their gel-less "stick-and-play" device for EEG monitoring. It's designed to be worn continuously for long periods while not interfering with the wearer's usual activities or drawing attention to its presence. To that end, the electrode portion of the device is 3D-printed using a polymer hydrogel to be 300 µm wide. It looks like a single strand of hair. (By the way, it can be printed using different biocompatible dyes to ensure the device matches the hair color of the wearer.) The electrode is attached to the scalp using a 3D-printable bioadhesive that, on testing, was found to be almost double the strength of commercial EEG gel. It stayed on after showering and exercise-induced sweating, but did not cause damage to the skin when it was removed.

The researchers tested the device's long-term adhesion and electrical performance and compared it to the current, standard EEG using multiple electrodes. Even while human test subjects performed their regular activities, the electrode remained securely attached to the scalp for 24 hours. Impedance remained stable with no noticeable increase after 12 or 24 hours, meaning that the quality of the brain activity signal didn't change. The hairlike device maintained better skin contact than the regular gel-dependent approach and eliminated motion artifacts.

"You don't have to worry if the position of the electrode has changed or if the impedance has changed because the electrodes haven't moved," said Zhou.

Currently, the hairlike EEG device is wired, so patients must be connected to a machine while their brain activity is recorded. However, the researchers hope to develop a wireless version and foresee many applications for the device.

"This technology holds promise for use in consumer health and wellness products, enabling the development of advanced wearable devices that can monitor mental health, stress levels, and cognitive functions discreetly," they said. "It could also be integrated into brain-computer interface (BCI) systems, enhancing their usability and comfort, thereby expanding their application in fields such as assistive technology for individuals with disabilities, virtual reality (VR) experiences, and even enhancing human-computer interaction in everyday tasks."

The study was published in the journal NPJ – Biomedical Innovations.

New Atlas, 5 May 2025

https://newatlas.com

New roadmap advances catalytic solutions to destroy 'forever chemicals'

2025-05-07

A team of researchers from Rice University, Carnegie Mellon University and other leading global institutions has outlined a bold new roadmap for harnessing heterogeneous catalysis to destroy per- and polyfluoroalkyl substances (PFAS), the so-called "forever chemicals" that have contaminated water supplies worldwide.

In an article published in Nature Water, the international team of environmental engineers, chemists and catalysis experts assessed current catalytic technologies for PFAS destruction, proposed a suite of innovations to overcome existing limitations and emphasized the urgent need for holistic performance metrics that reflect true environmental and public health benefits.

"Catalysis offers a promising path to completely break down PFAS molecules, but current approaches are still far from optimal," said Michael Wong, co-author and chair of the Department of Chemical and Biomolecular Engineering at Rice. "We need smarter design, better process integration and a more nuanced way of comparing technologies that accounts for energy, cost and toxicity reduction."

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

PFAS are synthetic compounds used in products from firefighting foams to cookware and personal care products. Their carbon-fluorine bonds are among the strongest in chemistry, making them extremely persistent in the environment and difficult to degrade. Conventional water treatments such as reverse osmosis and activated carbon filters only separate PFAS from water, meaning toxic waste is left behind.

"Heterogeneous catalysis—the use of solid materials to speed up chemical reactions—has the potential to not only separate but actually mineralize PFAS into harmless by-products," said Gregory Lowry, corresponding author and a Hamerschlag University Professor of Civil and Environmental Engineering at Carnegie Mellon. "But these systems face multiple hurdles, including poor selectivity, incomplete defluorination and high energy demands."

One of the team's key recommendations is a pretreatment step to simplify the complex soup of PFAS often found in industrial waste or contaminated groundwater. Using known homogeneous chemical reactions, they postulate that these mixtures can be transformed into a smaller set of better-understood compounds, paving the way for more effective catalytic destruction.

"Thinking of complex PFAS treatment as a multistep process that will require many steps makes catalyst design much more tractable," said Sarah Glass, co-first author and graduate student in civil and environmental engineering at Rice. "Designing and using treatment techniques that are really efficient for a certain step of degradation can improve overall efficiency and accelerate the development of real-world catalytic solutions."

The researchers proposed a sequential "treatment train," where simplified PFAS mixtures are processed through tailored catalytic steps. First, the process removes specific chemical head groups from the PFAS molecules. Next, it shortens their long perfluorinated carbon chains, stripping away the fluorine atoms—the key to their persistence. Finally, the remaining fluorinated fragments are broken down into safe, naturally occurring substances like carbon dioxide, water and fluoride ions.

Each step uses a specialized catalyst tailored to the chemical structure at that stage. For example, titanium-based materials are used to speed up oxidation, while palladium helps swap out fluorine atoms for hydrogen in a process called reductive hydrodefluorination. This approach ensures that even complex PFAS mixtures can be effectively destroyed rather than just absorbed into a solid, requiring additional treatment.

"Think of it as a relay race," said Thomas Senftle, co-author and the William Marsh Rice Trustee Associate Professor in Chemical and Biomolecular Engineering at Rice. "Each catalyst hands off a partially degraded PFAS to the next until the molecule is completely broken down. Our goal is total defluorination."

The researchers stressed the importance of creating catalysts that can target and break down PFAS without being distracted by other substances commonly found in contaminated water. To do this, they are exploring catalyst surfaces that better attract PFAS and are using computer models and machine learning to predict reactions and optimize catalyst design.

"We're still learning which PFAS break down under which conditions," said Pedro Alvarez, co-author, the George R. Brown Professor of Civil and Environmental Engineering and director of the Rice Water Technologies Entrepreneurship and Research Institute. "Data-driven simulations can dramatically speed up the discovery process."

The team also introduced a new energy metric called electrical energy per order of defluorination (EEOD) to fairly compare how efficiently different catalytic systems break fluorine-carbon bonds. Unlike traditional removal metrics, EEOD focuses on true degradation, not just separation.

The paper concludes with a call for interdisciplinary collaboration and open data sharing to refine PFAS treatment strategies, with the need for scalable, cost-effective destruction methods greater than ever.

"PFAS are a generational challenge," Wong said. "We owe it to future generations to find smart, sustainable solutions, and catalysis can be one of them."

Phys Org, 7 May 2025

https://phys.org

Spongy new material pulls drinkable water from thin air in emergencies

2025-05-08

One of the biggest difficulties in helping people affected by natural disasters is transporting and providing them with essential resources like safe drinking water. Researchers at Australia's RMIT University and five Chinese institutes have devised a simple and clever contraption that could solve that, by pulling potable water out of thin air.

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

The team's invention uses a newly developed composite material based on porous, lightweight balsa wood shaped into small cubes; these are installed into a cup with a domed lid, a simple cooling mechanism, and an activation system powered by the Sun.

The spongy material, known as WLG-15, also contains lithium chloride to improve water absorption, and iron oxide nanoparticles that help the sponge's surface layer to absorb sunlight, and turn the absorbed water into vapor. The latter also helps the water release from the material.

The device itself is pretty simple: when the cup's lid is open to the air, the WLG-15 material absorbs moisture from the atmosphere. When the lid is closed under sunlight, water is released into the cup. The domed lid initiates solar evaporation and facilitates the collection of the released water; a cooling plate, a heat sink block, and a cooling fan powered by a solar panel enhances condensation within the system.

The researchers noted that under lab conditions, their device absorbed about 0.03 fl oz (2 ml) of water per gram of WLG-15 material at 90% relative humidity, and released nearly all the water within 10 hours under the Sun. That doesn't seem like much, but when you consider that the blocks are awfully small and lightweight, it could prove to be effective in a larger configuration, or in an array of collection devices.

For reference, a set of nine little sponge cubes shown below – each of which weigh less than a gram – can release 0.5 fl oz (15 ml) into the cup. The researchers published the results of their work in the Journal of Cleaner Production in March.

According to the team, this level of efficiency is higher than most other known methods like fog harvesting and radiative cooling, and cheaper thanks to the use of widely available and inexpensive balsa wood. In a bigger setup, it could potentially find use as a portable water harvesting system for emergency aid in disaster-stricken areas, with solar energy powering the cooling system.

Dr. Junfeng Hou from Zhejiang A&F University, who led the Chinese institutes' collaboration with RMIT, noted that WLG-15 also worked just fine after being stored at sub-zero temperatures for weeks, and could be reused multiple times without much of a decline in efficiency. As such, the material could even be "deployed in real-world applications such as water collection in remote or arid regions."

If you've been reading New Atlas for a bit, you've probably come across commercially available atmospheric water generators (AWG) – electronic appliances that promise to do the same thing, with far greater speed and volumes. Why not just deploy those to disaster-stricken locations and far-flung areas where water is hard to come by?

They seem like an ideal solution for water-scarce regions, but the main reason is AWGs use substantial amounts of electricity to condense water vapor from air. Many water-stressed regions have unreliable or no electrical grid access, so you'd likely have trouble powering these machines. Solar-powered options exist, but add significant cost and complexity to the equation.

Plus, AWGs work best in environments with above-60% humidity; that may not be the case in many of the locations you're thinking of. And finally, these systems can be expensive, both to purchase upfront and to maintain with specialized technical expertise and custom parts. So while they might indeed do what it says on the tin, AWGs aren't necessarily an easily applicable solution for water scarcity.

Back to WLG-15: the researchers used AI to predict the air-to-water device's performance under a range of environmental conditions. Similar tech could also help them uncover more combinations of materials for efficient water capturing composites. The team is currently exploring ways to pilot production of this material with industry partners and test it in the field.

Oh, and incidentally, RMIT University has come up with another sponge-inspired innovation recently: a super strong-material inspired by sea sponges that could find use in constructing more durable buildings.

Source: RMIT University

New Atlas, 8 May 2025

https://newatlas.com

Physicists snap the first images of 'free-range' atoms

2025-05-07

MIT physicists have captured the first images of individual atoms freely interacting in space. The pictures reveal correlations among the "free-range" particles that until now were predicted but never directly observed. Their findings, appearing in the journal Physical Review Letters, will help scientists visualize never-before-seen quantum phenomena in real space.

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

The images were taken using a technique developed by the team that first allows a cloud of atoms to move and interact freely. The researchers then turn on a lattice of light that briefly freezes the atoms in their tracks, and apply finely tuned lasers to quickly illuminate the suspended atoms, creating a picture of their positions before the atoms naturally dissipate.

The physicists applied the technique to visualize clouds of different types of atoms, and snapped a number of imaging firsts. The researchers directly observed atoms known as "bosons," which bunched up in a quantum phenomenon to form a wave. They also captured atoms known as "fermions" in the act of pairing up in free space -- a key mechanism that enables superconductivity.

"We are able to see single atoms in these interesting clouds of atoms and what they are doing in relation to each other, which is beautiful," says Martin Zwierlein, the Thomas A. Frank Professor of Physics at MIT.

In the same journal issue, two other groups report using similar imaging techniques, including a team led by Nobel laureate Wolfgang Ketterle, the John D. MacArthur Professor of Physics at MIT. Ketterle's group visualized enhanced pair correlations among bosons, while the other group, from École Normale Supérieure in Paris, led by Tarik Yefsah, a former postdoc in Zwierlein's lab, imaged a cloud of noninteracting fermions.

The study by Zwierlein and his colleagues is co-authored by MIT graduate students Ruixiao Yao, Sungjae Chi, and Mingxuan Wang, and MIT assistant professor of physics Richard Fletcher.

Inside the cloud

A single atom is about one-tenth of a nanometer in diameter, which is one-millionth of the thickness of a strand of human hair. Unlike hair, atoms behave and interact according to the rules of quantum mechanics; it is their quantum nature that makes atoms difficult to understand. For example, we cannot simultaneously know precisely where an atom is and how fast it is moving.

Scientists can apply various methods to image individual atoms, including absorption imaging, where laser light shines onto the atom cloud and casts its shadow onto a camera screen.

"These techniques allow you to see the overall shape and structure of a cloud of atoms, but not the individual atoms themselves," Zwierlein notes. "It's like seeing a cloud in the sky, but not the individual water molecules that make up the cloud."

He and his colleagues took a very different approach in order to directly image atoms interacting in free space. Their technique, called "atom-resolved microscopy," involves first corralling a cloud of atoms in a loose trap formed by a laser beam. This trap contains the atoms in one place where they can freely interact. The researchers then flash on a lattice of light, which freezes the atoms in their positions. Then, a second laser illuminates the suspended atoms, whose fluorescence reveals their individual positions.

"The hardest part was to gather the light from the atoms without boiling them out of the optical lattice," Zwierlein says. "You can imagine if you took a flamethrower to these atoms, they would not like that. So, we've learned some tricks through the years on how to do this. And it's the first time we do it in-situ, where we can suddenly freeze the motion of the atoms when they're strongly interacting, and see them, one after the other. That's what makes this technique more powerful than what was done before."

Bunches and pairs

The team applied the imaging technique to directly observe interactions among both bosons and fermions. Photons are an example of a boson, while electrons are a type of fermion. Atoms can be bosons or fermions, depending on their total spin, which is determined by whether the total number of their protons, neutrons, and electrons is even or odd. In general, bosons attract, whereas fermions repel.

Zwierlein and his colleagues first imaged a cloud of bosons made up of sodium atoms. At low temperatures, a cloud of bosons forms what's known as a Bose-Einstein condensate -- a state of matter where all bosons share one and the same quantum state. MIT's Ketterle was one of the first to produce a Bose-Einstein condensate, of sodium atoms, for which he shared the 2001 Nobel Prize in Physics.

Zwierlein's group now is able to image the individual sodium atoms within the cloud, to observe their quantum interactions. It has long been predicted that bosons should "bunch" together, having an increased probability to be near each other. This bunching is a direct consequence of their ability to share one and the same quantum mechanical wave. This wave-like character was first predicted by physicist Louis de Broglie. It is the "de Broglie wave" hypothesis that in part sparked the beginning of modern quantum mechanics.

"We understand so much more about the world from this wave-like nature," Zwierlein says. "But it's really tough to observe these quantum,

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

wave-like effects. However, in our new microscope, we can visualize this wave directly."

In their imaging experiments, the MIT team were able to see, for the first time in situ, bosons bunch together as they shared one quantum, correlated de Broglie wave. The team also imaged a cloud of two types of lithium atoms. Each type of atom is a fermion, that naturally repels its own kind, but that can strongly interact with other particular fermion types. As they imaged the cloud, the researchers observed that indeed, the opposite fermion types did interact, and formed fermion pairs -- a coupling that they could directly see for the first time.

"This kind of pairing is the basis of a mathematical construction people came up with to explain experiments. But when you see pictures like these, it's showing in a photograph, an object that was discovered in the mathematical world," says study co-author Richard Fletcher. "So it's a very nice reminder that physics is about physical things. It's real."

Going forward, the team will apply their imaging technique to visualize more exotic and less understood phenomena, such as "quantum Hall physics" -- situations when interacting electrons display novel correlated behaviors in the presence of a magnetic field.

"That's where theory gets really hairy -- where people start drawing pictures instead of being able to write down a full-fledged theory because they can't fully solve it," Zwierlein says. "Now we can verify whether these cartoons of quantum Hall states are actually real. Because they are pretty bizarre states."

This work was supported, in part, by National Science Foundation through the MIT-Harvard Center for Ultracold Atoms, as well as by the Air Force Office of Scientific Research, the Army Research Office, the Department of Energy, the Defense Advanced Projects Research Agency, a Vannevar Bush Faculty Fellowship, and the David and Lucile Packard Foundation.

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https://sciencedaily.com

Fluorescence color-change strategy enables rapid detection of tertiary amines and opioids

2025-05-08

Researchers from the University of Science and Technology of China (USTC), led by Professor Zhang Guoqing, have developed a rapid

fluorochromic sensing method for detecting tertiary amines and opioids. Their study is published in the Journal of the American Chemical Society.

Detecting organic amines is critical for pharmaceutical analysis, food safety, biomedical diagnostics, and clinical testing. Traditional luminescence-based amine detection mainly relies on fluorescence quenching, limiting sensitivity and selectivity.

In contrast, the research team introduced a fluorescence color-change strategy. Upon light exposure, tertiary amines form exciplexes with photoactivated naphthalimide molecules, which then rearrange into stable photoinduced charge-transfer complexes (PCTCs). This interaction enables the differentiation of structurally similar tertiary amines based on their substituents and molecular flexibility.

The researchers systematically studied three types of tertiary amines—methylated, flexible-chain, and rigid amines—by exposing them to light in the presence of naphthalimide molecules.

They found that the photoluminescence quantum yield and emission color were strongly influenced by the amine substituents and molecular flexibility. Under 365 nm UV light, methylated amines rapidly emitted green fluorescence, while flexible-chain amines first displayed yellow fluorescence before eventually shifting to green.

This behavior, consistently observed across 24 different amine samples, suggests that methyl groups reduce steric hindrance and promote charge transfer with naphthalimide molecules. The proposed mechanism was further supported by DFT calculations and time-resolved fluorescence measurements.

Building on this mechanism, the researchers developed a portable visual method for detecting natural and synthetic opioids, including heroin, fentanyl, methamphetamine, and metonitazene. Compared to traditional approaches like the Marquis reagent test, their method is faster, simpler, and more suitable for on-site and real-time monitoring.

This work follows the group's earlier discovery of photoinduced charge-transfer complexes, offering further evidence of this phenomenon. It opens new possibilities for trace amine detection and rapid drug screening.

Phys Org, 8 May 2025

https://phys.org

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

The Chemistry Trick Poised to Slash Steel's Carbon Footprint

2025-04-18

Chemists are pioneering a clean, electrochemical method to make iron, a key step in decarbonizing the steel industry.

Their process, which uses saltwater and iron oxide instead of carbon-heavy blast furnaces, has been optimized to work with naturally sourced materials. By identifying low-cost, porous iron oxides that dramatically boost efficiency, the team is laying the groundwork for large-scale, eco-friendly steel production. And with help from engineers and manufacturers, they're pushing this green tech closer to the real world.

A Greener Future for Steel Production

Chemists at the University of Oregon are moving closer to a cleaner way to produce iron for steelmaking, an industry that ranks among the largest sources of carbon emissions worldwide.

Last year, UO chemist Paul Kempler and his team introduced a method for making iron using electrochemistry. The process relies on a series of chemical reactions that convert saltwater and iron oxide into pure iron metal.

In their latest study, the researchers focused on improving the process by identifying which types of iron oxides make the reaction more cost-effective, an essential step toward scaling the method for industrial use.

"We actually have a chemical principle, a sort of guiding design rule, that will teach us how to identify low-cost iron oxides that we could use in these reactors," Kempler said.

The research was published on April 9 in ACS Energy Letters.

The Global Demand for Steel

Almost 2 billion metric tons of steel were produced worldwide in 2024, used in everything from buildings to cars to infrastructure. Currently, the most fossil fuel-intensive part of that process is turning iron ore — the oxidized form of iron that's found in nature — into pure iron metal.

Traditionally done in blast furnaces that send carbon dioxide into the atmosphere, Kempler's team is developing a different approach to iron production.

Iron Production With a Valuable Byproduct

Their process starts with saltwater and iron oxide, which are cheap and available, and transforms them into iron metal through a series of chemical reactions. Those reactions conveniently also produce chlorine, a commercially valuable byproduct.

When Kempler and his team began developing their process a few years ago, they started with small quantities of iron oxides from chemical supply companies.

Those materials worked well in lab tests. But they didn't reflect the kind of iron-rich materials found naturally, which have much more variation in composition and structure.

Working With Earth-Derived Materials

"So then a very natural next question was: What happens if you actually try to work with something which was dug out from the earth directly, without being extra purified, extra milled, and so on?" said Ana Konovalova, who co-led the project as a postdoctoral researcher in Kempler's lab.

As the team experimented with different kinds of iron oxides, it was clear that some worked much better than others. But the researchers weren't sure what was driving the difference in the amount of iron metal they could generate from different starting materials. Was it the size of the iron oxide particles? The composition of the material? The presence or absence of specific impurities?

Testing Particle Structure and Density

Konovalova and graduate student Andrew Goldman found creative ways to test certain variables while keeping others the same.

For example, they took iron oxide powder and made it into nanoparticles. They put some of the nanoparticles through a heat treatment that made them much denser and less porous.

"It solidifies into this same secondary nanoparticle shape, but there are no more primary particles observed inside. It's essentially the same material, just in different stages," Konovalova said.

Faster Reactions, Lower Costs

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

In lab tests, the difference was striking: "With the really porous particles, we can make iron really quickly on a small area," Goldman said. "The dense particles just can't achieve the same rate, so we're limited in how much iron we can make per square meter of electrodes."

That's a key insight for making the process work at an industrial scale, where success often comes down to economics.

Large-scale electrochemical plants are expensive to build, and that cost scales with electrode area. To make it economically viable, the electrodes need to be able to generate enough product quickly enough to pay off the initial investment. The faster rate of reaction of the porous particles means the initial capital cost can be recouped faster, translating into a lower final cost for the iron product, ideally low enough to be competitive with conventional methods.

Surface Area Is the Secret Ingredient

The takeaway isn't that these specific nanoparticles are needed to make the electrochemical process work well, Kempler said. Rather, the study suggests that the surface area of the starting materials really matters. The porous nanoparticles had much more surface area for the reaction to take place, making the reaction run faster. Other iron oxides with a porous structure could also be cost-effective.

"The goal is to find something that's abundant, cheap and that's going to have a smaller environmental impact than the alternative," Kempler said. "We won't be satisfied if we invent something that's more damaging than the main way that we make iron today."

Collaborating to Bring Innovation to Market

To take their process beyond the lab, Kempler's lab is working with researchers in other fields. A collaboration with civil engineers at Oregon State University is helping them better understand what's needed for the product to work in real-world applications. And collaboration with an electrode manufacturing company is helping them address the logistical and scientific challenges of scaling up an electrochemical process.

Rethinking Industry With Sustainability in Mind

"I think what this work shows is that technology can meet the needs of an industrial society without being environmentally devastating," Goldman said. "We haven't solved all the problems yet, of course, but I think it's an example that serves as a nucleation point for a different way of thinking

about what solutions look like. We can continue to have industry and technology and medicine, and we can do it in a way that's clean — and that's awesome!"

Sci Tech Daily, 18 April 2025

https://scitechdaily.com

Self-Healing Polymer Changes from Solid to Liquid To Repair Damage

2025-05-02

What if there were a fabric that, like Superman, could take a bullet and self-heal? Such a super-dynamic, action-powered polymer might actually help protect real-life flyers in space.

Material scientists at Texas A&M University have developed just such a polymer with a unique self-healing property never before seen at any scale. When struck by a projectile, this material stretches so much that when the projectile manages to pass through, it takes only a small amount of the polymer with it. As a result, the hole left behind is much smaller than the projectile itself.

However, for now, this effect has only been observed under extreme temperatures and at the nanoscale.

"This is the first time a material at any scale has displayed this behavior," said Dr. Svetlana Sukhishvili, a professor in the Department of Materials Science and Engineering, who has been working on development of this polymer film with materials science and engineering professor Dr. Edwin (Ned) Thomas, and then-graduate student Dr. Zhen Sang. Their findings were published in the March/April issue of Materials Today.

"Besides being very cool, the new polymer will likely have many applications, including making the windows of space vehicles more resilient to the onslaught of micrometeoroids," Thomas said.

Space vehicles are frequently bombarded with micrometeoroids traveling at speeds of 10 kilometers per second. A micrometeoroid can create a hole in the window that, while small, is visible to the human eye. However, a window manufactured with a layer of this polymer could potentially sustain damage tinier than the meteoroid itself.

Thomas, who first suggested subjecting the polymer to ballistic testing, said a key goal of the research is to design a material that will

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

protect structures such as orbiting satellites and vehicles in space, with applications for military equipment and body armor on Earth.

The phenomenal behavior occurs in the new solid polymer film as it melts when impacted by a laser-launched high-speed projectile, and snaps back to its original shape when cooled. The polymer does this by absorbing much of the kinetic energy generated by the projectile, causing the film to stretch and liquify as the projectile continues its journey, finally piercing the film. Once pierced, the polymer quickly cools, its covalent bonds reform, and it returns to its original solid state, leaving a tiny hole.

"A major goal of our work was to see if we could simultaneously provide a material that would absorb a lot of kinetic energy per unit target mass from the high-speed projectile and be capable of very rapid healing of the punctured region," Thomas said. "We wanted the post-impact material to still be capable of performing its intended function, such as carrying air or liquids and remaining sealed against the loss of such fluids across the material membrane."

The material is a Diels-Adler Polymer or DAP, so-named by the researchers for its dynamic covalent bond networks that can be broken and reformed. It belongs to a class of materials called Covalent Adaptative Networks or CANs. While other Diels-Adler networks have been reported in the scientific literature, DAP's specific chemistry, topology and self-healing quality are novel. The DAP acronym could also refer to their polymer as a Dynamic Action-Powered material for its ability to self-heal.

"When we were synthesizing DAPs, we aimed to do it in such a way that the polymers would turn to liquids upon temperature increase," Sukhishvili said. "Although this feature was introduced to facilitate 3D printing, we thought that due to its ability to liquify upon heating, our polymers could show improved ballistic healing characteristics."

"Polymers are amazing materials, especially DAP materials," Thomas explained. "Because at low temperatures, they are stiff and strong; then at higher temperatures, they become elastic; and at still higher temperatures, they become an easily flowing liquid. That's a huge range of property behavior."

What's more, he said, the process reverses itself. "Nothing else on the planet can do that!"

The DAP structure is of long polymer chains containing double carbon bonds that break when severe strain and heat are applied, but quickly reform when cooled, albeit not necessarily in the same configuration.

"Think of the long polymer chains in the fabric as being like a bowl of Ramen noodle soup," said Sang, who worked on this project for his doctoral research and is first author on the paper. "You can stir it with chopsticks, then freeze it. When you unfreeze it, you can stir it, then refreeze. It will have the same ingredients as before, just in a slightly different appearance."

Sang, who is now an engineer at Apple, Inc., said it wasn't easy to do ballistic testing at such a small scale until he came across a new research methodology called LIPIT (laser-induced projectile impact testing), recently developed by Thomas and colleagues at MIT. Sang used LIPIT to laser-launch a tiny silica projectile 3.7 micrometers in diameter from a glass slide covered with a thin gold film resting on a one-square inch platform. His target consisted of a thin layer (75 to 435 nanometers) of the super DAP.

An ultrahigh-speed camera with a 3-nanosecond exposure time at 50 nanosecond intervals recorded the action. The research team then used scanning electron microscopy, laser scanning confocal microscopy and an infrared nano spectrometer to view the holes and assess the covalent bonding in the super polymer.

The results were puzzling at first, Sang said, because he could find no holes in the targeted polymer.

"Was I not aiming correctly? Were there no projectiles? What's wrong with my experiment, I asked myself," he said. However, when he placed the DAP sample under the infrared nano spectrometer, which combines chemical analysis with high-scale resolution, he was able to see the tiny perforations. "This was actually a surprising, surprising finding," Sang said. "A very exciting finding!"

He explained this behavior can't yet be recreated at the macro level because the strain rate during perforation of a very thin target material under impact is so much larger than at the nanoscale. "If this strain rate is really high, materials often have unexpected behavior that people don't usually see under normal circumstances," Sang said. "With the LIPIT apparatus that we're using, we're talking about a strain rate many orders of magnitude higher than for conventional scale bullets and targets. At that perspective, materials behave very differently."

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

Other coauthors on the paper are materials science doctoral student Hongkyu Eoh; former postdoctoral researchers Drs. Kailu Xiao, Wenpeng Shan and Jinho Hyon; and Dr. Dmitry Kurouski, associate professor in the department of biochemistry and biophysics at Texas A&M.

Sukhishvili and Thomas plan to continue researching the super DAP using different polymer compositions, temperature- and stress-responses.

"One could even imagine designing DAPs with characteristics such that it would be possible to absorb kinetic energy by breaking DAP bonds, then some of these broken bonds could very rapidly reform – by perhaps having just the right 'bond reform catalyst' present in the material – whereby the projectile would have to break these bonds a second (or even multiple times) before the material ultimately heals itself, and is ready for the next ballistic event.

"To date, no material has the requisite time response to deform, break, reform; and then deform, break and reform again during the sub-microsecond interval of a ballistic event," Thomas said.

Technology Networks, 5 May 2025

https://technologynetworks.com

Ultrasound unlocks a safer, greener way to make hydrogels

2025-05-08

Researchers at McGill University, in collaboration with Polytechnique Montréal, pioneered a new way to create hydrogels using ultrasound, eliminating the need for toxic chemical initiators. This breakthrough offers a faster, cleaner and more sustainable approach to hydrogel fabrication, and produces hydrogels that are stronger, more flexible and highly resistant to freezing and dehydration.

Hydrogels are gels composed of polymers that can absorb and retain large amounts of water. They are widely used in wound dressings, drug delivery, tissue engineering, soft robotics, soft contact lenses and more.

The new method, now published in Advanced Science, also promises to facilitate advances in tissue engineering, bioadhesives and 3D bioprinting.

Gel formation within minutes

Traditional hydrogel manufacturing relies on chemical initiators, some of which can be harmful, particularly in medical applications. Initiators are the chemicals used to trigger chemical chain reactions.

The McGill research team, led by Mechanical Engineering Professor Jianyu Li, has developed an alternative method using ultrasound. When applied to a liquid precursor, sound waves create microscopic bubbles that collapse with immense energy, triggering gel formation within minutes.

"The problem we aimed to solve was the reliance on toxic chemical initiators," said Li. "Our method eliminates these substances, making the process safer for the body and better for the environment."

This ultrasound-driven technique is dubbed "sonogel."

"Typical hydrogel synthesis can take hours or even overnight under UV light," said Li. "With ultrasound, it happens in just five minutes."

Revolutionizing biomedical applications

One of the most exciting possibilities for this technology is in noninvasive medical treatments. Because ultrasound waves can penetrate deep into tissues, this method could enable in-body hydrogel formation without surgery.

"Imagine injecting a liquid precursor and using ultrasound to solidify it precisely where needed," said Li. "This could be a game-changer for treating tissue damage and regenerative medicine. With further refinement, we can unlock new possibilities for safer, greener material production."

The technique also opens the door to ultrasound-based 3D bioprinting. Instead of relying on light or heat, researchers could use sound waves to precisely "print" hydrogel structures.

"By leveraging high-intensity focused ultrasound, we can shape and build hydrogels with remarkable precision," said Jean Provost, one of the co-authors of the study and assistant professor of engineering physics at Polytechnique Montréal.

Phys Org, 8 May 2025

https://phys.org

CHEMWATCH
Bulletin Board
Curiosities
MAY. 09, 2025

Food chemist takes top prize of annual Dance your PhD contest

2025-05-08

A food chemist from the University of Helsinki has won the 17th Dance your PhD contest with choreography that explores the unique sensations experienced when eating certain foods, such as fiery capsaicin found in chillis and the tingly cool of menthol in mint.

During the prize-worthy dance, Sulo Roukka, who was awarded a total of $2750 (£2070) for winning both the overall and chemistry category, transforms from a lab coat-clad scientist writing on a whiteboard to a red coat-tailed performer twirling and prancing among sequinned backing dancers and flashing lights. The music video also features a cameo by his PhD supervisor, food chemist Mari Sandell.

'I got to experience a Kylie Minogue fantasy,' Roukka, who studies how chemesthesis – sensations caused by the activation of receptors by chemicals – influences the human experience while eating particular foods, told Science.

As well as calling on friends to help with the music video, he enlisted dancers from one of the university's musical theatre groups but said his cousin's six-year-old daughter was upset to not have been included. 'If I ever do another PhD, I will make sure she's the first one to join for the next Dance Your PhD music video,' he added.

The Dance Your PhD competition is run by Science and the American Association for the Advancement of Science, and asks postgraduate students to explain their thesis through interpretive dance. The competition awards the best entries in biology, chemistry, physics and social sciences.

This year, there was also a special AI/quantum prize, for which the dance did not need to be based on a PhD thesis. The winner of this was Arfor Houwman at the University of Innsbruck, for his 1980s dance music-inspired video on laser cooling of ultracold atoms. Each category winner received $750 with Roukka receiving an extra $2000 as the overall winner.

Chemistry World, 8 May 2025

https://chemistryworld.com

CHEMWATCH

Bulletin Board

Technical Notes

MAY. 09, 2025

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

CHEMICAL EFFECTS

Profiling aerosol Polycyclic Aromatic Compounds (PACs) in a severely polluted European city: A comprehensive assessment of the residential biomass burning impact on atmospheric toxicity

Imbalance of phosphoric acid homeostasis in alveolar macrophages mediates lung toxicity of rare earth oxide nanoparticles

Human sperm as an in vitro toxicity model: a versatile tool for assessing the risk of environmental contaminants

ENVIRONMENTAL RESEARCH

Personal exposures to air pollutants and respiratory health among brick kiln workers and household members

Association of ambient air pollution with hospital admissions for major osteoarthritis diseases: A national case-crossover study in China

PHARMACEUTICAL/TOXICOLOGY

Power Outages and Carbon Monoxide Poisoning in Children

Incidence of respiratory diseases associated with per- and polyfluoroalkyl substances (PFAS) in PM2.5: New evidence from a population-based survey of Pearl River Delta (PRD), China

OCCUPATIONAL

Associations between long-term exposure to particulate matter and mortality from multiple causes among the oldest-old people

Agricultural Supervisors' Perspectives on Occupational Wildfire Smoke Rules

Long-term exposure to smoke PM2.5 and COPD caused mortality for elderly people in the contiguous United States