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

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ASIA PACIFIC

Agricultural chemical products and approved labels

2024-10-29

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.	141601
Product name	Seajet 032 Professional
Active constituent	457 g/L cuprous oxide
Applicant name	Chugoku Paints B.V.
Applicant ACN	N/A
Date of registration	21 August 2024
Product registration no.	94126
Label approval no.	94126/141601
Description of the application and its purpose, including the intended use of the chemical product	Registration of a 457 g/L cuprous oxide ready-to-use liquid marine antifouling paint product for moderate fouling areas

Application no.	144639
Product name	AC Antler Herbicide
Active constituents	90 g/L mefenpyrdiethyl, 30 g/L mesosulfuron-methyl
Applicant name	Axichem Pty Ltd
Applicant ACN	131 628 594
Date of registration	9 October 2024
Product registration no.	95090
Label approval no.	95090/144639

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Application no.	144639
Description of the application and its purpose, including the intended use of the chemical product	Registration of a 30 g/L mesosulfuron- methyl, 90 g/L mefenpyrdiethyl, 200 g/L aromatic hydrocarbon, oil-based suspension concentrate product for the post-emergent control of wild oats and annual Phalaris, and suppression of brome grass, barley grass and annual ryegrass in wheat

Read More

APVMA Gazette. 29-10-24

https://www.apvma.gov.au/news-and-publications/publications/gazette/ gazette-22-29-october-24

Veterinary chemical products and approved labels

2024-10-29

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 4: Veterinary products based on existing active constituents

Application no.	142762
Product name	Beast Pour-on for Horses
Active constituent	87 g/L permethrin (25:75 cis:trans)
Applicant name	Abbey Laboratories Pty Ltd
Applicant ACN	156 000 430
Date of registration	10 October 2024
Product registration no.	94555
Label approval no.	94555/142762



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Application no.	142762
purpose, including the intended use of	Registration of a 87 g/L permethrin (25:75 cis:trans) topical solution pouron product for the control of biting and nuisance flies on horses

Application no.	144301
Product name	Blue Wheelers and Dash Dogwash Hydrokill Flea and Tick Rinse concentrate for Dogs, cats, puppies, kittens and caged birds
Active constituents	10 g/L Pyrethrins, 30 g/L N-Octyl Bicycloheptene Dicarboximide, 18 g/L Piperonyl Butoxide
Applicant name	The Franchise Group Pty Ltd
Applicant ACN	007 449 587
Date of registration	15 October 2024
Product registration no.	94956
Label approval no.	94956/144301
Description of the application and its purpose, including the intended use of the chemical product	Registration of a 30 g/L N-Octyl Bicycloheptene Dicarboximide, 18 g/L Piperonyl Butoxide, 10 g/L Pyrethrin and 2 g/L Citronella Oil flea and tick rinse concentrate for aid in the control of Fleas (Ctenocephalides spp.), Adult brown dog tick (Rhipicephalus spp.), Paralysis tick (Ixodes holocyclus) and controls Lice (Trichodectes canis, Heterodoxus spp. and Felicola subrostraturm) on dogs and cats and caged birds

Read More

APVMA Gazette. 29-10-24

https://www.apvma.gov.au/news-and-publications/publications/gazette/gazette-22-29-october-24

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Approved active constituents

2024-10-29

NOV. 08, 2024

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 6: Approved active constituent

Application no.	142754
Active constituent	Pyroxasulfone
Applicant name	Zhejiang Zhongshan Chemical Industry Group Co Ltd
Applicant ACN	N/A
Date of approval	11 October 2024
Approval no.	94554
Description of the application and its purpose, including the intended use of the active constituent	Approval of the active constituent pyroxasulfone for use in agricultural chemical products

Application no.	141949
Active constituent	Flazasulfuron
Applicant name	Ishihara Sangyo Kaisha Ltd
Applicant ACN	N/A
Date of approval	14 October 2024
Approval no.	94265
Description of the application and its purpose, including the intended use of the active constituent	Approval of the active constituent flazasulfuron for use in agricultural chemical products

Application no.	143098
Active constituent	Triclabendazole
Applicant name	Vetsense Pty Ltd
Applicant ACN	150 968 871

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Application no.	143098
Date of approval	14 October 2024
Approval no.	94654
Description of the application and its purpose, including the intended use of the active constituent	Approval of the active constituent triclabendazole for use in veterinary chemical products

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APVMA Gazette. 29-10-24

https://www.apvma.gov.au/news-and-publications/publications/gazette/gazette-22-29-october-24

Variations to Schedule 20 of the Australian New Zealand Food Standards Code

2024-10-29

The APVMA has previously gazetted particular amendments which it had made to the APVMA MRL Standardand which have been proposed as variations to maximum residue limits (MRLs) for substances contained in agricultural and veterinary chemical products as set out as in Schedule 20 – Maximum residue limits of the Australia New Zealand Food Standards Code. This notice pertains to proposals (No. 2) gazetted on 9 July 2024 (No. APVMA 14).

Submissions have been sought on these proposals and the APVMA has written separately to each person or organisation that made a submission. All matters raised in the submissions have been resolved.

Under subsection 82(1) of the Food Standards Australia New Zealand Act 1991, the APVMA has, by legislative instrument, incorporated these variations to MRLs into Schedule 20. A copy of the Amendment Instrument (No. APVMA 2, 2024) accompanies this notice. For a complete and upto-date version of Schedule 20, including these amendments together with their Explanatory Statement, please refer to the Federal Register of Legislation.

Based on dietary exposure assessments and current health standards, the APVMA and Food Standards Australia New Zealand (FSANZ) are satisfied that these MRLs are not harmful to public health. MRLs contained in Schedule 20 provide the limits for residues of agricultural and veterinary chemicals that may legitimately occur in foods. By this means, Schedule 20

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permits the sale of treated foods and protects public health by minimising residues in foods consistent with the effective control of pests and diseases.

The agreement between the Australian Government and the New Zealand Government concerning a Joint Food Standards System, excludes MRLs for agricultural and veterinary chemicals in food from the system setting joint food standards. Australia and New Zealand independently and separately develop MRLs for agricultural and veterinary chemicals in food.

A Sanitary and Phytosanitary notification to the World Trade Organization (WTO) was also made in relation to the variations to MRLs in Schedule 20 and no comment was received in response to that notice OR comment was received in response to that notice which has been addressed.

A copy of these variations have been given to FSANZ.

The variations take effect as from the date of this notice.

This notice is published in accordance with subsection 82(7) of the Food Standards Australia New Zealand Act 1991.

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VOV. 08, 2024

APVMA Gazette. 29-10-24

https://www.apvma.gov.au/news-and-publications/publications/gazette/gazette-22-29-october-24

AMERICA

Environmental Defense Fund Applauds Governor Shapiro's Progress towards Implementing Methane Regulations

2024-10-16

Today at the Air Quality Technical Advisory Committe, the Pennsylvania Department of Environmental Protection presented Governor Shapiro's proposal on how to move a state plan forward to reduce methane emissions from existing oil and gas operations. The proposal is a significant step forward and demonstrates a proactive approach to reducing emissions from the second largest producer of natural gas in the country.

"Governor Shapiro is making meaningful progress towards quickly adopting new methane standards for existing oil and gas sources," said



John Rutecki, Regulatory and Legislative Affairs Manager, Appalachia at Environmental Defense Fund. "These efforts will improve air quality and help safeguard the climate while also growing local jobs and creating a framework that encourages industry innovation. This will meet Governor Shapiro's criteria of protecting jobs and our environment."

To ensure a balanced, transparent process, the next steps will include meaningful engagement sessions with stakeholders and review by the Citizens Advisory Council and Oil and Gas Technical Advisory Board. Environmental Defense Fund will remain engaged throughout this collaborative process.

"We encourage Governor Shapiro and PADEP to swiftly implement these protections. We also encourage an ambitious approach to further reduce methane emissions, beyond the federal rule, to fully realize the economic and climate benefits for Pennsylvania's future generations," said Rutecki.

Read More

Environmental Defense Fund, 16-10-24

https://www.edf.org/media/environmental-defense-fund-applauds-governor-shapiros-progress-towards-implementing-methane

Summary of public comments received on the risk management approach for certain triarylmethanes group

2024-10-11

Comments on the Risk Management Approach for Certain Triarylmethanes, assessed under the Chemicals Management Plan (CMP), were submitted jointly by the Forest Products Association of Canada (FPAC) and National Council for Air and Stream Improvement, Inc (NCASI).

Summarized public comments and responses are provided below, organized by topic.

Information on uses

Comment summary 1: 3 pulp and paper mills may be using triarylmethane dyes but given that suppliers do not always share information with end-users, it is unknown if other pulp and paper mills are using or could begin using triarylmethanes unknowingly.

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Response 1: It is recognized that supply chain transparency can pose a challenge in many sectors, including the pulp and paper sector.

Bill S-5: Strengthening Environmental Protection for a Healthier Canada Act received Royal Assent on June 13, 2023 to modernize the Canadian Environmental Protection Act, 1999 (CEPA). The modernized Act recognizes the importance of Canadians having information regarding the risks of toxic substances to the environment or to human health. Furthermore, the Government of Canada will release a strategy for enhancing the availability of information on chemicals of concern in products. The Strategy would promote the use of safer chemicals and sustainable business and consumer decision-making, support Canada's chemicals regulatory framework, and contribute to Canada's efforts to prevent the impact of pollution on the environment and human health.

When appropriate, the Government of Canada intends to apply the steps outlined in the Approach to disclose confidential information and promote transparency in chemicals management to release certain information publicly, taking into account the requirements of CEPA. This could occur in situations where it is in the interest of public health, public safety or the protection of the environment.

We also encourage users of products and chemicals to pursue disclosure requirements through their procurement processes with their suppliers.

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NOV. 08, 2024

Government of Canada, 11-10-24

https://www.canada.ca/en/environment-climate-change/services/evaluating-existing-substances/summary-public-comments-risk-management-approach-certain-triarylmethanes-group.html

Water quality advocates ask Virginia for more aggressive PFAS policies

2024-10-28

The federal government has now defined how much is too much when it comes to PFAS, or "forever chemicals," in drinking water. But that still leaves a lot of leeway as to how states will monitor or regulate PFAS found in rivers and streams.

In Virginia, laws passed so far require agencies to find and address specific sources of PFAS pollution when they have contaminated a public drinking water system. But clean water advocates want the state to require more



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monitoring now at facilities known to be possible sources of PFAS so that action can be taken more quickly when additional federal limits are finalized.

PFAS, or per– and polyfluoroalkyl substances, include thousands of synthetic chemicals that have been widely used since the 1940s in a variety of industrial and consumer products. That includes firefighting foam, nonstick cookware, water– and stain-repellent fabrics and some food packaging.

PFAS have been found in the drinking water or groundwater of nearly 2,800 communities nationwide, including dozens in the six-state Chesapeake Bay watershed. Much of the contamination has been found near military facilities or airports where firefighting foam laden with PFAS was deployed or stored.

Studies have linked long-term exposure to even low levels of some of the chemicals with serious health problems, including cancer and damage to reproductive and immune systems. But setting standards that define how much PFAS is too much has been a long process.

The U.S. Environmental Protection Agency in April set its first legally enforceable drinking water standards for six types of PFAS, which will go into full effect in the coming years.

Read More

Bay Journal, 28-10-24

https://www.bayjournal.com/news/pollution/water-quality-advocates-ask-virginia-for-more-aggressive-pfas-policies/article_6efca2ce-908d-11ef-b16b-7712e7a9df07.html

USEPA Issues Recommended Water Quality Criteria and Benchmarks for Certain PFAS in Surface Water

2024-10-28

On October 7, 2024, the United States Environmental Protection Agency ("EPA") issued recommended ambient surface water quality criteria and acute saltwater aquatic life benchmarks for PFOA and PFOS, as well as acute freshwater aquatic life benchmarks for eight PFAS. These are not regulatory standards, nor do they automatically become part of a State's water quality standards. According to EPA they "provide information that States and Tribes may consider when adopting water quality standards."

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As explained by EPA:

OV. 08, 2024

States must adopt into their standards water quality criteria that protect the designated uses of their water bodies. States can establish water quality criteria based on the EPA's recommended criteria, modify recommended criteria to reflect site-specific conditions, or develop proposed standards using on other scientifically defensible methods. A State's or Tribe's water quality criteria are not legally effective under the Clean Water Act until they have been adopted into a State's or Tribe's water quality standards and are approved by the EPA.

Read More

JDSupra, 28-10-24

https://www.jdsupra.com/legalnews/usepa-issues-recommended-water-quality-1372897

EPA Proposes Adding PFAS to TRI and Extends TSCA Reporting Deadline

2024-10-28

The EPA recently published a proposed rule to add 16 per- and polyfluoroalkyl substances (PFAS) and 15 PFAS categories to the Toxics Release Inventory (TRI), which is a list of toxic chemicals subject to reporting under the Emergency Planning and Community Right-to-Know Act (EPCRA) and the Pollution Prevention Act (PPA) to comply with the National Defense Authorization Act (NDAA) for fiscal year (FY) 2020. The proposed rule also addresses how PFAS categories should be treated.

The EPA also outlines what events may trigger the automatic addition of PFAS to TRI under the NDAA.

"This discussion does not propose to list chemicals to TRI pursuant to the NDAA, but rather describes what EPA documents and activities involving PFAS would trigger an automatic addition under the NDAA," according to the proposed rule.

Comments will be accepted on the proposed regulation until December 9, 2024.

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EHS Daily Advisor, 28-10-24

https://ehsdailyadvisor.blr.com/2024/10/epa-proposes-adding-pfas-to-tri-and-extends-tsca-reporting-deadline/

EUROPE

Pollution, over-use and climate change threaten water resilience in Europe

2024-10-21

Agriculture is the most significant pressure impacting both surface and groundwaters, according to the EEA report 'Europe's state of water 2024: the need for improved water resilience'. This results from water use and pollution from the intensive use of nutrients and pesticides, according to Member States' own monitoring. Agriculture is by far the highest net water consumer in Europe and, without changes in practices, demand from irrigated agriculture is likely to increase with climate change.

The EEA's report shows that, despite some progress, Europe's waters and aquatic ecosystems are still severely impacted by chemicals, predominantly by air pollution from coal-powered energy generation and diffuse pollution by nutrients and pesticides from agriculture. Habitat degradation is also widespread. Adding to the challenge to protect aquatic ecosystems is climate change, which is disrupting weather patterns and further increasing pressures on water resources and management.

Europe's state of water 2024: the need for improved water resilience

Only 37% of Europe's surface water bodies achieved 'good' or 'high' ecological status, a measure of aquatic ecosystem health, under EU's Water Framework Directive and only 29% achieved 'good' chemical status over the 2015-2021 period, according to data reported by EU Member States.

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European Environment Agency, 21-10-24

https://www.eea.europa.eu/en/newsroom/news/state-of-water

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Council urges Commission to take effective measures for Chemicals Strategy implementation

2024-10-14

Environment ministers today expressed their support for the CSS as a key part of the EU Green Deal. Large delegations asked the European Commission to accelerate its efforts to fulfil existing commitments and implement necessary measures. They highlighted the revision of the Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH) as a top priority and an essential step toward achieving the CSS objectives as well as the restriction of PFAS—forever chemicals. The delegations also stressed the need for an export ban of highly hazardous chemicals that are already banned in Europe and highlighted the need to strengthen the European Chemicals Agency (ECHA).

In October 2020, the European Commission adopted the EU Chemicals Strategy for Sustainability (CSS) as a key step towards achieving a zero-pollution, toxic-free environment. The strategy promised stricter regulations on harmful chemicals and limiting the use of forever chemicals, PFAS, to essential uses. It also aimed to stop the export of EU banned chemicals to less developed countries and overhaul the EU's REACH regulation to control entire chemical families instead of tackling substances one by one. However, four years later, despite strong support from both Parliament and the Council for the Chemicals Strategy, the Commission has dragged its feet, with little progress on key measures.

Read More

European Environment Bureau, 14-10-24

https://eeb.org/council-urges-commission-to-take-effective-measures-for-chemicals-strategy-implementation/

European Environment Agency | Understanding the data — what drives our material footprint?

2024-10-09

Housing and food are particular hotspots for resource consumption, accounting for 72% of the EU's material footprint and requiring the highest amount of material per Euro spent, according to the EEA briefing 'From data to decisions: material footprints in European policy making', which highlights how existing Eurostat data on our European material footprint can inform policymakers in formulating new measures to reduce our economic footprint on the environment.



The EEA briefing analyses the data and assesses the trends from 2010 to 2021 as a means of understanding how the use of biomass, metals, non-metallic minerals and fossils has contributed to the overall material footprint.

From data to decisions: material footprints in European policy making

To understand what drives material resource use in the EU, total consumption is assessed across six areas of consumption, namely housing, food, services, household goods and services, clothing and footwear, and personal mobility.

Using this information, policymakers can focus efforts to reduce material consumption where the highest potential for reduction lies and as a result reduce the demand for raw materials.

Why do we need to reduce our material footprint?

The level of resource use in the EU is very high, higher than in most other regions of the world. High resource use is responsible for severe environmental degradation across the world, linked to climate change, biodiversity loss and pollution. In our current linear economic model, prosperity is largely based on the use of resources extracted from nature.

Globally, the extraction and processing of natural resources to feed our production and consumption systems produce more than half of all greenhouse gas emissions and around 40% of particulate matter emissions – a type of pollution that is very harmful to human health. Extraction and processing also drive over 90% of land-based biodiversity loss.

It is, therefore, imperative to try to reduce primary resource consumption, as recognised by the EU's Eighth Environment Action Programme which is the EU's response to the environmental challenges posed by resource use and calls for a significant reduction of the EU's material footprint as soon as is possible.

Read More

European Environment Agency, 09-10-24

https://www.eea.europa.eu/en/newsroom/news/understanding-the-data

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EEB | Gender and Toxics: The hidden burden of mercury and other hazardous chemicals on women's health

2024-10-17

IOV. 08, 2024

Exposure to harmful chemicals, including mercury, claims the lives of over 1.5 million people globally each year. As research shows, the overwhelming majority among them are women.

Women around the world are exposed to significantly higher levels of toxic chemicals compared to men. Such an imbalance reveals yet another dark dimension of gender inequality that puts lives of the female part of the population at a constant unnecessary risk. These dynamics were confirmed by the latest UN report "Gender and Toxics", reviewing the existing gendered injustices.

Toxic substances in the modern world

Chemicals play a major role in today's scientific progress in the context of highly industrialised societies. While some substances have significantly improved the quality of human lives, including uses in the food industry, medicine and transportation, the overall pace of the chemical production growth remains concerning. In just 50 years, from 1950 to 2000, the volume of global production of chemicals increased more than 50 fold, while new chemicals are being registered every day. The efforts to protect humans from the harmful impact of numerous substances to which they are exposed every day are not keeping up with the speed of industrial development.

According to the UN report, we are witnessing "a planetary chemical crisis of unprecedented proportions" which is not only harming individuals and communities across the world but also exacerbating deeply rooted inequalities. The epidemic of chronic health conditions and deaths from chemical pollution goes hand in hand with the rapid growth of the chemical industry.

Read More

European Environmental Bureau, 17-10-24

https://meta.eeb.org/2024/10/17/the-hidden-burden-of-mercury-on-womens-health/



Air quality: Council gives final green light to strengthen

2024-10-14

standards in the EU

Today the Council formally adopted a directive setting updated air quality standards across the EU.

The new rules will contribute to the EU's objective on zero pollution by 2050 and will help prevent premature deaths due to air pollution. EU citizens will be able to seek compensation for damage to their health in cases where EU air quality rules are not respected.

Strengthening air quality standards

The revised directive prioritises the health of EU citizens: it sets new air quality standards for pollutants to be reached by 2030 which are more closely aligned with the WHO air quality guidelines. Those pollutants include, among others, particulate matter PM10 and PM2.5, nitrogen dioxide and sulphur dioxide, all known to cause respiratory problems. Member states may request that the 2030 deadline be postponed if specific conditions are met.

Air quality is assessed using common methods and criteria across the EU, and the revised directive brings further improvements to air quality monitoring and modelling.

The revised directive will also ensure early action, with air quality roadmaps that need to be prepared ahead of 2030 if there is a risk that the new standards will not be attained by that date.

The air quality standards will be reviewed regularly in line with latest scientific evidence to assess whether they continue to be appropriate.

Read More

Council of the European Union, 14-10-24

https://www.consilium.europa.eu/en/press/press-releases/2024/10/14/air-quality-council-gives-final-green-light-to-strengthen-standards-in-the-eu/

Pesticides: farming chemicals make insects sick at nondeadly doses – especially in hot weather

2024-10-28

The various regulatory systems for approving pesticides in operation around the world are crude and flawed. This has long been clear to

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scientists and it is deeply worrying, as this regulation is supposed to protect people and the environment from harm.

The EU regulatory system for pesticides is arguably the most rigorous in the world, yet it has repeatedly approved the use of pesticides that have subsequently been found to cause harm to humans or wildlife, leading to eventual bans. It often takes decades for the harm to accumulate before it is recognised.

The history of pesticide use is littered with such examples: DDT, parathion, paraquat, chlorpyrifos, neonicotinoids, chlorothalonil and many more. Most pesticides that were once deemed safe for humans and wildlife that aren't the target, like bees, have since been banned. This ought to tell us that the regulatory system is not working.

A new study offers yet more evidence. Research by the European Molecular Biology Laboratory shows how pesticide tests focus on the death of an animal and ignore any important "sublethal" effects.

Read More

NOV. 08, 2024

The Conversation, 28-10-24

https://theconversation.com/pesticides-farming-chemicals-make-insects-sick-at-non-deadly-doses-especially-in-hot-weather-241856

REACH Update

Hazardous chemicals found in cosmetic products

2024-10-30

Helsinki, 30 October 2024 - A pilot enforcement project by ECHA's Enforcement Forum found that 6 % of inspected cosmetic products contained hazardous substances banned under POPs and REACH regulations.

The national enforcement authorities in 13 European Economic Area (EEA) countries checked nearly 4 500 cosmetic products, mainly looking at the ingredients list, for the presence of perfluorooctanoic acid (PFOA), long chain perfluorocarboxylic acids (PFCAs) and related substances, and cyclic siloxanes D4 and D5. The authorities found that 285 of the inspected cosmetics included hazardous chemicals whose use is banned in these products. Those found were:

- Perfluorononyl dimethicone
- Perfluorooctylethyl triethoxysilane
- Perfluorononylethyl carboxydecyl PEG-10 dimethicone; and
- Cyclopentasiloxane (D5), cyclomethicone (a blend of D4, D5 and D6), cyclotetrasiloxane (D4).

These substances are not allowed in cosmetics because they have been identified as persistent organic pollutants (POPs) or (very) persistent, (very) bioaccumulative and toxic (PBT/vPvB) that adversely affect human health and the environment. Their use is banned under the Stockholm Convention on POPs or restricted under the REACH Regulation.

Based on national experience perfluorononyl dimethicone was primarily found in eyeliners and lipliners, in pencil or crayon form. D4 and D5 were found in hair conditioners and hair masks.

For example, perfluorononyl dimethicone degrades into PFOA and long chain perfluorocarboxylic acids. PFOA and siloxanes, D4 and D5, break down slowly in the environment and build up in humans and other species. PFOA is not only persistent in the environment but also toxic to reproduction and suspected of causing cancer. D4 is also suspected of damaging fertility.

Authorities' actions

The inspections were mainly done by checking the ingredients list - measures that can be easily used also by consumers. Consumers should be aware that the restricted substances were found in different types of cosmetic products, from various sellers and at all price ranges.

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The enforcement authorities have taken measures to remove the non-compliant products from the market. In most cases, the first step was issuing written advice to guide suppliers on how to comply with the law. At the time of writing the report, investigations were still ongoing in about half of the cases.

Background

IOV. 08, 2024

ECHA is responsible for the REACH and POPs regulations that also apply to cosmetic mixtures. This pilot project focused on the enforcement of PFCAs and related substances, PFOA and D4/D5 in cosmetics. The project contributes to the harmonised enforcement of integrated control of chemicals in cosmetics under the POPs and REACH regulations.

The inspections of this pilot enforcement project were conducted between November 2023 and April 2024 in 13 EEA countries.

Read More

ECHA, 30-10-24

https://echa.europa.eu/-/hazardous-chemicals-found-in-cosmetic-products

Brazil's Senate approved EU REACH like rules to increase chemical control

2024-10-16

Brazil's Senate approved on 15 October the creation of a National Inventory of Chemical Substances aiming at "reducing negative impacts" of toxic chemicals on human and environmental health.

The inventory and the associated public bodies to ensure compliance will put Latin America's largest economy close to the EU's Reach regulatory system regarding chemicals.

In the 27-country EU, the stringent Reach has since its inception at the end of the 2000s banned several chemicals and put hundreds of others in the so-called list of Substances of Very High Concern (SVHC).

While industry has repeatedly said it support the Reach principles, increased costs associated with complying with the regulation has put a burden in some small- and medium-sized enterprises (SMEs), a burden their peers in jurisdictions such China or the US do not have to face.

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REACH Update

Industry has also argued that while Reach may indeed avoid the entry of many toxic chemicals into the EU, those same chemicals are nonetheless still used in the manufacturing of many goods in overseas jurisdictions which end up entering the EU.

On Tuesday, the trade group representing Brazil's chemicals producers Abiquim welcomed the measure, arguing it had lobbying for the creation of the registry since 2014.

The bill, called in Parliament's jargon PL 6120/2019, now awaits presidential sanction from Brazil's President Luiz Inacio Lula da Silva, and after that it will come into force.

Read More

ICIS, 16-10-24

https://www.icis.com/explore/resources/news/2014/04/28/9775745/europe-benzene-market-poised-for-increase-in-may/?news_id=11041964

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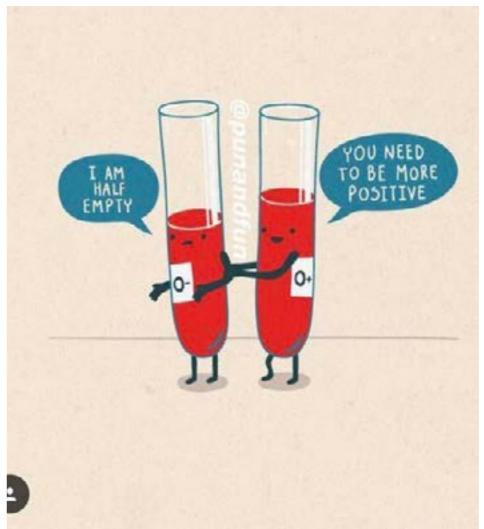
Janet's Corner

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Positivity

2024-11-08

NOV. 08, 2024



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Bulletin Board

Hazard Alert

Hexafluoroacetone

2024-11-08

USES [2,3]

Hexafluoroacetone is mostly employed in organic synthesis, but it is also the main chemical intermediate used in the production of hexafluoroisopropanol, as well as polymethyl methacrylates and polyesters for textile coating. It is also found in liquid form and is used in making solvents, adhesives, pharmaceutical products, other chemicals, and as a herbicide.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Routes of Exposure

The main routes of exposure to hexafluoroacetone are:

- Inhalation
- Contact with the skin and eyes;
- Skin absorption

HEALTH EFFECTS [4]

Acute Health Effects

- Hexafluoroacetone is toxic; may be fatal if inhaled, ingested or absorbed through skin.
- Vapours are extremely irritating and corrosive. Contact can severely irritate and burn the skin and eyes.
- Breathing hexafluoroacetone can irritate the nose and throat causing coughing and wheezing.
- Breathing hexafluoroacetone can irritate the lungs causing coughing and/or shortness of breath. Higher exposures can cause a build-up of fluid in the lungs (pulmonary oedema), a medical emergency, with severe shortness of breath.
- Exposure can cause headache, nausea, vomiting, dizziness and light-headedness.

Carcinogenicity

• Hexafluoroacetone has not been tested for its ability to cause cancer in animals.

Hexafluoroacetone is an organic compound with the formula CF3-CO-CF3. It comes in the form of a colourless, hygroscopic, non-flammable, highly reactive gas characterised by a musty odour. The most common form of this substance is hexafluoroacetone sesquihydrate (1.5 H2O). Hexafluoroacetone is a very reactive substance: it will react vigorously with water, forming corrosive acids. In the presence of humidity, reaction of hexafluoroacetone with most metals will generate white fumes of hydrogen gas. Hexafluoroacetone will also undergo violent reactions in the presence of alkali. [1,2]

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Other Effects

- There is limited evidence that hexafluoroacetone is a teratogen in animals. Until further testing has been done, it should be treated as a possible teratogen in humans.
- Hexafluoroacetone may damage the testes (male reproductive glands).

SAFETY

First Aid Measures [5]

- **If inhaled:** Move to fresh air. If the person is not breathing, give artificial respiration. Avoid mouth-to-mouth contact. Seek immediate medical attention.
- In case of skin contact: Remove all contaminated clothing.
 Immediately (within seconds) flush affected area for FIFTEEN (15) minutes. Seek immediate medical attention.
- In case of eye contact: Remove any contact lenses. Use nearest emergency eyewash immediately for at least FIFTEEN (15) minutes.
 Seek immediate medical attention and continue eye rinse during transport to hospital.
- If swallowed: DO NOT INDUCE VOMITING. Never give anything by mouth to an unconscious person. Rinse mouth with water. Seek immediate medical attention.

Workplace Controls & Practices [4]

Control measures include:

- Engineering controls are the most effective way of reducing exposure.
- The best protection is to enclose operations and/or provide local exhaust ventilation at the site of chemical release. Isolating operations can also reduce exposure.
- Where possible, automatically transfer hexafluoroacetone from cylinders or other storage containers to process containers.

The following work practices are recommended:

- Workers whose clothing has been contaminated by Hexafluoroacetone should change into clean clothing promptly.
- Contaminated work clothes should be laundered by individuals who have been informed of the hazards of exposure to hexafluoroacetone.
- Eye wash fountains should be provided in the immediate work area for emergency use.

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- · If there is the possibility of skin exposure, emergency
- shower facilities should be provided.

Personal Protective Equipment [5]

- Clothing: Avoid skin contact with hexafluoroacetone. Wear solvent-resistant gloves and clothing. Safety equipment suppliers/ manufacturers can provide recommendations on the most protective glove/clothing material for your operation. All protective clothing (suits, gloves, footwear, headgear) should be clean, available each day, and put on before work.
- Eye Protection: Wear non-vented, impact resistant goggles when
 working with fumes, gases, or vapours. Wear indirect-vent, impact and
 splash resistant goggles when working with liquids. Wear a face shield
 along with goggles when working with corrosive, highly irritating or
 toxic substances.
- Respiratory Protection: Where the potential exists for exposure over 0.1 ppm, use a MSHA/NIOSH approved supplied-air respirator with a full face piece operated in a pressure-demand or other positivepressure mode. For increased protection use in combination with an auxiliary self-contained breathing apparatus operated in a pressuredemand or other positive pressure mode.

REGULATION

United States

- ACIGH: American Conference of Governmental Industrial Hygienists has set a Threshold Limit Value (TLV) for hexafluoroacetone of 0.1 ppm, 0.68 mg/m3 TWA (Skin)
- NIOSH: National Institute for Occupational Safety and Health has established a Recommended Exposure Limit (REL) for hexafluoroacetone of 0.1 ppm TWA (Skin)

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Bulletin Board Gossip

Direct synthesis method uses recovered carbon dioxide and hydrogen to

2024-11-06

produce formic acid

With the goal of achieving a carbon-neutral society and eliminating greenhouse gas emissions by 2050, efforts are accelerating to utilize hydrogen as a key energy source. To achieve this goal, the technologies for hydrogen storage, transportation, and reproduction are actively being developed in Japan, including high-pressure hydrogen, liquid hydrogen, and liquid organic hydrogen carriers (LOHCs) such as methylcyclohexane.

One example is the transportation of hydrogen produced from lignite coal overseas to Japan, where it is used as liquid hydrogen in fuel cell vehicles, trains, forklifts, etc. Demonstration tests for these applications are already underway.

On the other hand, the use of high-pressure and liquid hydrogen, for example, presents challenges. It requires specialized equipment and heavy containers for safe storage and transportation, which pose safety risks and increased costs, limiting widespread adoption.

A researcher at AIST, in collaboration with the University of Tsukuba, has developed a highly efficient method for the direct formic acid synthesis from carbon dioxide and hydrogen. The research is published in the journal Organometallics.

Formic acid has attracted significant attention as one of the promising hydrogen carriers. In the conventional method, formic acid is first produced from carbon dioxide and hydrogen as a stable "formate salt" under basic conditions and later, the "formate salt" is converted to formic acid through acid treatment.

However, these methods involve multiple steps to manage the generated heat and to remove by-products, leading to high production costs, which complicates the cost-effective supply of hydrogen.

In this study, the researchers developed a simple and efficient method for the direct synthesis of formic acid from carbon dioxide and hydrogen using the iridium catalyst in hexafluoroisopropanol (HFIP).

Until now, direct synthesis with iridium catalysts faced challenges due to the rapid decomposition of formic acid into hydrogen and carbon dioxide in water. In contrast, they discovered that HFIP inhibits the formic acid decomposition and increases the formation rate of iridium hydride

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complexes, the key intermediates in the synthesis, by more than four times compared to that of water.

This breakthrough enables the direct, efficient production of formic acid without the need for formate intermediates. Furthermore, this achievement paves the way for formic acid to be used as a sustainable hydrogen source.

By integrating it with AIST's flow-based power generation system, this innovation could accelerate the development of carbon-neutral hydrogen storage and production solutions.

Phys Org, 6 November 2024

https://phys.org

Breaking the Rules of Chemistry: New Theory Shatters Old Ideas About Crystal Formation

2024-11-02

A new crystallization theory shows that the solvent, not the solute, controls crystal formation. This two-step process improves predictions of crystal growth and has practical applications in areas like medicine and technology.

Do you remember that old high school chemistry experiment where salt crystals would form from a saltwater solution—or the one where sugar crystals grew into rock candy from sugar water? It turns out that your understanding of how crystals formed in those solutions might be wrong.

A new theory "demystifies" the crystallization process and shows that the material that crystallizes is the dominant component within a solution – which is the solvent, not the solute. The theory could have implications for everything from drug development to understanding climate change.

"Crystals are ubiquitous – we use them in everything from technology to medicine – but our actual understanding of the crystallization process has been lacking," says James Martin, professor of chemistry at North Carolina State University and author of a paper in Matter that outlines the theory.

High School Chemistry Revisited

"The prevailing ideas around dissolving and precipitating are that they're essentially the reverse of each other, but they aren't. In reality, they are completely different processes," Martin says.

"Using the high school chemistry experiment with getting precipitate out of a solution as an example: when I dissolve salt (the solute) into water (the solvent), the water is dominant. It dissolves the salt by essentially ripping it apart," Martin says. "If I then want to grow a salt crystal from that solution,

the dominant phase must become the salt – which is the solvent at that

Thermodynamic phase diagrams, which describe concentration and temperature-dependent transition points in solutions, can be used to illustrate the new theory, dubbed the transition-zone theory.

The theory demonstrates that crystallization happens in two steps: first a melt-like pre-growth intermediate forms. Then that intermediate can organize into the crystal structure.

"To grow a crystal out of a solution, you have to quickly separate the solvent and solute," Martin says. "When we refer to the 'melt' here, we're talking about the pure phase of the solvent prior to crystal formation. The difference here is that my theory shows you get better, faster crystal growth by moving your solution toward conditions that emphasize the solvent; in other words, the solvent – not the impurity within it – controls the rate of crystal growth."

Applications and Practical Implications

point and is the one that forms the crystal."

Martin applied his theory to a number of different solutions, concentrations, and temperature conditions and found that it accurately describes the rate and size of crystal formation.

"The main issue with previous descriptions of crystallization was the perception that crystals grow by having independent solute particles diffuse to, and then attach to a growing crystal interface," Martin says. "Instead, it is necessary to understand cooperative ensembles of the solvent to describe crystal growth."

According to Martin, the important aspect of the new theory is its focus on understanding how solute impurities disrupt that cooperative ensemble of solvent.

"By understanding the interplay of temperature and concentration, we can predict exactly how fast and large crystals will grow out of solution."

Martin believes the phase diagrams could have important applications for not just crystal formation, but for preventing crystal formation, such as preventing kidney stones from growing.

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"Crystals underpin technology – they're all around us and impact our daily lives," Martin says. "This theory gives researchers simple tools to understand the 'magic' of crystal growth and make better predictions. It's an example of how foundational science lays the foundation for solving all kinds of real-world problems."

Sci Tech Daily, 2 November 2024

https://scitechdaily.com

Al-driven mobile robots team up to tackle chemical synthesis

2024-11-06

Researchers at the University of Liverpool have developed Al-driven mobile robots that can carry out chemical synthesis research with extraordinary efficiency.

In a study published in the journal Nature, researchers show how mobile robots that use AI logic to make decisions were able to perform exploratory chemistry research tasks to the same level as humans, but much faster. The paper is titled "Autonomous mobile robots for exploratory synthetic chemistry."

The 1.75-meter-tall mobile robots were designed by the Liverpool team to tackle three primary problems in exploratory chemistry: performing the reactions, analyzing the products, and deciding what to do next based on the data.

The two robots performed these tasks in a cooperative manner as they addressed problems in three different areas of chemical synthesis—structural diversification chemistry (relevant to drug discovery), supramolecular host-guest chemistry, and photochemical synthesis.

The results found that with the AI function, the mobile robots made the same or similar decisions as a human researcher but these decisions were made on a far quicker timescale than a human, which could take hours.

Professor Andrew Cooper from the University of Liverpool's Department of Chemistry and Materials Innovation Factory, who led the project explained, "Chemical synthesis research is time consuming and expensive, both in the physical experiments and the decisions about what experiments to do next, so using intelligent robots provides a way to accelerate this process.

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"When people think about robots and chemistry automation, they tend to think about mixing solutions, heating reactions, and so forth. That's part of it, but the decision making can be at least as time-consuming.

"This is particularly true for exploratory chemistry, where you're not sure of the outcome. It involves subtle, contextual decisions about whether something is interesting or not, based on multiple datasets. It's a time-consuming task for research chemists but a tough problem for AI."

Decision-making is a key problem in exploratory chemistry. For example, a researcher might run several trial reactions and then decide to scale up only the ones that give good reaction yields, or interesting products. This is hard for AI to do as the question of whether something is "interesting" and worth pursuing can have multiple contexts, such as novelty of the reaction product, or the cost and complexity of the synthetic route.

Dr. Sriram Vijayakrishnan, a former University of Liverpool Ph.D. student and the Postdoctoral Researcher with the Department of Chemistry who led the synthesis work, explained, "When I did my Ph.D., I did many of the chemical reactions by hand. Often, collecting and figuring out the analytical data took just as long as setting up the experiments. This data analysis problem becomes even more severe when you start to automate the chemistry. You can end up drowning in data."

"We tackled this here by building an Al logic for the robots. This processes analytical datasets to make an autonomous decision—for example, whether to proceed to the next step in the reaction. This decision is basically instantaneous, so if the robot does the analysis at 3:00 am, then it will have decided by 3:01 am which reactions to progress. By contrast, it might take a chemist hours to go through the same datasets."

Professor Cooper added, "The robots have less contextual breadth than a trained researcher, so in its current form, it won't have a 'Eureka!' moment. But for the tasks that we gave it here, the Al logic made more or less the same decisions as a synthetic chemist across these three different chemistry problems, and it makes these decisions in the blink of an eye.

"There is also huge scope to expand the contextual understanding of the AI, for example, by using large language models to link it directly to relevant scientific literature."

In the future, the Liverpool team wants to use this technology to discover chemical reactions that are relevant to pharmaceutical drug synthesis, as well as new materials for applications such as carbon dioxide capture.

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Two mobile robots were used in this study, but there is no limit to the size of the robot teams that could be used. Hence, this approach could scale to the largest industrial laboratories.

This new research builds on the world's first "mobile robotic chemist," reported by Professor Cooper's team in 2020 (Nature), which performed almost 700 catalysis experiments over eight days, working 24/7.

Phys Org, 6 November 2024

https://phys.org

Detecting evidence of lung cancer in exhaled breath

2024-11-06

Exhaled breath contains chemical clues to what's going on inside the body, including diseases like lung cancer. And devising ways to sense these compounds could help doctors provide early diagnoses -- and improve patients' prospects. In a study in ACS Sensors, researchers report developing ultrasensitive, nanoscale sensors that in small-scale tests distinguished a key change in the chemistry of the breath of people with lung cancer. November is Lung Cancer Awareness Month.

People breathe out many gases, such as water vapor and carbon dioxide, as well as other airborne compounds.

Researchers have determined that declines in one exhaled chemical -- isoprene -- can indicate the presence of lung cancer.

However, to detect such small shifts, a sensor would need to be highly sensitive, capable of detecting isoprene levels in the parts-per-billion (ppb) range.

It would also need to differentiate isoprene from other volatile chemicals and withstand breath's natural humidity.

Previous attempts to engineer gas sensors with characteristics like these have focused on metal oxides, including one particularly promising compound made with indium oxide.

A team led by Pingwei Liu and Qingyue Wangset out to refine indium oxide-based sensors to detect isoprene at the level at which it naturally occurs in breath.

The researchers developed a series of indium(III) oxide (In2O3)-based nanoflake sensors.

In experiments, they found one type, which they called Pt@InNiOx for the platinum (Pt), indium (In) and nickel (Ni) it contains, performed best.

These Pt@InNiOx sensors:

- Detected isoprene levels as low as 2 ppb, a sensitivity that far surpassed earlier sensors.
- Responded to isoprene more than other volatile compounds commonly found in breath.
- Performed consistently during nine simulated uses.

More importantly, the authors' real-time analysis of the nanoflakes' structure and electrochemical properties revealed that Pt nanoclusters uniformly anchored on the nanoflakes catalyzed the activation of isoprene sensing, leading to the ultrasensitive performance.

Finally, to showcase the potential medical use of these sensors, the researchers incorporated the Pt@InNiOx nanoflakes into a portable sensing device. Into this device they introduced breath collected earlier from 13 people, five of whom had lung cancer. The device detected isoprene levels lower than 40 ppb in samples from participants with cancer and more than 60 ppb from cancer-free participants. This sensing technology could provide a breakthrough in non-invasive lung cancer screening and has the potential to improve outcomes and even save lives, the researchers say.

Science Daily, 6 November 2024

https://sciencedaily.com

Tiny Gold "Frying Pans" Kill Bacteria on Implants, Reducing Antibiotic Need

2024-11-02

Gold nanorods heated by NIR light create antibacterial surfaces on implants, reducing infection risks during surgeries and potentially decreasing antibiotic resistance.

A new technology developed at Chalmers University of Technology in Sweden may play a crucial role in combating antibiotic resistance, especially in surgical procedures like hip and knee implant insertions. The technique involves heating tiny gold nanorods with near-infrared (NIR) light to sterilize the implant surface by killing bacteria. Researchers have recently published a study that deepens the understanding of how

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these gold rods respond to light and how to accurately measure their temperature.

Infections can occur during surgical procedures, with the risk increasing significantly when foreign materials, such as knee prostheses, are implanted into the body. The presence of the material weakens the body's immune system and antibiotic treatments are commonly used. If infected, high doses of antibiotics are often required with long treatment times, sometimes lifelong. This entails a risk of increased antibiotic resistance, which is seen by the WHO as one of the greatest threats to human health.

Heat kills the bacteria on the implant surface

The technology developed by the researchers at Chalmers is a method in which nanometre-sized rods of gold are attached to the implant surface. When near-infrared (NIR) light hits the surface of the implant, the rods heat up and act as tiny heating elements. Because the heating elements are so small, there is a very local heating, which kills any bacteria on the surface of the implant without heating the surrounding tissue.

"The gold rods absorb the light, the electrons in the gold are set in motion, and finally the nanorods emit heat. You could say that the gold nanorods work like small frying pans that fry the bacteria to death," says Maja Uusitalo, a doctoral student at Chalmers and lead author of the study, which has been published in the journal Nano Letters.

NIR light is invisible to the naked eye but has the ability to penetrate human tissue. This property allows the gold nanorods to be heated on the surface of the implant inside the body by illuminating the skin. The gold rods are sparsely distributed and cover only about ten percent of the implant's surface. This means that the material's beneficial properties, such as the ability to attach to bone, are largely retained.

"The trick is to tailor the size of the rods. If you make them a little smaller or a little bigger, they absorb light of the wrong wavelengths. We want the light that is absorbed to penetrate skin and tissue well. Because once the implant is inside the body, the light must be able to reach the surface of the prosthesis," says Martin Andersson, Professor and research leader at Chalmers.

Precise measurements for gold rod temperature

To increase the understanding of how the technology works, and how the NIR-heated gold nanorods affect both bacteria and human cells, the researchers needed to measure the temperature of the rods. Due to their

tiny size, it is impossible to measure with a regular thermometer, instead the researchers used X-rays to study how the gold atoms move. The method enables precise measurement of the temperature of the gold rods and how the temperature can be regulated using the intensity of the NIR light.

Maja Uusitalo

Maja Uusitalo, PhD student at the Division of Applied Chemistry, Department of Chemistry and Chemical Engineering, Chalmers University of Technology. Credit: Chalmers University of Technology | Mats Hulander

"The temperature must not exceed 120 degrees Celsius, as higher temperatures cause the nanorods to lose their shape and transform into spheres. As a result, they lose their optical properties and can no longer absorb NIR light effectively, which prevents the rods from heating up" says Maja Uusitalo.

She points out that the heating is very local with low energy transfer to the surroundings. This is crucial to avoid causing any damage to the surrounding tissue.

The researchers hope that the method can be used on many different implant materials, such as titanium or different plastics.

Gold rods become antibacterial when activated

The gold nanorods themselves are completely passive on the surface before the NIR light heats them. Only then are the rods activated, becoming hot and triggering the antibacterial effect.

"We can control when the surface should be antibacterial and when it should not. When we turn off the light, the surface is no longer antibacterial and reverts to its original state. This is an advantage because many antibacterial surfaces usually have negative effects on healing," says Martin Andersson.

The goal is to eventually bring this technology into healthcare.

"We primarily believe in using NIR light for heating shortly after the implant is placed and the wound is sutured. By heating up the gold nanorods, we can eliminate any bacteria that may have settled on the prosthesis during surgery," says Martin Andersson.

All bacteria die from the heat from the gold nanorods, but even ordinary cells can be damaged during treatment.

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"If a few human cells are destroyed during the NIR heating process the body quickly regenerates new ones, so the impact on healing is minimal," says Martin Andersson.

The technology with NIR-heated gold nanorods has previously been studied in cancer research, but the research group at Chalmers is the first to use the technology to create an antibacterial surface on implants with high precision and control.

Sci Tech Daily, 2 November 2024

https://scitechdaily.com

Safe, efficient method for synthesizing allenes opens up new possibilities for drug development

2024-10-31

A research team jointly led by Professor Sung You Hong and Professor Jan-Uwe Rohde has unveiled a novel method for synthesizing allenes—a series of compounds integral to drug development and synthetic chemistry without relying on hazardous, highly reactive chemicals.

Allenes exhibit a distinctive structure in which carbon atoms are double-bonded, making them essential for various applications in medicinal chemistry. The new synthesis method utilizes more stable organic halides instead of unstable organometallic compounds, enhancing safety in chemical reactions. Organic (pseudo) halides are compounds in which halogen elements, such as bromine and iodine, are covalently bonded to organic materials, allowing for more predictable reactivity compared to previously used alternatives.

Under nickel-catalyzed reduction conditions, the research team successfully synthesized an allene compound with a consistent structure by sequentially combining three components: 1,3-enyne, alkyl iodide and aryl iodide. Importantly, this method produced only the desired compound, avoiding the formation of irregular structures. The findings are published in ACS Catalysis.

This process showcases excellent chemo- and regioselectivity in allene formation, enabling the efficient synthesis of complex allene compounds. Chemoselectivity ensures that only the targeted chemical reaction occurs, while regioselectivity allows for precise control over where this reaction takes place within the molecule.

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The research team's approach to multi-component reactions—where

three or more compounds are combined simultaneously—has proven to be a valuable synthetic pathway. They successfully extended this method to create more complex structures and demonstrated a broad range of functional group tolerance with various allene compounds, establishing the method's stability with substances possessing diverse chemical properties.

"Our research has revealed that reduced nickel complexes play a crucial role in the key stages of this reaction," noted first authors Ji Hwan Jean and Gun Ha Kim. "We directly identified and studied nickel organometallic complexes, which are known for their instability and high reactivity."

Professor Hong said, "We can now synthesize complex allene compounds in a safe and straightforward manner," adding, "This opens up new possibilities in the field of synthetic chemistry."

Professor Rohde expressed optimism about future applications, saying, "A deeper understanding of these catalysts will pave the way for the development of coupling reactions that link two compounds to form novel entities."

Phys Org, 31 October 2024

https://phys.org

A smart 'insect screen' for sun protection and cool comfort

2024-11-06

A research team consisting of Professors Junsuk Rho from the Department of Mechanical Engineering, the Department of Chemical Engineering, and the Department of Electrical Engineering and PhD candidates Byoungsu Ko and Jaebum Noh from the Department of Mechanical Engineering at POSTECH collaborated with a research team led by Professor Heon Lee and PhD candidate Dongwoo Chae from the Department of Materials Science and Engineering at Korea University. Together, they developed a transparent radiative cooling film featuring a perforated structure resembling an insect screen, designed to regulate solar heat and lower interior temperatures. This breakthrough was recently published in Advanced Functional Materials, an international journal in materials science.

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Typically, objects exposed to sunlight heat up, but there is a technique -- "radiative cooling" -- that allows them to release heat and cool down naturally without using any external power.

Researchers have been exploring ways to integrate this cooling effect into transparent films such as glass.

However, they have encountered challenges as these films often transmit solar heat, limiting their cooling effectiveness.

To address this challenge, a joint research team from POSTECH and Korea University engineered a film combining a perforated silver (Ag) substrate, a Bragg mirror, and a polydimethylsiloxane (PDMS) coating.

This film achieves both transparency and radiative cooling performance.

The Bragg mirror, a multi-layer thin-film structure, is designed to reflect near-infrared light, which is responsible for much of the sun's heat.

To maintain visibility, the team created a perforated design, akin to an insect screen, by puncturing micrometer-scale holes in the silver substrate to allow light to pass through.

For effective emission of far-infrared radiation within the atmospheric window, they added a high-absorption, silicon-based PDMS coating.

Constructed with these three layers -- a perforated silver substrate, a Bragg mirror, and a PDMS coating -- the film effectively provides cooling while maintaining visibility.

In testing, glass with this film stayed 22.1°C cooler than glass coated solely with PDMS.

Professor Junsuk Rho of POSTECH stated, "This technology is ready for mass production and has significant potential in architecture and environmental applications." He continued, "Most importantly, it efficiently dissipates heat and reduces energy consumption, positioning it as a key technology for a sustainable future."

The research was conducted with support from the POSCO Holdings N.EX.T IMPACT Metasurface-based Planar Optics Technology Lab and the Leading Research Lab of the Ministry of Science and ICT and the National Research Foundation of Korea.

Science Daily, 6 November 2024

https://sciencedaily.com

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Steeped in chemistry

2024-01-25

As a keen tea drinker I was intrigued by a January 2020 tweet in which @ andrechemist wondered if a tetrahedral teabag produced a better cup of tea. The question sent me into the literature to see what chemists knew about the shape of teabags and the resulting brew. In fact, just what did chemists know about making tea more generally?

Quite a lot as it turns out. This should not have surprised me as tea is the most popular beverage in the world after water (a statistic nearly every paper on tea I read cited). In the end I wrote my own version of George Orwell's 1946 essay, 'A Nice Cup of Tea' for Nature Chemistry. That essay grew into my book Steeped: The chemistry of tea.

There is a vast chemical literature on tea: I read some 500 papers. To flesh out what I was reading, I did some experiments of my own. I measured cooling curves for teapots of different materials, spiked my tea with extra doses of its naturally occurring amino acid I-theanine to see if it affected the flavour (researchers disagreed, but I could taste the difference) and sampled heavy water to determine if it is sweet (it is). Given its price tag I drew the line at buying deuterium-depleted water to see if that produced an exceptional cup of tea as one author suggested, and a lack of snow the past two winters kept me from scraping it off plum blossoms to reproduce a famously extraordinary cup detailed in an 8th century Chinese manuscript.

The biggest challenge I faced in writing Steeped – beyond the daunting scope of the literature – was how to present the chemistry in such a way that someone who had not taken a chemistry course could appreciate what was happening in a cup of tea on the molecular level. I settled on highlighting four big ideas that chemists use to explain the behaviour of molecules: atoms make up everything, opposites attract, getting close matters, and molecular function depends on molecular structure. I wrote an introductory chapter that fleshes out these concepts and provides a short course in how to read chemical structures. In case people were daunted by even that much chemistry, I wrote a three paragraph TL;DR that was just enough (I hoped) to get them through. I wanted not only to help non-chemists navigate the chemistry in the book, but to let them catch a glimpse of the world as chemists see it. I hope that readers without a science background will be able to wield these concepts to understand other everyday chemistry.

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Researching Steeped changed my own tea making habits. My experiments measuring the cooling curves drove home to me the importance of pre-warming the teapot or the cup whenever possible. If I don't, the temperature in my favorite Japanese cast-iron tetsukyūsu quickly drops below the optimum temperature for extracting caffeine and other desirable compounds. These days I reach more often for a double-walled glass pot that not only keeps the tea hot while it brews, but also keeps it at a drinkable temperature longer without the need for a tea cozy.

I have also become a more agitated brewer of tea. I repeatedly dunk teabags and swish my tea basket infuser as the tea steeps in order to expose the tea leaves more evenly to the solvent and extract more catechins—tea's signature antioxidants. Finally I unscrew the lid on my travel mug when I can to inhale the volatile calming compounds such as linalool found in the steam.

While writing Steeped certainly enhanced my enjoyment of a cup of tea, there were several disquieting discoveries along the way. There are the remains of lots of bugs in my tea – the DNA of hundreds of different insects have been identified in tea leaves. I also now know how closely the white film that appears on tea when water is heated in the microwave resembles bathtub scum. Though that also means that the remedy is the same for both, some citric acid to chelate those hard water ions.

I particularly enjoyed encountering other women connected to the chemistry of tea. The earliest paper I read was from 1885, a careful analysis of an infusion of tea by Wilhelmina Green, a chemist I wish I knew more about. And while the invention of the modern teabag is usually credited to Thomas Sullivan in 1908, a US patent for such a teabag was issued to Roberta Lawson and Mary McLaren five years earlier.

And to answer the question that kicked off this project, it is not so much the shape of the teabag that matters as the size. To use one of the big ideas of chemistry, the tea leaves need enough space to get close to the water. Agitate well and enjoy a better cup of tea.

Chemistry World, 25 January 2024

https://chemistryworld.com

Ozempic drug alleviates osteoarthritic knee pain

2024-11-07

The 'Ozempic drug,' semaglutide, has been found to reduce moderately severe pain caused by knee osteoarthritis and improve physical

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functioning following weight loss, according to the results of a recent

clinical trial by Novo Nordisk, the drug's manufacturer.

Osteoarthritis in the knee joints is painful and restrictive, and with obesity, the risk of developing the condition is increased. But joint stress isn't the only contributing problem. Fat is chemically active and constantly releases inflammation-causing proteins that travel to the joints.

Novo Nordisk, the Danish pharmaceutical company that manufactures the wonder diabetes-and-weight-loss drug semaglutide, sold as Ozempic (for diabetes) and Wegovy (for weight loss), recently published the results of a phase 3 clinical trial of the drug's effect on obese adults with moderate knee osteoarthritis.

"Obesity-related knee osteoarthritis is a progressive condition that can lead to pain and stiffness of the knee and impair critical daily functions such as walking or moving around," said Henning Bliddal, MD, from The Parker Institute at the Copenhagen University Hospital and the study's lead and corresponding author. The Parker Institute researches disorders of the musculoskeletal system.

"The risk of developing the condition is more than four times higher in people with obesity. Weight reduction, along with physical activity, is often a recommended approach to managing painful symptoms, but adherence can be challenging. There is a significant need for non-surgical and sustainable treatment options for those living with obesity-related osteoarthritis. The STEP 9 trial aimed to provide rigorous evidence as to how semaglutide may help these people."

The 68-week STEP 9 trial included 407 adult participants (81.6% women) at 61 sites in 11 countries. Participants were included if they had been diagnosed, by clinical exam and radiological imaging, with moderate knee osteoarthritis and at least moderate pain. Pain was measured using the Western Ontario and McMaster Universities Osteoarthritis Index (WOMAC) questionnaire that scores three areas: pain, stiffness, and physical function. Scores for each subscale are tallied, with a possible range of zero to 20 for pain, zero to eight for stiffness, and zero to 68 for physical function. Usually, a sum of the scores for all three subscales gives a total WOMAC score. They were randomized to receive a once-weekly subcutaneous (under the skin) injection of 2.4 mg of semaglutide or placebo, in addition to counseling on physical activity and eating a reduced-calorie diet.

The trial participants' mean baseline body weight was 239.5 lb (109 kg). Semaglutide led to a -13.7% mean change from baseline body weight at

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week 68 compared with -3.2% with placebo. Semaglutide also produced a mean change from baseline in WOMAC score of -41.7 points at the trial's end versus -27.5 with placebo. Those taking semaglutide also had a greater improvement in physical functioning scores at week 68 compared with placebo, with a mean change of 12 vs. 6.5 points.

"Obesity is a complex metabolic disease associated with multiple comorbid conditions, including knee osteoarthritis," said Anna Windle, PhD, senior vice president of clinical development, medical and regulatory affairs at Novo Nordisk. "The STEP 9 results are encouraging and provide important information about the effect of semaglutide, a glucagon-like peptide-1 receptor agonist, on knee osteoarthritis outcomes in people with obesity. We look forward to working with regulatory authorities on next steps based on these findings."

At present, semaglutide is not approved as a treatment for osteoarthritis pain.

The study was published in The New England Journal of Medicine.

New Atlas, 7 November 2024

https://newatlas.com

Potential New Treatment Suggested for Aggressive Prostate Cancer

2024-11-06

Researchers have identified how mutations to CDK12 drive prostate cancer development and reported a promising treatment.

When researchers at the University of Michigan Rogel Cancer Center first identified a new subtype of aggressive prostate cancer, they knew they needed to understand how this genetic alteration was driving cancer and how to target it with treatment.

In two new papers, both published in Cell Reports Medicine, they do both, describing the mechanisms of how alterations in the CDK12 gene drive prostate cancer development and reporting on a promising degrader that targets CDK12 and a related gene to destroy tumors.

Researchers previously found loss of the CDK12 gene in about 7% of patients with metastatic prostate cancer, suggesting this alteration may be linked to a more-aggressive form of the disease. This was discovered from DNA and RNA sequencing from patient tumor samples. CDK12 also plays a role in some ovarian cancers.

To understand how CDK12 loss impacts cells on a molecular level, researchers created a mouse model to try to parallel the genetic alterations they were seeing in human prostate cancers.

"What was quite surprising was when we created CDK12 loss in a mouse prostate, this caused precursor lesions to form in the mouse prostate. Then, when we added loss of the p53 oncogene, the mice developed bona fide invasive prostate cancer," said senior author Arul M. Chinnaiyan, M.D., Ph.D., director of the Michigan Center for Translational Pathology and S.P. Hicks Professor of Pathology at Michigan Medicine. "It will be an addition to the field to have a genetically engineered mouse model that parallels what we see in human prostate cancer."

With the mouse model, researchers then discovered the mechanism of how CDK12 loss induces DNA damage. The loss of this gene activates other known cancer driver genes, causing them to be overexpressed at a high level while also causing DNA to be replicated very rapidly. The collision of these two processes leads to DNA damage.

"These back-to-back studies taken together are quite impressive. We created an animal model and then deciphered the mechanisms of how CDK12 loss actually drives prostate cancer," Chinnaiyan said.

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The team also found that a partner gene, CDK13, is important in targeting the alteration therapeutically. They developed a potential therapy designed to degrade CDK12 and CDK13. Testing in cell lines and mice showed the degrader specifically binds to CDK12 and CDK13 and stops the growth of cancer cells over normal cells. The degrader can be absorbed orally and would not need to be delivered intravenously. This is notable as most protein degraders are too large to be absorbed orally, which has limited their potential in drug development.

Further, they found that knocking down CDK12/13 activated the AKT pathway, which plays a role in cancer development. Combining the CDK12/13 degrader with existing therapies targeting AKT resulted in a synergistic effect in destroying cancer cells. This suggests the potential to combine a CDK12/13 degrader with other approved therapies.

"It's well known that single therapies for cancer treatment have been challenging. Oftentimes patients develop resistance. If we can find the right combination, we could prevent resistance mechanisms from occurring. That's one of the benefits of finding an FDA-approved agent to combine with CDK12/13 degraders," Chinnaiyan said. "This study also highlights an international collaboration with Ke Ding, Ph.D., a medicinal chemist at the Shanghai Institute of Chemistry, in the development of orally bioavailable CDK12/13 degraders."

Technology Networks, 6 November 2024

https://technologynetworks.com

How Much Magnesium You Should Take in a Day, with an Expert Doctor's Detailed Wisdom

2024-04-16

Magnesium is "the relaxation mineral," but—no surprise—many Americans aren't getting enough. A doctor reveals the daily magnesium requirement, the best magnesium supplements, and natural ways to increase magnesium intake.

With nearly half of Americans falling short of their daily magnesium needs, it's no surprise that magnesium supplements have been trending. In fact, the global magnesium supplements market was projected to value at \$107 million in 2024 and anticipated to climb to \$130 million by 2031. That's a greater-than 20% jump over just a few years.

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So, what's the cause of this widespread magnesium shortfall? According to experts like Mark Hyman, MD, a leader in functional medicine, there are multiple reasons we're not getting the recommended amounts of magnesium:

- Our meals are more processed and less nutrient-dense than ever before.
- The soil where our food grows is increasingly stripped of magnesium.
- Our consumption of coffee, alcohol, and sugar—all of which can diminish magnesium levels—is on the rise.

So by the time you see your doctor for muscle cramps or spasms, poor sleep, unexplained weight problems, urinary issues or another symptom of low magnesium, it's likely you'll discuss much magnesium should you take per day, and the best ways to get more magnesium.

Keep reading for clinical recommendations on magnesium intake.

What is magnesium?

Magnesium is a mineral involved in at least 300 enzyme reactions within the human body—and according to some studies, up to 600. This means magnesium is fundamental for muscle and nerve function, regulating blood sugar and blood pressure, and producing protein, bone, and DNA.

Given its central role in so many physiological functions, it's clear why a magnesium deficiency can lead to symptoms such as fatigue, muscle cramps, mental issues, irregular heart rhythms, and increased stress.

Here's how much magnesium you should take per day

The recommended dietary allowances for magnesium are specific to age, gender, and physiological conditions, says the National Institutes of Health:

- Men between 19 and 30 years old should consume 400 milligrams of magnesium
- Men 31 years and older should consume 420 milligrams of magnesium
- Women between 19 and 30 years old should consume 310 milligrams of magnesium
- Women 31 years and older should consume 320 milligrams of magnesium
- For pregnant individuals over age 18, an increased daily requirement of 350-360 milligrams is recommended.

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The National Institutes of Health has set the upper limit of magnesium that you should take in supplement form at 350 milligrams. (Dr. Hyman suggests a daily supplemental magnesium intake of 300 milligrams.) However, consult your healthcare provider to determine the optimal amount for your unique needs, as some individuals may benefit from higher doses.

When selecting magnesium supplements, magnesium glycinate is often recommended for its ability to cross the blood-brain barrier, which can be beneficial for reducing anxiety and improving sleep quality.

If constipation is a concern, magnesium citrate may offer relief, though be cautious because excessive amounts could lead to diarrhea.

Magnesium L-threonate has also been shown to benefit brain health in a 2022 study.

Magnesium carbonate, oxide, or gluconate are forms that research suggests are less efficiently absorbed by the body.

How to get more magnesium?

Magnesium supplements can work, but experts suggest adding magnesium-rich foods to your diet is the best way to increase magnesium intake:

- Dark leafy greens (spinach, kale)
- Nuts and seeds (pumpkin seeds, almonds, chia seeds)
- Whole grains (brown rice, quinoa)
- · Legumes (black beans, chickpeas)
- Avocado
- Dark chocolate

Additionally, an Epsom salt bath is a relaxing way to absorb magnesium through the skin.

Is it OK to take magnesium every day?

It is generally safe to take magnesium every day, provided you stick within the dosage guidelines recommended by your healthcare provider. Consistent, moderate intake supports your body without leading to adverse side effects.

Who shouldn't take magnesium?

People suffering from kidney disease, heart disease, intestinal disorders, diabetes, or those on specific medications such as bisphosphonates, antibiotics, diuretics, and proton pump inhibitors—which can impact magnesium levels—should seek medical advice before beginning any magnesium supplementation.

Magnesium risks

While magnesium is beneficial, excessive intake can lead to several risks, including:

- Diarrhea and abdominal cramping
- Nausea and vomiting
- Interference with certain medications, such as antibiotics and blood pressure medications
- In severe cases, irregular heartbeat and cardiac arrest.

To minimize risks, always follow the recommended dietary allowance and guidelines set by your healthcare provider if you have concerns about your magnesium intake.

The Healthy, 16 April 2024

https://thehealthy.com

Gene Repair via CRISPR May Trigger Unwanted Defects

2024-11-06

The CRISPR molecular scissors have the potential to revolutionize the treatment of genetic diseases. This is because they can be used to correct specific defective sections of the genome. Unfortunately, however, there is a catch: under certain conditions, the repair can lead to new genetic defects – as in the case of chronic granulomatous disease. This was reported by a team of basic researchers and physicians from the clinical research program ImmuGene at the University of Zurich (UZH).

Chronic granulomatous disease is a rare hereditary disease that affects about one in 120,000 people. The disease impairs the immune system, making patients susceptible to serious and even life-threatening infections. It is caused by the absence of two letters, called bases, in the DNA sequence of the NCF1 gene. This error results in the inability to produce an enzyme complex that plays an important role in the immune defense against bacteria and molds.

The CRISPR tool works...

The research team has now succeeded in using the CRISPR system to insert the missing letters in the right place. They performed the experiments in cell cultures of immune cells that had the same genetic defect as people with chronic granulomatous disease. "This is a promising result for the use of CRISPR technology to correct the mutation underlying this disease," says team leader Janine Reichenbach, professor of somatic gene therapy at the University Children's Hospital Zurich and the Institute for Regenerative Medicine at UZH.

... but unfortunately, it's not perfect

Interestingly however, some of the repaired cells now showed new defects. Entire sections of the chromosome where the repair had taken place were missing. The reason for this is the special genetic constellation of the NCF1 gene: it is present three times on the same chromosome, once as an active gene and twice in the form of pseudogenes. These have the same sequence as the defective NCF1 and are not normally used to form the enzyme complex.

CRISPR's molecular scissors cannot distinguish between the different versions of the gene and therefore occasionally cut the DNA strand at multiple locations on the chromosome – at the active NCF1 gene as well as at the pseudogenes. When the sections are subsequently rejoined, entire gene segments may be misaligned or missing. The medical consequences are unpredictable and, in the worst case, contribute to the development of leukemia. "This calls for caution when using CRISPR technology in a clinical setting," says Reichenbach.

Safer method sought

To minimize the risk, the team tested a number of alternative approaches, including modified versions of CRISPR components. They also looked at using protective elements that reduce the likelihood of the genetic scissors cutting the chromosome at multiple sites simultaneously. Unfortunately, none of these measures were able to completely prevent the unwanted side effects.

"This study highlights both the promising and challenging aspects of CRISPR-based therapies," says co-author Martin Jinek, a professor at the UZH Department of Biochemistry. He says the study provides valuable insights for the development of gene-editing therapies for chronic granulomatous disease and other inherited disorders. "However, further



technological advances are needed to make the method safer and more effective in the future."

Technology Networks, 6 November 2024

https://technologynetworks.com

Gamma radiation converts methane into complex organic molecules and could explain the origin of life

2024-11-06

Gamma radiation can convert methane into a wide variety of products at room temperature, including hydrocarbons, oxygen-containing molecules, and amino acids, according to a new article published in the journal Angewandte Chemie International Edition.

This type of reaction probably plays an important role in the formation of complex organic molecules in the universe—and possibly in the origin of life. It also opens up new strategies for the industrial conversion of methane into high value-added products under mild conditions.

With these research results, the team led by Weixin Huang at the University of Science and Technology of China (Hefei) has contributed to our fundamental understanding of the early development of molecules in the universe.

"Gamma rays, high-energy photons commonly existing in cosmic rays and unstable isotope decay, provide external energy to drive chemical reactions of simple molecules in the icy mantles of interstellar dust and ice grains," states Huang. "This can result in more complex organic molecules, presumably starting from methane (CH4), which is widely present throughout the interstellar medium."

Although higher pressures and temperatures reign on Earth and on planets in the so-called habitable zone, most studies of cosmic processes are only simulated under vacuum and at extremely low temperatures. In contrast, the Chinese team studied the reactions of methane at room temperature in the gas and aqueous phases under irradiation with a cobalt-60 emitter.

The composition of the products varies depending on the starting materials. Pure methane reacts—with very low yield—to give ethane, propane and hydrogen. The addition of oxygen increases the conversion, resulting mainly in CO2 as well as CO, ethylene, and water.

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In the presence of water, aqueous methane reacts to give acetone and tertiary butyl alcohol; in the gas phase, it gives ethane and propane. When both water and oxygen are added, the reactions are strongly accelerated. In the aqueous phase, formaldehyde, acetic acid, and acetone are formed. If ammonia is also added, acetic acid forms glycine, an amino acid also found in space.

"Under gamma radiation, glycine can be made from methane, oxygen, water, and ammonia, molecules that are found in large amounts in space," says Huang. The team developed a reaction scheme that explains the routes by which the individual products are formed. Oxygen (·O2–) and ·OH radicals play an important role in this. The rates of these radical reaction mechanisms are not temperature-dependent and could thus also take place in space.

In addition, the team was able to demonstrate that various solid particles that are components of interstellar dust—silicon dioxide, iron oxide, magnesium silicate, and graphene oxide—change the product selectivity in different ways. The varied composition of interstellar dust may thus have contributed to the observed uneven distribution of molecules in space.

Silicon dioxide leads to a more selective conversion of methane to acetic acid. Huang says, "Because gamma radiation is an easily available, safe, and sustainable source of energy, this could be a new approach for using methane as a carbon source that can be efficiently converted into value-added products under mild conditions—a long-standing challenge for industrial synthetic chemistry."

Phys Org, 6 November 2024

https://phys.org

A smart 'insect screen' for sun protection and cool comfort

2024-11-06

A research team consisting of Professors Junsuk Rho from the Department of Mechanical Engineering, the Department of Chemical Engineering, and the Department of Electrical Engineering and PhD candidates Byoungsu Ko and Jaebum Noh from the Department of Mechanical Engineering at POSTECH collaborated with a research team led by Professor Heon Lee and PhD candidate Dongwoo Chae from the Department of Materials Science and Engineering at Korea University. Together, they developed a transparent radiative cooling film featuring a perforated structure

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resembling an insect screen, designed to regulate solar heat and lower interior temperatures. This breakthrough was recently published in

Advanced Functional Materials, an international journal in materials

science.

Typically, objects exposed to sunlight heat up, but there is a technique -- "radiative cooling" -- that allows them to release heat and cool down naturally without using any external power.

Researchers have been exploring ways to integrate this cooling effect into transparent films such as glass.

However, they have encountered challenges as these films often transmit solar heat, limiting their cooling effectiveness.

To address this challenge, a joint research team from POSTECH and Korea University engineered a film combining a perforated silver (Ag) substrate, a Bragg mirror, and a polydimethylsiloxane (PDMS) coating.

This film achieves both transparency and radiative cooling performance.

The Bragg mirror, a multi-layer thin-film structure, is designed to reflect near-infrared light, which is responsible for much of the sun's heat.

To maintain visibility, the team created a perforated design, akin to an insect screen, by puncturing micrometer-scale holes in the silver substrate to allow light to pass through.

For effective emission of far-infrared radiation within the atmospheric window, they added a high-absorption, silicon-based PDMS coating.

Constructed with these three layers -- a perforated silver substrate, a Bragg mirror, and a PDMS coating -- the film effectively provides cooling while maintaining visibility.

In testing, glass with this film stayed 22.1°C cooler than glass coated solely with PDMS.

Professor Junsuk Rho of POSTECH stated, "This technology is ready for mass production and has significant potential in architecture and environmental applications." He continued, "Most importantly, it efficiently dissipates heat and reduces energy consumption, positioning it as a key technology for a sustainable future."

The research was conducted with support from the POSCO Holdings N.EX.T IMPACT Metasurface-based Planar Optics Technology Lab and the

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Leading Research Lab of the Ministry of Science and ICT and the National Research Foundation of Korea.

Science Daily, 6 November 2024

https://sciencedaily.com

Bioinspired hydrogels harness sunlight: A step closer to artificial photosynthesis

2024-11-06

NOV. 08, 2024

Mimicking how plants convert sunlight into energy has long been a dream for scientists aiming to create renewable energy solutions. Artificial photosynthesis is a process that seeks to replicate nature's method, using sunlight to drive chemical reactions that generate clean energy. However, creating synthetic systems that work as organically as natural photosynthesis has been a significant challenge until now.

Now, researchers from the Japan Advanced Institute of Science and Technology (JAIST) and the University of Tokyo have designed a new type of bioinspired hydrogel that can generate hydrogen and oxygen by splitting water molecules using sunlight. Their study was published online in Chemical Communications.

This design can be a potential game changer in the quest for clean energy, as hydrogen is seen as a promising fuel for the future. Moreover, this advancement in hydrogen production could be compared to other clean energy technologies like solar photovoltaics and electrolysis-based hydrogen production.

These methods rely on external energy sources, whereas the hydrogel system mimics nature by using sunlight directly to split water, potentially improving efficiency and reducing costs.

The research team, led by Associate Professor Kosuke Okeyoshi, along with his doctoral student Reina Hagiwara at JAIST, and Professor Ryo Yoshida at the University of Tokyo, designed these hydrogels with carefully structured polymer networks. These networks help control the transfer of electrons, which is crucial for splitting water into hydrogen and oxygen.

The hydrogels are packed with functional molecules, such as ruthenium complexes and platinum nanoparticles, which work together to simulate the natural process of photosynthesis.

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"The biggest challenge was figuring out how to arrange these molecules so they could transfer electrons smoothly," says Prof. Okeyoshi. "By using a

polymer network, we were able to prevent them from clumping together, which is a common issue in synthetic photosynthesis systems."

Adding further, first-author Reina Hagiwara, a Ph.D. student at JAIST,

Adding further, first-author Reina Hagiwara, a Ph.D. student at JAIST, says, "What's unique here is how the molecules are organized within the hydrogel. By creating a structured environment, we've made the energy conversion process much more efficient."

One of the key breakthroughs in this study is the hydrogels' ability to prevent the functional molecules from aggregating—a major issue in previous artificial photosynthesis systems. As a result, the team was able to significantly boost the activity of the water-splitting process and produce more hydrogen compared to older techniques.

This design has major implications for clean energy. Hydrogen, when produced using just water and sunlight, could become a key player in future energy systems, offering a renewable alternative to fossil fuels.

As Prof. Okeyoshi explains, "Hydrogen is a fantastic energy source because it is clean and renewable. Our hydrogels offer a way to produce hydrogen using sunlight, which could help sustainably reshape energy technologies."

By making artificial photosynthesis more active, this study moves us closer to a future where renewable hydrogen could power industries, transportation, and energy storage systems.

Despite these promising results, the researchers note that there is still work to be done. Scaling up the production of these hydrogels and ensuring their long-term stability will be important next steps.

"We have shown the potential, but now we need to refine the technology for industrial use," says Prof. Okeyoshi. "The possibilities are exciting, and we're eager to continue pushing forward."

The team also plans to explore precise integration in the hydrogels to further enhance their energy conversion efficiency.

Phys Org, 6 November 2024

https://phys.org



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Al-powered system detects toxic gases with speed and precision

2024-11-05

NOV. 08, 2024

Researchers at the University of Virginia School of Engineering and Applied Science developed an Al-powered system that mimics the human sense of smell to detect and track toxic gases in real time. Using advanced artificial neural networks combined with a network of sensors, the system quickly identifies the source of harmful gases like nitrogen dioxide (NO?) that poses severe respiratory health risks.

According to the World Health Organization, outdoor air pollution, including NO2, contributes to approximately 4.2 million premature deaths globally each year, primarily due to respiratory conditions like asthma and chronic obstructive pulmonary disease (COPD).

Graphene-Based Sensors Mimic Human Smell

The innovative system relies on nano-islands of metal catalysts embedded on graphene surfaces. This device functions like an artificial nose, reacting with targeted toxic gas molecules. As nitrogen dioxide molecules bind to the graphene, the conductivity of the sensor changes, allowing the system to detect gas leaks with extreme sensitivity.

"Nano-islands of metal catalysts are tiny clusters of metal particles deposited on a surface, such as graphene, that enhance chemical reactions by increasing the surface area for gas molecules to interact, enabling precise detection of toxic gases," said Yongmin Baek, a research scientist in the Department of Electrical and Computer Engineering who is leading the R&D for the sensors.

Kyusang Lee, associate professor of electrical and computer engineering and materials science engineering, and one of the lead researchers on the project, explains, "By integrating Al with state-of-the-art gas sensors, we're able to pinpoint gas leaks with unprecedented accuracy, even in large or complex environments. The artificial olfactory receptors are able to detect tiny changes in gas concentrations and communicate that data to a near-sensor computing system, which uses machine learning algorithms to predict the source of the leak."

Neural Net Optimizes Sensor Placement

The system's artificial neural network analyzes data from the sensors in real-time, based on the optimized sensor placement to ensure coverage and efficiency of system. This optimization is enabled by a "trust-region"

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Bayesian optimization algorithm," a machine learning technique that breaks down complex problems into smaller regions to find the most efficient sensor positions. This ensures fewer resources are used while providing faster and more accurate gas leak detection.

Electrical and computer engineering Ph.D. student Byungjoon Bae adds, "Our Al-powered system has the potential to make industrial settings, urban areas and even residential buildings safer by constantly monitoring air quality. It's a major step forward in preventing long-term health risks and protecting the environment."

Science Daily, 5 November 2024

https://sciencedaily.com

Cancer Breathalyzer: Nanotech Breath Test for Cancer Could Save Lives

2024-11-06

Detecting early-stage lung cancer may become easier thanks to an innovative approach that analyzes exhaled breath.

Researchers developed an ultrasensitive nanoscale sensor capable of detecting isoprene levels in breath, a biomarker for lung cancer. By incorporating platinum-based nanoclusters, the Pt@InNiOx sensor achieved high sensitivity, with a detection threshold of just 2 parts per billion, surpassing previous sensors.

Exhaled Breath as a Diagnostic Tool

Exhaled breath holds valuable chemical clues about our health, including indicators of diseases like lung cancer. Developing ways to detect these compounds could enable doctors to make earlier diagnoses and improve outcomes for patients.

In a study published today (November 6) in ACS Sensors, researchers describe creating ultrasensitive, nanoscale sensors that, in preliminary tests, successfully identified a key chemical change in the breath of individuals with lung cancer. This research arrives timely as November marks Lung Cancer Awareness Month.

Breath Gases and Their Diagnostic Potential

When we breathe out, we release various gases, including water vapor, carbon dioxide, and other airborne compounds. Among these, researchers

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have found that reduced levels of a specific chemical, isoprene, may signal lung cancer.

Detecting these small changes requires highly sensitive sensors capable of measuring isoprene levels in the parts-per-billion (ppb) range. Additionally, these sensors must distinguish isoprene from other volatile chemicals in the breath and withstand natural humidity.

Earlier efforts to create such sensors focused on metal oxides, particularly a promising compound made with indium oxide. With this in mind, a research team led by Pingwei Liu and Qingyue Wang aimed to refine indium oxide-based sensors to detect isoprene at the levels naturally found in breath.

Advancing Sensor Sensitivity With Indium Oxide

The researchers developed a series of indium(III) oxide (In2O3)-based nanoflake sensors. In experiments, they found one type, which they called Pt@InNiOx for the platinum (Pt), indium (In), and nickel (Ni) it contains, performed best. These Pt@InNiOx sensors:

- Detected isoprene levels as low as 2 ppb, a sensitivity that far surpassed earlier sensors.
- Responded to isoprene more than other volatile compounds commonly found in breath.
- Performed consistently during nine simulated uses.

More importantly, the authors' real-time analysis of the nanoflakes' structure and electrochemical properties revealed that Pt nanoclusters uniformly anchored on the nanoflakes catalyzed the activation of isoprene sensing, leading to ultrasensitive performance.

Portable Device Development for Real-World Testing

Finally, to showcase the potential medical use of these sensors, the researchers incorporated the Pt@InNiOx nanoflakes into a portable sensing device. Into this device, they introduced breath collected earlier from 13 people, five of whom had lung cancer. The device detected isoprene levels lower than 40 ppb in samples from participants with cancer and more than 60 ppb from cancer-free participants. This sensing technology could provide a breakthrough in non-invasive lung cancer



screening and has the potential to improve outcomes and even save lives, the researchers say.

Sci Tech Daily, 6 November 2024

https://scitechdaily.com

Scientists find key to engineering water-responsive biopolymers

2024-11-05

Scientists at the Advanced Science Research Center at the CUNY Graduate Center (CUNY ASRC) have developed a novel approach to better understand and predict the behaviors of water-responsive materials—solid matter that can change shape by absorbing or releasing water in response to humidity fluctuations. These materials, commonly found in nature, have the potential to revolutionize a range of industries, from robotics and smart textiles to bioelectronics and clean energy generation systems.

Despite water-responsive materials' growing popularity in research and development, a gap exists in the theoretical understanding of how these materials generate mechanical stress when they absorb and release water. A research team led by Professor Xi Chen at the CUNY ASRC Nanoscience Initiative and City College of New York's Chemical Engineering Department has pioneered a new quantitative method to correlate the structure of confined water with the macroscopic water-responsive properties of materials like silk.

"Water-responsive materials that react to humidity changes are highly promising for use as actuators in robotics and for energy harvesting applications, yet we lack the theories to explain or predict the stress they generate," said Chen.

"Our research shows that nanoconfinement of water plays a crucial role in determining the behavior of regenerated silk fibroin films. The important parameters highlighted in the study, will allow us to better predict material performance and engineering for future use in water-responsive actuators" said Darjan Podbevšek, the paper's first author and a postdoctoral research associate in Chen's and Raymond Tu's labs. Tu is a co-corresponding author of the paper and a Chemical Engineering professor at CUNY's City College of New York.

CHEMWATCH

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The study, published in Nature Communications, introduces a groundbreaking approach to explain water-responsive materials' behavior, focusing on how water's molecular structure within these materials affects stress generation. Previous studies have only qualitatively explained hydration and dehydration-induced stress in WR materials, but this new approach quantitatively demonstrates that the water structure, rather than the material's structural properties, is the main factor governing stress.

The team discovered that all the samples began to exert force when they reached a critical threshold at which their bound and mobile water ratios reached a specific value, consistent among all samples. This finding highlights the importance of the different water populations in biomaterials and suggests universal guidelines for predicting and engineering water-responsive behavior in biopolymers.

"This breakthrough not only helps us understand how water-responsive materials work, but also opens doors to exciting new applications in tissue engineering, biocompatible materials, optical coatings, and beyond," said Tu.

The study provides key insights that could be applied to a wide range of hygroscopic and water-absorbent materials, with significant implications for industries like biomedical engineering, food preservation, and cosmetics.

Phys Org, 5 November 2024

https://phys.org

UCLA Chemists Shatter 100-Year-Old Chemistry Rule – Textbooks Need a Rewrite

2024-11-03

UCLA chemists have overturned a century-old rule in organic chemistry that limited molecular design by proving that anti-Bredt olefins can be synthesized and stabilized. This finding opens new paths in drug discovery and innovation.

- According to Bredt's rule, double bonds cannot exist at certain
 positions on organic molecules if the molecule's geometry deviates too
 far from what we learn in textbooks.
- This rule has constrained chemists for a century.



 A new paper in Science shows how to make molecules that violate Bredt's rule, allowing chemists to find practical ways to make and use them in reactions.

UCLA Chemists Challenge Century-Old Rule

UCLA chemists have discovered a major flaw in a fundamental rule of organic chemistry that has held for 100 years. They say it's time to rewrite the textbooks.

Organic molecules, which are primarily made of carbon, have specific shapes and arrangements of atoms. Molecules called olefins contain double bonds, or alkenes, between two carbon atoms. Typically, these atoms and their attached groups lie in the same 3D plane, and deviations from this structure are rare.

The rule being questioned, known as Bredt's rule, was established in 1924. It asserts that molecules cannot have a double bond at the "bridgehead" position—the junction of a bridged bicyclic molecule—because this position would distort the geometry of the double bond. Bredt's rule has constrained the design of synthetic molecules by preventing chemists from creating certain structures. Since olefins play a critical role in pharmaceutical research, Bredt's rule has limited the types of molecules that scientists could envision, potentially holding back innovations in drug discovery.

Researchers Break the Mold With Anti-Bredt Olefins

A new paper published on November 1 by UCLA scientists in the journal Science has invalidated that idea. They show how to make several kinds of molecules that violate Bredt's rule, called anti-Bredt olefins, or ABOs, allowing chemists to find practical ways to make and use them in reactions.

"People aren't exploring anti-Bredt olefins because they think they can't," said corresponding author Neil Garg, the Kenneth N. Trueblood Distinguished Professor of Chemistry and Biochemistry at UCLA. "We shouldn't have rules like this — or if we have them, they should only exist with the constant reminder that they're guidelines, not rules. It destroys creativity when we have rules that supposedly can't be overcome."

Practical Applications: Developing Useful Chemical Reactions

Garg's lab treated molecules called silyl (pseudo)halides with a fluoride source to induce an elimination reaction that forms ABOs. Because ABOs are highly unstable, they included another chemical that can "trap" the

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unstable ABO molecules and yield products that can be isolated. The resulting reaction indicated that ABOs can be generated and trapped to give structures of practical value.

"There's a big push in the pharmaceutical industry to develop chemical reactions that give three-dimensional structures like ours because they can be used to discover new medicines," Garg said. "What this study shows is that contrary to one hundred years of conventional wisdom, chemists can make and use anti-Bredt olefins to make value-added products."

Sci Tech Daily, 3 November 2024

https://scitechdaily.com

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<u>Environmental behavior and risk of the emerging organic contaminants</u> <u>halogenated carbazoles in chemical industrial park clusters</u>

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