CHEMWATCH

Bulletin Board

Contents

MAY. 31, 2024

(click on page numbers for links)

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GOSSIP

CURIOSITIES

TECHNICAL NOTES

CHEMWATCH
Bulletin Board
Contents
MAY. 31, 2024

ASIA PACIFIC

Japan Launches GHS Classification Information Collection Project, Requiring Companies to Provide Test Reports

2024-05-24

Recently, in order to strengthen the management of chemical substances, the Japanese government, in collaboration with the National Institute of Technology and Evaluation (NITE) and other relevant departments, has launched the GHS Classification Information Collection Project of 2024 Public-Private Cooperation. This project requires companies to provide test reports for chemical substances.

Since 2006, the Japanese government has implemented the GHS classification of chemical substances and has released the classification results for approximately 3,300 substances. However, due to the increasing variety of chemical substances and a lack of relevant testing information, more and more substances are unable to be effectively classified. This project aims to improve the information and enhance the accuracy and safety of chemical substance management.

1. The Substances to be Accepted must Meet the Following Conditions:

Target substances of the government GHS classification project

This includes substances scheduled for the current year's government GHS classification project as well as substances classified in previous years with results published by NITE.

Substances lacking reliable international information

Information sources are divided into three lists. List 1 includes information from Japanese laws and regulations or other international organizations. List 2 includes internationally recognized standards (such as OECD, etc.) and GLP (Good Laboratory Practice) test reports. List 3 includes non-GLP test reports and papers. If a substance lacks List 1 information, it is considered to lack reliable international information.

2. Test Information Required from Companies

Physical and chemical hazards of the substance

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 31, 2024

Testing methods shall comply with the international organizations or standard institutions such as the United Nations Recommendations on the Transport of Dangerous Goods (UNRTDG), the International Organization for Standardization (ISO), Japanese Industrial Standards (JIS), etc.

Human health hazards of the substance

Testing methods shall comply with the internationally recognized guidelines (such as OECD test guidelines). The tested substances shall have a certain purity, preferably conducted in GLP-compliant facilities.

Environmental hazards of the substance

Testing methods shall comply with the internationally recognized guidelines (such as OECD test guidelines). The tested substances shall have a certain purity, preferably conducted in GLP-compliant facilities.

Read More

CIRS, 24-05-24

https://www.cirs-group.com/en/chemicals/japan-launches-ghs-classification-information-collection-project-requiring-companies-to-provide-test-reports

Taiwan GHS: 22 Standards to Be Revised to Adopt UN GHS Rev.8

2024-05-20

Taiwan is undertaking a comprehensive update of the CNS 15030 serial standards, which are expected to be finalized and published by the end of 2024.

Taiwan's Bureau of Standards, Metrology and Inspection (BSMI) of the Ministry of Economic Affairs (MOEA) is responsible for revising CNS 15030 serial standards to align with UN GHS Rev.8. In addition to introducing a new hazard class for desensitized explosives, 21 out of the current 29 CNS 15030 serial standards will be updated.

Read More

Chemlinked, 20-05-24

https://chemical.chemlinked.com/news/chemical-news/taiwan-ghs-22-standards-to-be-revised-to-adopt-ghs-rev8

Chemicals added to the Inventory following issue of assessment certificate (early listing) - 24 May 2024

2024-05-24

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

Chemicals added to the inventory following issue of assessment certificate.

AICIS Approved Chemical Name (AACN)	Siloxanes and Silicones, di-Me, vinyl group-terminated, polymers with alkyl acrylate and branched alkyl acrylate
Defined Scope of Assessment	The chemical has been assessed: as a polymer meeting the polymer of low concern (PLC) definition (Schedule 2 of the Industrial Chemicals (General) Rules 2019) and as a polymer that is not a high molecular weight polymer that has lung overloading potential (within the meaning given by the Industrial Chemicals Categorisation Guidelines) as a component of lubricants
Listing date	17 May 2024
CAS number	71119-07-8
Chemical name	Phenol, 2-ethoxy-4-(ethoxymethyl)-
Molecular formula	C11H16O3

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 31, 2024

AICIS Approved Chemical Name (AACN)	Siloxanes and Silicones, di-Me, vinyl group-terminated, polymers with alkyl acrylate and branched alkyl acrylate
Defined Scope of Assessment	The chemical has been assessed: as a fragrance component imported into Australia at up to 1 tonne/year as imported in fragrance formulations at up to 1% concentration for reformulation into continuous action air fresheners and fine fragrances at up to 0.5% concentration, instant action air fresheners at up to 0.1% concentration, and other cosmetic and household products at up to 0.02% concentration as imported in end use cosmetic and household products at up to 0.5% concentration in continuous action air fresheners and fine fragrances, up to 0.1% concentration in instant action air fresheners, and up to 0.02% concentration in other cosmetic and household products
Listing date	22 May 2024

Published date: 24 May 2024

Read More

AICIS, 24-05-24

https://www.industrialchemicals.gov.au/news-and-notices/chemicals-added-inventory-following-issue-assessment-certificate-early-listing-24-may-2024

AMERICA

Toxic Downpour: "Forever Chemicals" Rain on All Five Great Lakes

2024-05-18

A study on PFAS in the Great Lakes shows uniform pollution levels from precipitation and differing rates of chemical removal across the lakes, emphasizing the need for enhanced regulatory measures.

Perfluoroalkyl and polyfluoroalkyl substances (PFAS), commonly referred to as "forever chemicals," are enduring environmental contaminants

found in air, water, and soil. Their chemical stability allows them to circulate through the water cycle, infiltrating sources of drinking water and precipitation. Research reported in the American Chemical Society's journal Environmental Science & Technology indicates that precipitation deposits roughly equal quantities of PFAS into each of the Great Lakes; however, the lakes eliminate the chemicals at different rates.

Consuming PFAS has been linked to negative health outcomes. And in April 2024, the U.S. Environmental Protection Agency (EPA) designated two forever chemicals — PFOS and PFOA — as hazardous substances, placing limits on their concentrations in drinking water. The Great Lakes are a major freshwater source for both the U.S. and Canada, and the EPA reports that the surrounding basin area is home to roughly 10% and 30% of each country's population, respectively. Previous studies demonstrated that these lakes contain PFAS. But Marta Venier at Indiana University and colleagues from the U.S. and Canada wanted to understand where the compounds come from and where they go.

Research Methodology and Findings

Between 2021 and 2022, 207 precipitation samples and 60 air samples were taken from five sites surrounding the Great Lakes in the U.S.: Chicago; Cleveland; Sturgeon Point, N.Y.; Eagle Harbor, Mich.; and Sleeping Bear Dunes, Mich. During the same period, 87 different water samples were collected from the five Great Lakes. The team analyzed all the samples for 41 types of PFAS and found.

Read More

Sci Tech Daily, 18-05-24

https://scitechdaily.com/toxic-downpour-forever-chemicals-rain-on-all-five-great-lakes/

Register for EPA Webinars on Reducing Lead Exposure in Your Community

2024-05-23

Join the U.S. Environmental Protection Agency (EPA) for webinars on the dangers of lead and ways to reduce and prevent lead exposure. The webinars will focus on the Lead Awareness Curriculum, an adaptable resource for educating and protecting communities from potential lead exposure.

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 31, 2024

These webinars are intended for community leaders with experience educating and training members of their communities. The webinars will teach attendees how to use and modify theLead Awareness Curriculumto educate their communities about lead, lead exposure, and actions to reduce and prevent childhood lead exposure. Prior knowledge of lead or lead exposure is not needed to use the curriculum and attendees will receive a digital certificate of participation after completing the session.

Read More

US EPA, 23-05-24

https://www.epa.gov/lead/final-strategy-reduce-lead-exposures-and-disparities-us-communities

EPA Finalizes New Rule Clarifying Public Awareness of Water Quality

2024-05-17

The U.S. Environmental Protection Agency (EPA) announced a new regulation to make annual drinking water quality reports more accessible and understandable for the public. This initiative, set to take effect in 2027, will enhance the clarity of these reports, support translation into various languages and provide more detailed information about lead contamination.

According to a recent release, the EPA's final rule will ensure that water systems serving over 10,000 customers distribute these reports twice annually. Currently, these systems are required to deliver reports only once a year. The rule also encourages electronic delivery methods.

"EPA is taking action today to help ensure that the American public has improved access to information about the drinking water in their communities by strengthening requirements for annual drinking water quality reports," acting Assistant Administrator for EPA's Office of Water Bruno Pigott said in a statement. "Today's announcement will ensure these reports are easier to understand and easier to access in additional languages to provide all people with the information they want and need about their water."

This regulatory update is part of the broader effort under the America's Water Infrastructure Act of 2018, which tasked the EPA with revising the Consumer Confidence Report Rule. These reports, also known as Drinking Water Quality Reports, inform residents about the quality of their local

drinking water and any contaminants present. The new rule includes a reporting requirement that mandates states to submit compliance monitoring data annually to the EPA.

In improving these reports, the EPA aims to support the Safe Drinking Water Act's "right-to-know" provisions, enabling the public to make better decisions in general.

Read More

Environmental Protection, 17-05-24

https://eponline.com/Articles/2024/05/17/EPA-Finalizes-New-Rule-Clarifying-Public-Awareness-of-Water-Quality.aspx

Minister Guilbeault imposes strict benzene pollution controls in the pursuit of environmental justice for Aamjiwnaang First Nation and Sarnia, Ontario

2024-05-17

Minister Guilbeault issued an Interim Order to the petrochemical industry in Sarnia, Ontario, responding to the significant danger to human health of volatile organic compounds, including benzene, originating from these facilities.

Aamjiwnaang First Nation and Sarnia have experienced poor air quality conditions that have spiked in recent months, according to monitoring done by Environment and Climate Change Canada, the Province of Ontario, and Aamjiwnaang First Nation. The high levels of toxic air pollution led to the closure of the Aamjiwnaang's Band Office and community services buildings, including their daycare and resource centre. The situation can lead to a variety of serious health issues for local residents and merits an immediate response to protect the community.

This is why Minister Guilbeault has published an Interim Order under existing authorities in the Canadian Environmental Protection Act. These efforts are also consistent with Canada's commitments in relation to the United Nations Declaration of the Rights of Indigenous Peoples.

The Order requires that petrochemical production facilities in Sarnia with fenceline concentrations of benzene above 29 micrograms per cubic metre (µg/m3) measured in any of the two-week sampling periods beginning on March 1, 2023, and ending on February 29, 2024, at any sampling location established in accordance with Ontario regulations

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 31, 2024

implement vapour-control measures, including fully closed vent systems with vapour control on certain storage tanks that store benzene. The Order will be in effect for 14 days, pending Governor in Council approval, which would extend the Order for up to two years. The Order is complementary to the Government of Ontario's efforts to reduce benzene pollution in Sarnia. The Aamjiwnaang First Nation community, which is bordered by Sarnia's refinery and petrochemical district, will directly benefit from this Order, which will reduce benzene emissions and their accompanying health impacts.

The Government of Canada is also releasing a "what we heard" public consultation update on the proposed Reduction in the Release of Volatile Organic Compounds (Storage and Loading of Volatile Petroleum Liquids) Regulations that informed the Interim Order. The government thoroughly consulted with Aamjiwnaang First Nation, other Indigenous peoples, industry, provinces and territories, and other stakeholders in drafting these regulations. These proposed Regulations are designed to further reduce emissions of volatile organic compounds, including benzene, from the petroleum and petrochemical industry in Canada. The Government of Canada is now working to finalize the Regulations in the months ahead. Once finalized, the Regulations would apply to terminals, refineries, upgraders, petrochemical facilities, and bulk fuel facilities that store volatile petroleum liquids in tanks that meet or exceed a specified capacity or load and unload volatile petroleum liquids that exceed a specified daily or annual quantity. The Regulations would set a timeline to install abatement equipment and would also further reduce air pollution from hundreds of sources across Canada.

Read More

Government of Canada, 17-05-24

https://www.canada.ca/en/environment-climate-change/news/2024/05/minister-guilbeault-imposes-strict-benzene-pollution-controls-in-the-pursuit-of-environmental-justice-for-aamjiwnaang-first-nation-and-sarnia-ontario.html

Brazil – New technical regulation on materials in contact with food

2024-04-09

The National Health Surveillance Agency (ANVISA in Portuguese) has published Resolution RDC No. 854/2024 on Provides requirements for

sanitary conditions applicable to packaging, coatings, utensils, lids and metal equipment intended to come into contact with food.

This Technical Regulation applies to packaging, coatings, utensils, utensils, lids and equipment made of metal materials, coated or uncoated, that come into contact with food and its raw materials during production, preparation, transport, distribution and storage. Printing inks, varnishes on tableware and enamels used on the external surface shall not be subject to the provisions of these regulations, provided that they do not come into direct contact with food, nor with the user's mouth in the form of habitual use.

Read More

OFFICIAL DIARY OF THE UNION, 09-04-2024

https://www.in.gov.br/en/web/dou/-/resolucao-da-diretoria-colegiada-rdc-n-854-de-4-de-abril-de-2024-552792277

EUROPE

Environmental groups call for a new EU deal: green, social and fit for a one-planet economy

2024-05-13

A new deal for Europe

Calls for an Industrial Deal in the Antwerp Declaration and demands for social rights made by the La Hulpe Declaration are yet the latest indicators that relevant EU actors envisage the need for a new deal. Meanwhile, Heads of State prepare the Strategic Agenda that will guide the EU's priorities for the next five years. Yet, these high-level debates fail to acknowledge the environmental dimension – and that long-term sustainability needs to underpin our social and economic policy.

The upcoming EU mandate requires a comprehensive approach that integrates environmental concerns with social and economic priorities. Without addressing the interconnected climate, biodiversity and pollution crises, any other pact, deal or declaration would be incomplete and a gross oversight on the side of EU leaders. Extreme weather events, critical changes to earth systems, biodiversity loss and shortage of natural resources are already threatening us and will starkly increase in the next ten years.

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 31, 2024

This is why we developed, in consultation with civil society and with decision makers across Member States, the European institutions and wider stakeholders, a European Pact for the Future to offer an agenda of hope, an actionable and viable programme for our common future, and transformational change without leaving anyone behind.

Patrick ten Brink, Secretary General at the EEB said:

"The ongoing triple crisis on pollution, climate and biodiversity, and the increasing frequency of resource-related conflicts, are at the heart of all the challenges facing Europe today. All of our priorities depend on our success in tackling this question.

Europe cannot give up on its position as a global environmental leader. In fact, its competitive strength lies in its forward-looking policy agenda, rooted in robust social and environmental standards– we should not undermine this; we should build on it. The European Green Deal was a starting point, catalysing part of the transformational change we need, strengthening the EU's international credibility, and was proving to be a tool for EU competitiveness globally – we should move further. Don't stop now."

Read More

European Environmental Bureau, 13-05-24

https://eeb.org/environmental-groups-call-for-a-new-eu-deal-green-social-and-fit-for-a-one-planet-economy/

Toy safety: Council adopts position on updated rules

2024-05-15

The Council has adopted its position (negotiating mandate) on the toy safety regulation that updates the rules to protect children from risks related to the use of toys. While the current legislation makes EU toy safety rules among the strictest in the world, the proposed legislation aims to increase protection from harmful chemicals (e.g. endocrine disruptors) and reinforce the enforcement rules with a new digital product passport.

The Council position supports the general objectives of the proposal but introduces several improvements to clarify the obligations of economic operators and online marketplaces; it sets out the contents of the digital product passport and warnings and increases the number of substances whose presence in toys is prohibited.

Although the current rules are amongst the safest in the world, under the Belgian Presidency, we managed to strengthen the requirements for economic operators and providers of online marketplaces. Particular safety requirements, including chemical requirements, have been enhanced, refining new or existing risks. Safety of toys deserves our utmost attention and we should certainly keep protecting our children from non-compliant products being manufactured or imported.

Pierre-Yves Dermagne, Belgian Deputy Prime Minister and Minister for the Economy and Employment

Commission proposal: protection from chemicals and the digital passport

The negotiating mandate adopted today sets out the Council's position on a proposal tabled by the Commission in July 2023. The Commission proposal for a toy safety regulation aims to update the existing directive with measures to increase protection from harmful chemical products, expanding the ban on carcinogenic, mutagenic and products toxic for reproduction (CMRs) to other dangerous chemical products such as endocrine disruptors and chemicals that affect the respiratory system or other organs.

The proposed legislation aims to reduce the number of non-compliant and unsafe toys on the EU market by strengthening the enforcement of the legal requirements, in particular for imported toys. The Commission proposal introduces a digital product passport (DPP) that will include information on the safety of the toy, so that border control authorities can scan all digital passports using a new IT system. The Commission will be able to update the regulation and order the removal of certain toys from the market if any new risks not provided for in the current text arise in future.

Council position: Obligations of economic operators

In the Council's negotiating mandate, the obligations of economic operators have been aligned with the general product safety regulation (GPSR) and with the new realities of the increasing volume of online sales.

To that end, manufacturers will be required to mark the warnings in a language or languages that can be easily understood by consumers and other end-users, as determined by Member States. Manufacturers will also have to inform other economic operators in the distribution chain of any product conformity issues. Furthermore, toy importers will have to inform the producer and the market surveillance authorities if they suspect that

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 31, 2024

a toy presents a risk. The Council mandate also clarifies the obligations of 'fulfilment service providers' (the companies that take care of the logistical elements of selling products, such as warehousing, picking, packaging or shipping). They are considered economic operators, since fulfilment service providers play an important role in the placing of toys on the market, and in particular toys from third countries or those purchased online. Their obligations will be limited to their role in the supply chain.

Providers of online marketplaces

The Council position considers that providers of online marketplaces play an important role when intermediating the sale or promotion of toys between traders and consumers. Therefore, toys that do not conform with the toy safety regulation will be regarded as illegal content for the purposes of the digital services act (DSA). The negotiating mandate also sets out toy-specific obligations for providers of online marketplaces, in addition to those required by the existing legal framework (like the DSA and the GPSR). For instance, it requires that the interfaces of online marketplaces be designed and organised in a way that allows economic operators to display the CE marking, any warning necessary for the consumer prior to purchase and the weblink or data carrier (i.e. QR or bar code) which provides a link to the digital product passport.

Digital product passport and warnings

The negotiating mandate further aligns the provisions related to the digital product passport with the ecodesign for sustainable products regulation (ESPR). The Council position introduces a definition of 'digital product passport' to clarify what information must be contained in the digital product passports and the technical characteristics of the data carrier. The scope of the technical requirements relating to the digital product passport for toys will be determined by the implementing acts adopted by the Commission.

The Council position also clarifies the requirements as regards the minimum size, visibility and legibility of warning notices, so that they are visually accessible to the general population.

Chemicals

The Council position aligns the toy safety regulation with the regulation on the classification, labelling and packaging (CLP) of chemical products. To that end, it limits the general ban on the presence of substances classified as carcinogenic, mutagenic or toxic for reproduction (CMR

substances) in toys to those that have been subject to harmonised classification. Furthermore, it introduces a ban on certain categories of skin sensitisers (chemical substances that provoke an allergic response following skin contact), a ban on toys that have a biocidal function, and a ban on the treatment of toys with biocidal products (except for toys that are intended to be placed permanently outdoors). Biocidal products are substances including preservatives, insecticides, disinfectants and pesticides used for the control of harmful organisms. Certain preservatives are allowed in some kind of toy materials.

Finally, as regards allergenic fragrances, the negotiating mandate updates the specific rules governing their use in toys (including a prohibition on the intentional use of fragrances in toys), as well as the labelling of certain allergenic fragrances.

Read More

Council of the European Union, 15-05-24

https://www.consilium.europa.eu/en/press/press-releases/2024/05/15/toy-safety-council-adopts-position-on-updated-rules/

Upcoming GB active substance expiry dates

2024-05-23

The active substance/product type combinations listed below are due to expire under the GB BPR on the following dates:

- 1-[[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolan-2-yl]methyl]-1H-1,2,4-triazole (Propiconazole) (CAS 60207-90-1 EC 262-104-4) in product type 9

31 May 2025

- Carbon dioxide (CAS 124-38-9 EC 204-696-9) in product type 15

31 May 2025

- Iodine (CAS 7553-56-2 EC 231-442-4) in product types 1, 4 and 22

31 August 2025

- n-decanoic acid (Decanoic acid) (CAS 334-48-5 EC 206-376-4) in product types 18 and 19

31 August 2025

- n-octanoic acid (Octanoic acid) (CAS 124-07-2 EC 204-677-5) in product type 18

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 31, 2024

31 August 2025

- Polyvinylpyrrolidone iodine (CAS 25655-41-8 EC 607-771-8) in product type 1, 4 and 22

31 August 2025

Once the approvals expire, the active substances will no longer be able to be used in biocidal products of the relevant product types in GB. In addition articles treated with such products will no longer be able to be placed on the market in GB.

If you hold an affected GB BPR product authorisation or Control of Pesticides Regulations (COPR) product approval, we will contact you about cancelling or revoking your authorisation or approval. You will have an opportunity to submit comments or additional information and we will take account of these when finalising our decision.

If you are aware of any disproportionate negative impacts that are likely to arise from the expiry of any of the active substance/product type combinations listed above, please contact us.

Read More

UK HSE, 23-05-24

https://www.hse.gov.uk/biocides/index.htm

GB active substance expiry dates postponed

2024-05-24

Active substance expiry dates postponed in GB until 31 January 2027

As previously updated, the active substance expiry dates for all biocidal active substance/product type combinations which expire between 1 January 2024 – 31 December 2026, are able to be postponed until 31 January 2027. The expiry date postponements are subject to a timely renewal application being submitted and accepted.

The requirements have now been met for the active substance/product type combinations listed below:

- Azoxystrobin (CAS 131860-33-8 EC 603-524-3) in product types 7, 9 and 10

From 31 October 2025 to 31 January 2027

- Ethyl butylacetylaminopropionate (CAS 52304-36-6 EC 257-835-0) in product type 19

From 31 October 2025 to 31 January 2027

- Transfluthrin (CAS 118712-89-3 EC 405-060-5) in product type 18

From 31 October 2025 to 31 January 2027

- Nonanoic acid (CAS 112-05-0 EC 203-931-2) in product type 2

From 30 September 2025 to 31 January 2027

Read More

UK HSE, 23-05-24

https://www.hse.gov.uk/biocides/index.htm

CHEMWATCH
Bulletin Board

Harmonised classification and labelling consultations

2024-05-22

Parties concerned are invited to comment on hazard classes open for consultation, which are indicated in the substance table below.

The indicated hazard classes were assessed and concluded by the dossier submitter in their proposal for harmonised classification and labelling (CLH) of the substance.

A hazard class may be open for commenting even if the dossier submitter did not conclude that it warrants a classification. The CLH consultation lasts for 60 days (unless specified otherwise).

Name	EC Number	CAS Number	Hazard classes	Start of	Deadline for	
	208-826-5 [1] 233-195-8 [2] 431-460-4 [3]	542-75-6 [1] 10061-01-5 [2] 10061-02-6 [3]	Physical hazards			Details
propyl	247-125-9	25606-41-1				

Read More

ECHA, 22-05-24

https://echa.europa.eu/harmonised-classification-and-labelling-consultation

Commission adopts EU-wide restriction on cyclosiloxanes

2024-05-24

On 16 May 2024, the European Commission adopted a restriction on siloxanes D4, D5 and D6. This measure will protect our environment by reducing up to 90 % of the emissions of these very persistent and very bioaccumulative substances. The restriction will start applying after 6 June 2026.

D4, D5, and D6 are used in various consumer and professional products, including cosmetics, dry cleaning, waxes and washing and cleaning products.

REACH Update

MAY. 31, 2024

The restriction proposal was prepared by ECHA in January 2019. The scientific committees for Risk Assessment and Socio-Economic Analysis supported the proposal in their 2020 opinions.

Read More

ECHA, 23-05-24

https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=OJ%3AL_202401328&qid=1715919472757#msdynttrid=piE2SWc4qZ1vey2B87b08gF8UbZD6Ee5YMF_hIlNPKw

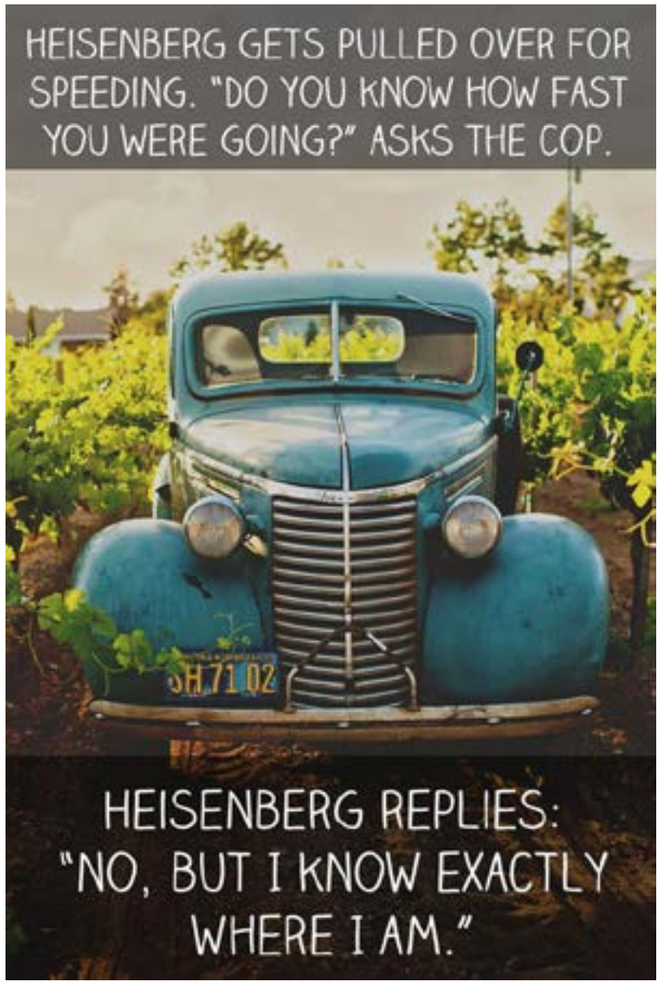
CHEMWATCH
Bulletin Board

Janet's Corner

MAY. 31, 2024

Speeding Heisenberg

2024-05-31



https://www.buzzfeed.com

Dibenzofuran

2024-05-31

USES [2,3]

Dibenzofuran is used as an insecticide and to make other chemicals.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Exposure Sources

- Dibenzofuran has been detected in emissions from combustion of coal, biomass, refuse, diesel fuel, and tobacco.
- It is also found in leachates from commercial coal tar and is formed from the incomplete combustion of propane.
- Dibenzofuran also is a photolytic product of environmental photolysis of chlorinated biphenyl ethers in surface waters by sunlight.
- The primary stationary sources that have reported emissions of dibenzofuran in California are lumber and wood products manufacturers, and manufacture of fabricated metal ordnance and accessories.
- It may be found in coke dust, grate ash, fly ash, and flame soot.

Routes of Exposure

- Occupational exposure may occur through inhalation and dermal contact, particularly at sites engaged in combustion/carbonisation processes, such as coal tar and coal gasification operations.
- Dibenzofuran is released to the ambient air from combustion sources. The general public may be exposed to dibenzofuran through the inhalation of contaminated air or through the consumption of contaminated drinking water or food.
- Since it has been found in tobacco smoke, you can be exposed if you smoke cigarettes or breathe cigarette smoke.

HEALTH EFFECTS [4]

Acute Health Effects

- Dibenzofuran causes skin irritation.
- Exposure to dibenzofuran can irritate the eyes, nose and throat.

Dibenzofuran is a heterocyclic organic compound with the molecular formula C12H8O. It is an aromatic compound that has two benzene rings fused to a central furan ring. All the numbered carbon atoms have a hydrogen atom bonded to each of them. It is a volatile white solid that is soluble in non-polar organic solvents. Dibenzofuran is created from the production of coal tar. [1,2]

CHEMWATCH
Bulletin Board
Hazard Alert
MAY. 31, 2024

Carcinogenicity

Dibenzofuran has not been tested for its ability to cause cancer in animals. The U.S. Environmental Protection Agency has determined that there is not enough information available to classify dibenzofuran as a cancer causing substance.

Other Effects

Repeated contact with Dibenzofuran can cause:

- Skin growths;
- Rashes (may be made worse by exposure to sunlight); and
- Changes in skin colour.

SAFETY

First Aid Measures [5]

- **Inhalation:** If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
- **Skin Contact:** Wash off with soap and plenty of water. Consult a physician.
- **Eye Contact:** Flush eyes with water as a precaution.
- **Ingestion:** Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Workplace Controls & Practices [4]

- Ensure there are appropriate engineering controls in place.
- Handle in accordance with good industrial hygiene and safety practice.
- Wash hands before breaks and at the end of workday.

Personal Protective Equipment [5]

The following personal protective equipment is recommended when handling dibenzofuran:

Eye/face Protection:

- Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin Protection:

- Handle with gloves.

- Gloves must be inspected prior to use.
- Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product.
- Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices.
- Wash and dry hands.
- The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.
- Full contact Material: Nitrile rubber

Body Protection:

- Complete suit protecting against chemicals.
- The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory Protection:

- For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator.
- For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges.
- Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

REGULATION

United States

No occupational exposure limits have been established by dibenzofuran.

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CHEMWATCH
Bulletin Board
Hazard Alert
MAY. 31, 2024

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Carbon Nanotube Yarns Generate Electricity from Waste Heat

2024-05-30

In line with global efforts towards sustainability, the development of energy harvesting technologies has become a top research priority. Although renewable energy sources like wind and solar power have recently taken the spotlight, waste heat also stands as a largely untapped source of energy. Using thermoelectric materials, industrial waste heat can be harvested and converted into electrical energy, which can help increase the efficiency of industrial processes.

Unfortunately, this approach is less straightforward for "low-grade" waste heat (waste heat reaching temperatures below 200 °C). The main problem is that the thermoelectric materials available at this temperature range are quite limited. Most thermoelectric inorganic materials are either toxic, prohibitively expensive to produce, or too rigid for applications that call for flexibility (such as wearable electronics).

Against this backdrop, a research team including Research Associate Professor Hiroo Suzuki from Okayama University, Japan, have been studying the application of carbon nanotube (CNT) yarns in thermoelectric conversion. In a recent study, whose findings were , they addressed a major roadblock in this particular area: the lack of high-performance n-type CNT yarns (CNT yarns with an excess of electrons) for low-grade waste heat, as opposed to p-type CNT yarns (yarns with excess of positive charge carriers). This paper was co-authored by Jun Kametaka, Takeshi Nishikawa, and Yasuhiko Hayashi, all from Okayama University.

"Constructed from CNTs, CNT yarns are well-suited for practical applications as the yarn-like structure allows for the fabrication of flexible thermoelectric devices such as fabric-based modules," explains Dr. Suzuki. "Although recent reports have showcased p-type CNT yarns with a remarkable thermoelectric power factor, the absence of similar n-type CNT yarns imposes limitations for device configurations involving π-type modules, which require both p- and n-type CNTs to achieve high efficiency."

To tackle the abovementioned problem, the research team sought to establish a novel doping (impurity addition) method to efficiently produce n-type CNT yarns. They selected 4-(1, 3-dimethyl-2, 3-dihydro-1H-benzimidazole-2-yl) phenyl) dimethylamine (N-DMBI) as a promising dopant owing to its high stability in air, which is essential in most practical applications.

CHEMWATCH
Bulletin Board
Gossip
MAY. 31, 2024

First, the researchers spun CNT yarns using a dry spinning technique. These yarns then underwent a "Joule annealing process," which subjects the material to an electric current until it reaches a precisely controlled high temperature. The logic underlying this processing step is that the transient heat increases the crystallinity of the CNTs, thus reducing their thermal conductivity. In turn, this improves their thermoelectric performance. Moreover, Joule annealing greatly enhances the mechanical properties of the yarn.

Next, the team sought to establish an optimal N-DMBI doping protocol for the CNT yarns. "The optimization of the doping process involved rigorous selection of a suitable solvent. We evaluated ten different options, including nonpolar solvents, polar aprotic solvents, and polar protic solvents," comments Dr. Suzuki. "We ultimately identified o-dichlorobenzene as the most suitable solvent for N-DMBI doping at low temperatures, based on an analysis of the resulting Seebeck coefficient of the CNT yarns."

After extensive experimentation, the team reported that the annealed, n-doped CNT yarns achieved a remarkably high thermoelectric power factors within temperatures ranging from 30 to 200 °C, along with a high figure of merit (a numerical expression representing the performance or efficiency of a material). They further tested this n-type material in a prototype π-type thermoelectric generator, which could produce electricity even at only 55 °C and a temperature difference of 20 °C.

"Achieving power generation at low temperatures with small temperature differences is significant for the development of thermoelectric modules that can tap into various thermal sources, such as waste heat from industrial facilities, thermal dissipation from vehicles, and even body heat," remarks Dr. Suzuki. "Our research can thus help address energy problems faced by society, contributing to energy saving through the efficient use of otherwise wasted energy. Furthermore, thermoelectric generators can be used as a local energy source to drive IoT devices, such as flexible health sensors."

Overall, the insights obtained through this study will lead to the development of better organic thermoelectric materials, paving the way for more efficient energy harvesting from waste heat. Further efforts

in this field can ultimately contribute to our collective stride towards sustainability.

Technology Networks, 30 May 2024

https://technologynetworks.com

New method uses light to enable the generation of non-canonical amino acids

2024-05-30

UC Santa Barbara researchers are building out the repertoire of chemical reactions, using light. In a paper published in the journal Nature, chemistry professor Yang Yang and collaborators at the University of Pittsburgh report a method using photobiocatalysis to produce non-canonical (not naturally occurring) amino acids that are valuable building blocks of peptide therapeutics, bioactive natural products and novel functional proteins.

"So many efforts have been made in the field of biocatalysis, and we are now at a point where we can rationally design entirely new enzymatic reactions which are unprecedented in either chemistry or biology," Yang said.

Most efforts in the field of biocatalysis, or the acceleration of chemical reactions via enzymes—nature's privileged catalysts—have leaned toward optimizing natural enzyme functions that are useful to synthetic chemistry, or repurposing natural enzymes to facilitate unnatural reactions known to synthetic chemistry. Despite a decade of extensive research, there are only a handful of examples of enzymatic reactions that are both new-to-nature and new-to-synthetic chemistry.

"What we are interested in is essentially to discover entirely new enzymatic reactions and general modes of enzyme catalysis," Yang added.

Enter photobiocatalysis, in which light is used to excite enzymes to generate energy (often in the form of free radicals) to convert one molecule into another. A relatively young field of chemistry, photobiocatalysis takes advantage of the selectivity and efficiency of enzymes and combines that with the versatility and sustainability of light to create new processes, and in this case, non-canonical amino acids.

CHEMWATCH
Bulletin Board
Gossip
MAY. 31, 2024

Interacting catalytic processes

For this study, the research team focused on pyridoxal-phosphate (PLP)-dependent enzymes, a large family of enzymes responsible for the metabolism of amino acids. The team developed an interacting, triple catalytic cycle in which a photocatalyst—an iridium-based compound—is exposed to light, initiating a process that generates a transient free radical, while a second cycle using light regenerates the photocatalyst.

Concurrently, the biocatalysis cycle using a PLP enzyme modifies the amino acid substrate via a series of activation steps unique to PLP biochemistry. The free radical generated from photochemistry comes into play here, entering the enzyme active site and engaging the enzymatic intermediate to enable new chemistry. This cooperation between the enzyme and the photocatalyst allows the production of a non-canonical amino acid product.

The altering of—in this case—common amino acid molecular structures adds new features and capabilities to these acids. In creating a new carbon-carbon bond to the critical "alpha carbon," of the amino acid, Yang said, it becomes possible to use this "backbone" to design a range of novel amino acids that could in turn perform new, unique and desirable functions as the basis of new therapeutics and natural products.

"This is the first demonstration of pyridoxical biocatalysis via radical-mediated alpha functionalization of abundant amino acid substrates," Yang pointed out.

Additionally, the highly efficient process is both stereoselective, meaning it can select for a preferred three-dimensional "shape" of the resulting amino acid, and it eliminates the extra steps of adding and removing "protecting groups," or compounds that mask certain reactive areas on molecules to prevent unwanted chemical reactions in those regions.

"We've uncovered interesting interactions between the photocatalyst and the enzyme," said Yang, whose group is studying how to further improve the interactions between the two catalysts. "I think this is going to lead to new fundamental science, both from a synthetic chemistry standpoint and also an enzymology standpoint."

Phys Org, 30 May 2024

https://phys.org

Promethium Discovery Set to Rewrite Chemistry Textbooks

2024-05-29

Scientists have made a significant breakthrough in understanding the properties of promethium, a rare earth element with elusive characteristics despite its use in modern technology.

Researchers have uncovered the properties of a rare earth element that was first discovered 80 years ago at the very same laboratory. Their discoveries open a new pathway for the exploration of elements critical in modern technology, from medicine to space travel.

Promethium was discovered in 1945 at Clinton Laboratories, now the Department of Energy's Oak Ridge National Laboratory, and continues to be produced at ORNL in minute quantities. Some of its properties have remained elusive despite the rare earth element's use in medical studies and long-lived nuclear batteries. It is named after the mythological Titan who delivered fire to humans and whose name symbolizes human striving.

Groundbreaking Research at ORNL

"The whole idea was to explore this very rare element to gain new knowledge," said Alex Ivanov, an ORNL scientist who co-led the research. "Once we realized it was discovered at this national lab and the place where we work, we felt an obligation to conduct this research to uphold the ORNL legacy."

The ORNL-led team of scientists prepared a chemical complex of promethium, which enabled its characterization in solution for the first time. Thus, they exposed the secrets of this extremely rare lanthanide, whose atomic number is 61, in a series of meticulous experiments.

Their landmark study, published on May 22 in the journal Nature, marks a significant advance in rare earth research and might rewrite chemistry textbooks.

Characteristics of Lanthanides

"Because it has no stable isotopes, promethium was the last lanthanide to be discovered and has been the most difficult to study," said ORNL's Ilja Popovs, who co-led the research. Most rare earth elements are lanthanides, elements from 57 — lanthanum — to 71 — lutetium — on the periodic table. They have similar chemical properties but differ in size.

CHEMWATCH
Bulletin Board
Gossip
MAY. 31, 2024

The other 14 lanthanides are well understood. They are metals with useful properties that make them indispensable in many modern technologies. They are workhorses of applications such as lasers, permanent magnets in wind turbines and electric vehicles, X-ray screens and even cancer-fighting medicines.

"There are thousands of publications on lanthanides' chemistry without promethium. That was a glaring gap for all of science," said ORNL's Santa Jansone-Popova, who co-led the study. "Scientists have to assume most of its properties. Now we can actually measure some of them."

Unique Research Capabilities

The research relied on unique resources and expertise available at DOE national laboratories. Using a research reactor, hot cells and supercomputers, as well as the accumulated knowledge and skills of 18 scientists in different fields, the authors detailed the first observation of a promethium complex in solution.

The ORNL scientists bound, or chelated, radioactive promethium with special organic molecules called diglycolamide ligands. Then, using X-ray spectroscopy, they determined the properties of the complex, including the length of the promethium chemical bond with neighboring atoms — a first for science and a longstanding missing piece to the periodic table of elements.

Promethium is very rare; only about a pound occurs naturally in the Earth's crust at any given time. Unlike other rare earth elements, only minute quantities of synthetic promethium are available because it has no stable isotopes.

For this study, the ORNL team produced the isotope promethium-147, with a half-life of 2.62 years, in sufficient quantities and at a high enough purity to study its chemical properties. ORNL is the United States' only producer of promethium-147.

Notably, the team provided the first demonstration of a feature of lanthanide contraction in solution for the whole lanthanide series, including promethium, atomic number 61. Lanthanide contraction is a phenomenon in which elements with atomic numbers between 57 and 71 are smaller than expected. As the atomic numbers of these lanthanides increase, the radii of their ions decrease. This contraction creates distinctive chemical and electronic properties because the same charge is limited to a shrinking space. The ORNL scientists got a clear promethium

signal, which enabled them to better define the shape of the trend — across the series.

"It's really astonishing from a scientific viewpoint. I was struck once we had all the data," said Ivanov. "The contraction of this chemical bond accelerates along this atomic series, but after promethium, it considerably slows down. This is an important landmark in understanding the chemical bonding properties of these elements and their structural changes along the periodic table."

Many of these elements, such as those in the lanthanide and actinide series, have applications ranging from cancer diagnostics and treatment to renewable energy technologies and long-lived nuclear batteries for deep space exploration.

Implications for Technology and Science

The achievement will, among other things, ease the difficult job of separating these valuable elements, according to Jansone-Popova. The team has long worked on separations for the whole series of lanthanides, "but promethium was the last puzzle piece. It was quite challenging," she said. "You cannot utilize all these lanthanides as a mixture in modern advanced technologies, because first you need to separate them. This is where the contraction becomes very important; it basically allows us to separate them, which is still quite a difficult task."

The research team used several premier DOE facilities in the project. At ORNL, promethium was synthesized at the High Flux Isotope Reactor, a DOE Office of Science user facility, and purified at the Radiochemical Engineering Development Center, a multipurpose radiochemical processing and research facility. Then, the team performed X-ray absorption spectroscopy at the National Synchrotron Light Source II, a DOE Office of Science user facility at DOE's Brookhaven National Laboratory, specifically working at the Beamline for Materials Measurement, which is funded and operated by the National Institute of Standards and Technology.

The team also performed quantum chemical calculations and molecular dynamics simulations at the Oak Ridge Leadership Computing Facility, a DOE Office of Science user facility at ORNL, using the lab's Summit supercomputer, the only computational resource capable of providing the necessary calculations at the time. In addition, the researchers used resources of the Compute and Data Environment for Science at ORNL. They expect future calculations to be performed on ORNL's Frontier, the

CHEMWATCH
Bulletin Board
Gossip
MAY. 31, 2024

world's most powerful supercomputer and the first exascale system, which is able to perform more than a quintillion calculations each second.

Popovs emphasized that the ORNL-led accomplishments can be attributed to teamwork. Each of the Nature paper's 18 authors was critical to the project, he said.

The achievement sets the stage for a new era of research, the scientists said. "Anything that we would call a modern marvel of technology would include, in one shape or another, these rare earth elements," Popovs said. "We are adding the missing link."

Sci Tech Daily, 29 May 2024

https://scitechdaily.com

Researchers create materials with unique combo of stiffness, thermal insulation

2024-05-29

Researchers have demonstrated the ability to engineer materials that are both stiff and capable of insulating against heat. This combination of properties is extremely unusual and holds promise for a range of applications, such as the development of new thermal insulation coatings for electronic devices.

"Materials that have a high elastic modulus tend to also be highly thermally conductive, and vice versa," says Jun Liu, co-corresponding author of a paper on the work and an associate professor of mechanical and aerospace engineering at North Carolina State University. "In other words, if a material is stiff, it does a good job of conducting heat. And if a material is not stiff, then it is usually good at insulating against heat.

"But there are instances where you'd want materials that are stiff, but are also good insulators," Liu says. "For example, you might want to create thermal insulation coatings to protect electronics from high temperatures. Historically, that's been a challenge.

"We've now discovered a range of materials that are both stiff and excellent thermal insulators. What's more, we can engineer the materials as needed to control how stiff they are and how thermally conductive they are."

Specifically, the researchers were working with a subset of the class of materials called two-dimensional hybrid organic-inorganic perovskites (2D HOIP).

"These are thin films consisting of alternating organic and inorganic layers in a highly ordered crystalline structure," says Wei You, co-corresponding author of this paper and professor of chemistry and applied physical sciences at the University of North Carolina at Chapel Hill. "And we can tune the composition of either the inorganic or organic layer."

"We found that we can control the elastic modulus and thermal conductivity of some 2D HOIPs by replacing some of the carbon-carbon chains in the organic layers with benzene rings," says Qing Tu, co-corresponding author of this paper and an assistant professor of materials science and engineering at Texas A&M University. "Basically -- within this specific subset of layered materials -- the more benzene rings we add, the stiffer the material gets, and the better able it is to insulate against heat."

"While discovering these materials in itself holds tremendous potential for a range of applications, as researchers we are particularly excited because we've identified the mechanism that is responsible for these characteristics -- namely the critical role that the benzene rings play," says Liu.

In experiments, the researchers found at least three distinct 2D HOIP materials that became less thermally conductive the stiffer they got.

"This work is exciting because it suggests a new pathway for engineering materials with desirable combinations of properties," Liu says.

The researchers also discovered another interesting phenomenon with 2D HOIP materials. Specifically, they found that by introducing chirality into the organic layers -- i.e., making the carbon chains in those layers asymmetrical -- they could effectively maintain the same stiffness and thermal conductivity even when making substantial changes to the composition of the organic layers.

"This raises some interesting questions about whether we might be able to optimize other characteristics of these materials without having to worry about how those changes might influence the material's stiffness or thermal conductivity," says Liu.

Science Daily, 29 May 2024

https://sciencedaily.com

CHEMWATCH
Bulletin Board
Gossip
MAY. 31, 2024

Yes, Plant-Based Diets Really Are Better for Your Health, Review Finds

2024-05-16

The health benefits of vegetarianism and veganism are unmistakable, according to a new review.

After reassessing 48 previously published papers on the health effects of plant-based diets, researchers from the University of Bologna concluded that such lifestyles reduce the risk of cardiovascular diseases and certain cancers.

Before millions are encouraged to forgo their fish and red meat, however, the researchers stress that more thorough studies are still needed to account for the potential risks of such restrictive diets.

The findings were published in PLOS One.

Vegans, vindicated

Ischemic heart disease is the leading cause of death globally. As a suboptimal diet (insufficient intake of fruit and vegetables, excessive intake of red meat, etc.) is a strong risk factor for the disease and other conditions like gastric cancer, the World Health Organization has called on governments around the world to promote healthy diets to reduce disease incidence and severity.

To test whether vegetarian and vegan diets meet such healthy criteria, the researchers from the University of Bologna reread 48 previously published reviews and meta-analyses. These reviews assessed dozens of studies, including randomized controlled clinical trials, that had investigated the risks plant-based diets pose to blood pressure, cardiovascular events, pregnancies, cholesterol and other health qualities.

The Bologna researchers' own "umbrella review" of the papers concluded that, overall, plant-based diets were firmly associated with better health outcomes regarding blood pressure, blood sugar management and body mass index scores. In turn, the diets appeared to lower the overall incidences of ischemic heart disease and gastrointestinal and prostate cancers.

There were fewer benefits for pregnant people, however. Among the pregnant women studied in the literature, those sticking to vegetarian diets experienced no significant differences in their risk of gestational

diabetes and hypertension compared to the women who ate meat during their pregnancies.

Nonetheless, the Bologna researchers say that, overall, their findings suggest plant-based diets are associated with significant health benefits, even independent of other healthy lifestyle factors, such as exercise.

"Certainly long term wellbeing depends on a healthy lifestyle which includes not only healthy diet but also regular physical exercise and avoidance of risky habits (i.e., tobacco smoke and drug abuse)," Davide Gori, an associate professor at the Department of Biomedical and Neuromotor Sciences at the University of Bologna, told Technology Networks.

"Therefore, we mentioned that, to a certain extent, the results we have observed could be related to a generally more healthy lifestyle followed by vegetarians and vegans."

"Nevertheless," he continued, "it is important to underline that the results shown in our paper strongly support the importance of diet per se, which means that adhering to a vegetarian or to a vegan diet, independently from other factors, significantly reduce the risk of cardiovascular diseases and of underlying conditions (i.e., hypercholesterolemia, hyperglycemia/diabetes, overweight) and of cancers (i.e., gastrointestinal, pancreatic, prostate)."

As for those keen on a healthy, plant-rich lifestyle but unwilling to give up the occasional chicken sandwich, Gori says that, while the odd bite of meat could fit into a healthy routine, the review's findings can't guarantee so.

"The occasional consumption of meat or fish or poultry should not significantly alter the benefits of a healthy plant rich diet, but this cannot be assumed by our study since we deliberately included only articles focusing completely on vegan or vegetarian diet allowing, in some cases, animal derived products (i.e., ovo-vegetarian or lacto-vegetarian regimen) but not sporadic [consumption] of fish, meat and poultry," he said.

According to Gori, more thorough studies that account for such dietary flexibility will be needed before such conclusions can be made. These studies should also ideally research the potential vitamin deficiency risks posed by plant-based diets, say the Bologna researchers, to test the safety

CHEMWATCH
Bulletin Board
Gossip
MAY. 31, 2024

of the diets and their suitability for people with particular nutritional needs.

Technology Networks, 16 May 2024

https://technologynetworks.com

Cheap, dirty leftovers can release pure oxygen: Hexagonal manganites show promise for production on an industrial scale

2024-05-30

New materials for producing oxygen may challenge traditional production methods. This is exciting news, because pure oxygen is in demand for many areas in industry and medicine.

"We have identified materials that can store and release pure oxygen much faster and at much lower temperatures than known materials currently used for this purpose," says Professor Sverre Magnus Selbach at the Norwegian University of Science and Technology (NTNU's) Department of Materials Science and Engineering.

Oxygen is an element, so it cannot be made, only released. The most common method is to distill oxygen directly from the air, but it can also be extracted from materials that have oxygen bound in them.

Retrieving oxygen from materials

Many materials absorb oxygen from the air. When these materials are heated up, they release this oxygen, and small changes in the materials can change their properties.

As the chemical process speeds up, scientists refer to "the kinetics being faster" in the material. The fact that this process can take place at low temperatures is a big advantage. Not only does it mean that less energy is required for heating, but also that reactors can be made from cheaper materials that will need less maintenance than if they had to be exposed to higher temperatures.

"Both of these improvements in material properties make the materials more competitive," says Frida Hemstad Danmo. The research was part of her doctoral work.

The research results have now been published in the journal Chemistry of Materials.

The wonder material

So, what kind of wonder material are we talking about? It might be a little surprising. Have you heard of hexagonal manganites?

Probably not. Almost no one has heard of hexagonal manganites. Fortunately, the researchers at NTNU have. The material is not only very suitable for extracting oxygen, it can also be made quite cheaply and efficiently.

"Because oxygen is absorbed so quickly into the material, we can use bulk materials that can be made in large quantities using cheaper methods than those required to make nanoparticles," explains Danmo.

If the oxygen transport was not already so rapid in these hexagonal manganites, the process would have required nanoparticles to increase surface area and provide the oxygen with a 'shorter way' in and out of the material.

Nanoparticles are more complicated to produce and cannot be made in large quantities as easily as bulk material.

Impurities in the material are unproblematic

The hexagonal manganites they have developed are so-called "high-entropy materials." This means that they are neither pure nor have a particularly well-ordered crystal structure, and this is where the secret lies.

Not only are the materials quite cheap, they are also not that particular when it comes to chemical composition. Impurities and small defects in the material are therefore not a problem. Things don't have to be so precise, the process works anyway, and it makes it possible to achieve cheaper production on an industrial scale.

The researchers used five to six different rare earth metals in the mix they experimented with, and the result was much better than when well-ordered materials with just one or two rare earth metals were used.

"The high-entropy materials are actually more stable than those with simpler chemical composition. The reason is the entropy, i.e. the disorder that comes from having many different elements in the crystal structure instead of fewer," says Selbach.

"All spontaneous processes will increase the disorder of the universe. Interestingly, it is the disorder itself that also provides such rapid oxygen absorption, since our materials are not sensitive to precise chemical

CHEMWATCH
Bulletin Board
Gossip
MAY. 31, 2024

composition. Focusing on high entropy is a paradigm shift for this particular class of materials, and something that has given us exceptional properties," says Danmo.

Using cheaper and available materials

These types of materials are not currently used in the industry, but a great deal of research is being done on them precisely because the potential for cheaper oxygen production is so great.

"Industry can use cheaper raw materials, such as oxides of recycled rare earth metals or low-quality ore. These raw materials remain after more expensive elements such as neodymium and dysprosium are extracted for use in electric motors in windmills and electric cars," says Selbach.

Industry may even be able to use waste materials from the production of electric motors.

In collaboration with Danmo, Aamund Westermoen conducted much of the experimental work. Senior Engineer Elvia Anabela Chavez Panduro contributed measurements at NTNU, and Kenneth Marshall and Dragos Stoian at the European Synchrotron Radiation Facility (ESRF) in France helped with the synchrotron measurements made at the Swiss–Norwegian Beamlines facility in Grenoble.

Phys Org, 30 May 2024

https://phys.org

Ultrasonic coffee-maker produces the perfect cold brew in minutes

2024-05-08

A high-tech method for producing cold brew coffee that uses ultrasonic waves to extract flavour could cut the time required from 24 hours to just a few minutes.

Cold brew coffee, which is made by steeping coffee grounds in cold water, is gaining popularity because it results in a less bitter drink than traditional methods using hot water. But the technique is also a headache for coffee shops as they need refrigerator space and must allow up to 24 hours to make a brew.

Now Francisco Trujillo at the University of New South Wales in Sydney and his colleagues have found a unique way to quickly extract a cold shot of

coffee – by bombarding the grounds with ultrasonic waves. The resulting drink can be ready in less than 3 minutes.

Trujillo says the initial idea for using ultrasound, which smashes up the grounds in a process called acoustic cavitation, was that it might allow the extraction of more antioxidants. This turned out not to be the case, but their initial set up, requiring around £15,000 of ultrasonic equipment, produced a surprisingly good coffee.

"There's nothing like it," says Trujillo. "The flavour is nice, the aroma is nice and the mouth feel is more viscous and there's less bitterness than a regular espresso shot. And it has a level of acidity that people seem to like. It's now my favourite way to drink coffee."

The researchers have refined their process to work with existing espresso machines at a fraction of the cost of their initial equipment. They say their preferred technique for a cold espresso is 60 seconds of ultrasound, pumping a small amount of water every 12 seconds, but they also experimented with a 3-minute brew.

Trujillo says there are some important differences that make the ultrasonic cold espresso unique. Firstly, unlike a traditional hot espresso shot, the coffee grounds aren't tamped down. The cold ultrasonic espresso shot also isn't transparent and is a different colour when compared with a traditional cold brew, since the sound waves emulsify the oils in the coffee.

Samples of the new cold brew were tested by the Queensland Alliance for Agriculture and Food Innovation at the University of Queensland, where it was assessed for aroma, texture, flavour and aftertaste.

Trujillo says the ultrasonic 1-minute shot had generally similar ratings to a 24-hour cold brew but scored lower in aroma intensity, suggesting the cold shot may be under-extracted. On the other hand, he says, the 3-minute shot scored the same on aroma intensity as a 24-hour cold brew but with a slightly greater bitterness, indicating that the 3-minute brew was over-extracted. Somewhere between 1 and 3 minutes, and tweaking other parameters, will make a perfect cold brew, he says.

New Scientist, 8 May 2024

https://newscientist.com

CHEMWATCH
Bulletin Board
Gossip
MAY. 31, 2024

New Drug Affecting Sperm Motility Shows Promise as Male Birth Control Pill

2024-05-28

A novel, non-hormonal sperm-specific approach offers a promising option for reversible human male contraception.

The world's population has increased by more than 2.6-fold in the last 60 years. The growing trend continues – projections indicate that the number of people living on our planet will grow to 9 billion by 2037 from 8 billion in 2022. These numbers underscore the need for considering family planning; however, there have been limited breakthroughs in contraception in recent decades. Specifically for men, there are no oral contraceptive pills available.

In a study published in the journal Science, researchers at Baylor College of Medicine and collaborating institutions show in animal models that a novel, non-hormonal sperm-specific approach offers a promising option for reversible human male contraception.

"Although researchers have been investigating several strategies to develop male contraceptives, we still do not have a birth control pill for men," said corresponding author Dr. Martin Matzuk, director of the Center for Drug Discovery and chair of the Department of Pathology and Immunology at Baylor. "In this study we focused on a novel approach – identifying a small molecule that would inhibit serine/threonine kinase 33 (STK33), a protein that is specifically required for fertility in both men and mice."

Previous research has shown that STK33 is enriched in the testis and is specifically required for the formation of functional sperm. In mice, knocking out the Stk33 gene renders the mice sterile due to abnormal sperm and poor sperm motility. In men, having a mutation in the STK33 gene leads to infertility caused by the same sperm defects found in the Stk33 knockout mice. Most importantly, mice and men with these mutations have no other defects and even have normal testis size.

"STK33 is therefore considered a viable target with minimal safety concerns for contraception in men," said Matzuk, who has been on faculty at Baylor for 30 years and is Baylor's Stuart A. Wallace Chair and Robert L. Moody, Sr. Chair of Pathology and Immunology. "STK33 inhibitors have been described but none are STK33-specific or potent for chemically disrupting STK33 function in living organisms."

Finding an effective STK33 inhibitor

"We used DNA-Encoded Chemistry Technology (DEC-Tec) to screen our multi-billion compound collection to discover potent STK33 inhibitors," said first author Dr. Angela Ku, staff scientist in the Matzuk lab. "Our group and others have used this approach before to uncover potent and selective kinase inhibitors."

The researchers uncovered potent STK33-specific inhibitors, from which they successfully generated modified versions to make them more stable, potent and selective. "Among these modified versions, compound CDD-2807 turned out to be the most effective," Ku said.

"Next, we tested the efficacy of CDD-2807 in our mouse model," said co-author Dr. Courtney M. Sutton, postdoctoral fellow in the Matzuk lab. "We evaluated several doses and treatment schedules and then determined sperm motility and number in the mice as well as their ability to fertilize females."

Compound CDD-2807 effectively crossed the blood-testis barrier and reduced sperm motility and numbers and mice fertility at low doses. "We were pleased to see that the mice did not show signs of toxicity from CDD-2807 treatment, that the compound did not accumulate in the brain, and that the treatment did not alter testis size, similar to the Stk33 knockout mice and the men with the STK33 mutation," Sutton said. "Importantly, the contraceptive effect was reversible. After a period without compound CDD-2807, the mice recovered sperm motility and numbers and were fertile again."

"In our paper, we also present the first crystal structure for STK33," said co-author Dr. Choel Kim, associate professor of biochemistry and molecular pharmacology and member of the Dan L Duncan Comprehensive Cancer Center at Baylor. "Our crystal structure showed how one of our potent inhibitors interacts with STK33 kinase in three dimensions. This enabled us to model and design our final compound, CDD-2807, for better drug-like properties."

"This study was a tour de force by our team in the Center for Drug Discovery at Baylor and our collaborators," said co-author Dr. Mingxing Teng, assistant professor of pathology and immunology and of biochemistry and molecular pharmacology at Baylor. Teng also is a Cancer Prevention Research Institute of Texas Scholar and a member of the Dan L Duncan Comprehensive Cancer Center at Baylor. "Starting with

CHEMWATCH
Bulletin Board
Gossip
MAY. 31, 2024

a genetically validated contraceptive target, we were able to show that STK33 is also a chemically validated contraceptive target."

"In the next few years, our goal is to further evaluate this STK33 inhibitor and compounds similar to CDD-2807 in primates to determine their effectiveness as reversible male contraceptives," Matzuk said.

Technology Networks, 28 May 2024

https://technmologynetworks.com

Novel method for mass production of recombinant proteins uses mono-sodium glutamate

2024-05-30

Mass production of recombinant proteins using yeast cell "factories" needs methanol, a compound that requires safe handling, carries the risk of catching fire, and sometimes produces harmful byproducts. Researchers at the Department of Biochemistry (BC), Indian Institute of Science (IISc), have now developed an alternative safer process that instead relies on a common food additive called mono-sodium glutamate (MSG).

Recombinant proteins, such as vaccine antigens, insulin and monoclonal antibodies, are mass-produced by growing modified bacterial, viral or mammalian cells in large bioreactors. The most widely used organism is the yeast Pichia pastoris (now called Komagataella phaffii). It contains a unique promoter—a specific gene region which can be activated by methanol. This promoter codes for an enzyme called alcohol oxidase (AOX).

To mass-produce a recombinant protein, the gene coding for that protein is spliced into the yeast genome right next to the AOX promoter. The yeast cells are then fed glycerol or glucose as the carbon source. Once enough cells have formed, methanol is added, which then activates the AOX promoter, and the cells start producing the recombinant protein in copious amounts.

Most industries use this methanol-induced process for producing recombinant proteins. However, methanol is highly flammable and hazardous, requiring stringent safety precautions, points out PN Rangarajan, Professor at BC and corresponding author of the study published in Microbial Cell Factories. Methanol also metabolizes to form hydrogen peroxide which can induce oxidative stress in the yeast cells or damage the recombinant proteins.

To solve this problem, Trishna Dey, a former Ph.D. student at BC, started looking for alternatives. After an extensive search, the team found that mono-sodium glutamate (MSG), a USFDA approved food additive, can activate a different promoter in the yeast genome that codes for an enzyme called phosphoenolpyruvate carboxykinase (PEPCK). Activating this promoter with MSG led to protein production similar to methanol activation of the AOX promoter.

Optimizing the cell culture medium for this new and untested process was challenging, says Neetu Rajak, first author and Ph.D. student at BC. For a long time, the yeast cells grew poorly in shake flasks and produced very little recombinant protein. "There was a time when we almost gave up because we thought it was not going to work," recalls Rangarajan.

The group eventually figured out that using MSG alone was not enough. Vedanth Bellad and Yash Sharma, project assistants at BC and co-authors, explain that they tried supplementing the culture with various other compounds, until one finally did the trick: ethanol.

Adding ethanol helped the cells grow faster, which increased the biomass and the amount of recombinant protein produced. Ethanol is also safer for yeast cells compared to methanol, as it does not produce toxic byproducts when broken down.

To test their process, the team tried producing the SARS-CoV-2 receptor binding domain—a widely-used vaccine antigen that has been successfully expressed in yeast and mammalian cells. They found that their new expression system produced twice the amount of antigen compared to the methanol-induced process.

The researchers hope that this novel and indigenous expression system can be used in biotech industries to mass-produce valuable proteins including milk and egg proteins, baby food supplements and nutraceuticals, apart from therapeutic molecules.

Phys Org, 30 May 2024

https://phys.org

Why warm drinks taste more alcoholic than cold ones

2024-05-01

Chemists have found a link between the taste of a beverage and the shapes formed by its water and ethanol molecules, which explains why spirits like whisky taste more alcoholic at warmer temperatures

CHEMWATCH
Bulletin Board
Gossip
MAY. 31, 2024

Beer is most refreshing when it is ice-cold, while spirits like whisky taste most alcoholic at warmer temperatures – and those shifts in flavour may be due to the way water and ethanol molecules cluster together within a beverage.

Lei Jiang at the Chinese Academy of Sciences and his colleagues wanted to study how factors like temperature and alcohol by volume (ABV) affect molecular behaviour in drinks like beer, rice wine and the whisky-like Chinese spirit baijiu – and what that may mean for their taste.

They first measured the surface tension of these alcoholic beverages while increasing the drinks' ABV levels. Then they used nuclear magnetic resonance imaging and computer simulations to "zoom in" on combinations, or clusters, of water and ethanol molecules in beverages at different ABVs and temperatures. Finally, they conducted taste tests in partnership with Chinese baijiu company Wuliangye.

Jiang says that what they found surprised them, defying what chemists once thought was "common sense". While he and his colleagues expected surface tension to evenly decrease as the ABV of a drink increased, it actually changed in discrete "steps".

The researchers uncovered that these jumps happened when clusters of water and ethanol molecules changed shape, shifting from compact, pyramid-like structures to long, chain-like ones. Jiang says that colder and less alcoholic liquids had a greater proportion of pyramid clusters and were associated with a more refreshing flavour.

"When the temperature drops, the structure becomes more compact, which is why chilled beer has a more stimulating taste," he says.

In warmer drinks and those with higher ABVs, more chain-like clusters dominated, and their flavour was more pungent and ethanol-heavy.

Gavin Sacks at Cornell University in New York says the study found novel details about the chemistry of ethanol and water in beverages, but that connecting molecular clusters to taste is very complicated. The burning flavour of ethanol stimulates the same taste receptors that sense heat. As a result, it is difficult to isolate which chemical property of a warm drink – the way its molecules cluster, its temperature and how it interacts with

other liquids in the human mouth – is responsible for changes in its taste, he says.

New Scientist, 1 May 2024

https://newscientist.com

Luxury perfumes linked to child labour, BBC finds

2024-05-29

A BBC investigation into last summer's perfume supply chains found jasmine used by Lancôme and Aerin Beauty's suppliers was picked by minors.

All the luxury perfume brands claim to have zero tolerance on child labour.

L'Oréal, Lancôme's owner, said it was committed to respecting human rights. Estée Lauder, Aerin Beauty's owner, said it had contacted its suppliers.

The jasmine used in Lancôme Idôle L'Intense - and Ikat Jasmine and Limone Di Sicilia for Aerin Beauty - comes from Egypt, which produces about half the world's supply of jasmine flowers - a key perfume ingredient.

Industry insiders told us the handful of companies that own many luxury brands are squeezing budgets, resulting in very low pay. Egyptian jasmine pickers say this forces them to involve their children.

And we have discovered the auditing systems the perfume industry uses to check on supply chains are deeply flawed.

The UN Special Rapporteur on contemporary forms of slavery, Tomoya Obokata, said he was disturbed by the World Service's evidence, which includes undercover filming in Egyptian jasmine fields during last year's picking season.

"On paper, they [the industry] are promising so many good things, like supply chain transparency and the fight against child labour. Looking at this footage, they are not actually doing things that they promised to do."

Heba - who lives in a village in the district of Gharbia, the heart of Egypt's jasmine region - wakes her family at 03:00 to begin picking the flowers before the sun's heat damages them.

Heba says she needs her four children - aged from 5 to 15 - to help. Like most jasmine pickers in Egypt, she is what is known as an "independent picker" and works on a smallholder farm. The more she and her children can pick, the more they earn.

On the night we filmed her, she and her children managed to pick 1.5kg of jasmine flowers. After paying a third of her earnings to the land owner, she was left with roughly US$1.5 [£1.18] for that night's work. This is worth less

than ever before, given inflation in Egypt is at an all-time high, and pickers are often living below the poverty line.

Heba's 10-year-old daughter Basmalla has also been diagnosed with a severe eye allergy. At a medical consultation we attended with her, the doctor told her that her vision will be affected if she continues jasmine picking without treating the inflammation.

Once the jasmine has been picked and weighed, it is transferred via collection points to one of several local factories which extract oil from the flowers - the main three being A Fakhry and Co, Hashem Brothers and Machalico. Each year, it is the factories that set the price for the jasmine picked by people like Heba.

It is difficult to say exactly how many of the 30,000 people involved in Egypt's jasmine industry are children. But during the summer of 2023 the BBC filmed across this region and spoke to many residents who told us the low price for jasmine meant they needed to include their children in their work.

We witnessed that, at four different locations, a significant number of pickers working on smallholder farms - which supply the main factories - were children under the age of 15. Multiple sources also told us that there were children working on farms directly owned by the Machalico factory, so we went undercover to film there and found pickers who told us their ages ranged from 12 to 14.

It is illegal for anyone under the age of 15 to work in Egypt between the hours of 19:00 and 07:00.

The factories export the jasmine oil to international fragrance houses where the perfumes are created. Givaudan, based in Switzerland is one of the largest, and has a longstanding relationship with A Fakhry and Co.

But it is the perfume companies above them - which include L'Oréal and Estée Lauder - which hold all the power, according to independent perfumer Christophe Laudamiel and several other industry insiders.

Known as "the masters", they set the brief and a very tight budget for the fragrance houses, he said.

"The masters' interest is to have the cheapest oil possible to put in the fragrance bottle," and then to sell it at the highest possible price, said Mr Laudamiel, who spent years working inside one of the fragrance houses.

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

"They actually don't govern the salary or the wages of the harvesters, nor the actual price of jasmine, because they are beyond that," he explained.

But he said that because of the budget that they set, the pressure on wages "trickles down" - to the factories, and ultimately, the pickers.

"There's a big disconnect between the preciousness that is talked about in the marketing talk, and what is actually given to the harvesters," he added.

In their promotional material, the perfume companies and fragrance houses paint a picture of ethical sourcing practices. Every employer in the supply chain has also signed a letter of commitment to the UN, pledging to abide by its guidelines regarding safe working practices and eliminating child labour.

The issue, according to a senior executive with fragrance house Givaudan, is the lack of oversight the perfume companies have of their supply chains.

Speaking on condition of anonymity, the executive said these companies relied on the fragrance houses to instruct third-party auditing companies to check for due diligence.

The auditing firms most often mentioned by the conglomerates and fragrance houses on their websites, and in letters to the UN, are Sedex and UEBT. Their audit reports are not publicly available but by posing as a buyer looking for ethically sourced jasmine, we managed to get the factory A Fakhry and Co to send both of them to us.

The report from UEBT, based on a visit to the factory last year, shows there was an indication of a human rights issue, but it doesn't go into detail. Despite this, the company was given a "verification", which means it can say it offers "responsibly sourced jasmine oil".

UEBT, in its response to this, said: "One company has been issued a responsible sourcing attestation, subject to an action plan… valid till mid 2024, and will be withdrawn if… not implemented."

The Sedex report gave the factory a glowing assessment, but it was clear from its write-up that the visit had been pre-announced, and only the factory site itself had been audited, and not the smallholder farms it sourced jasmine from.

Sedex told us that it was "firmly against all forms of labour rights abuses. But no one tool alone can or should be relied on to uncover and remediate all environmental and human rights risks or impacts."

Lawyer Sarah Dadush, founder of the Responsible Contracting Project, which seeks to improve human rights in global supply chains, said the BBC's investigation "reveals… that those systems aren't working".

The issue, she said, is that "the auditors are only auditing what they're paid to audit", and this might not include the price paid to the labour force - "a major root cause" of child labour.

A Fakhry and Co told us that child labour is prohibited in both its farm and factory, but that the vast majority of its jasmine is sourced from independent collectors. "In 2018, under the monitoring of the UEBT, we commenced the Jasmine Plant Protection Products Mitigation Project, which imposes a prohibition on individuals under the age of 18 working on the farms." It added that "by any comparable standards in Egypt, jasmine picking is well-remunerated".

Machalico said it does not use pickers under the age of 18, and said it had increased the price it pays for jasmine for the past two years, and will do so again this year. Hashem Brothers said our report was "based on misleading information".

Givaudan, the fragrance house which makes Lancôme Idôle L'Intense, described our investigation as "deeply alarming", adding "it's incumbent upon us all to continue taking action to remove the risk of child labour entirely".

Firmenich, the fragrance house which makes Ikat Jasmine and Limone Di Sicilia for Aerin Beauty, and in summer 2023 sourced jasmine from Machalico, told us it was now using a new supplier in Egypt. It added that it will "support initiatives that seek to collectively address this issue with industry partners and local jasmine farmers".

We also put the findings of the investigation to the perfume masters.

L'Oréal said it was "actively committed to respecting the most protective internationally recognised human rights standards", adding that it "never request[s] Fragrance Houses to go lower than the market price for ingredients at the expense of farmers. Despite our strong commitments… we know that in certain parts of the world where L'Oréal suppliers operate there are risks to our commitments being upheld."

It added: "Whenever an issue arises, L'Oréal works proactively to identify the underlying causes and the way to resolve the issue. In January 2024, our partner performed an on-site human rights impact assessment to

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

identify potential human rights violations and find ways to prevent and mitigate them, with a focus on the child labour risks."

L'Oréal has provided the BBC with an additional statement:

"L'Oréal is seeking to ensure that decent wages are paid to the farmers, that their children have access to education, and human rights laws, policies and practices are in place to stop children from working.

"Ahead of this year's harvest in June, a detailed action plan is in place with suppliers and our teams will be in Egypt evaluating their success."

Estée Lauder said: "We believe the rights of all children should be protected. And we have contacted our suppliers to investigate this very serious matter. We recognise the complex socio-economic environment surrounding the local jasmine supply chain, and we are taking action to gain better transparency and to work toward improving the livelihoods of sourcing communities."

Back in Gharbia, jasmine picker Heba was shocked when we told her the price perfume was selling for on the international market.

"People here are worth nothing," she said.

"I don't mind people using perfume, but I want the people using this perfume to see in it the pain of children. And to speak up."

But lawyer Sarah Dadush said the responsibility does not lie with the consumer.

"This is not a problem that should be for us to solve. We need law… we need corporate accountability, and that cannot just be on the consumers."

BBC, 29 May 2024

https://bbc.com

World-first tooth-regrowing drug will be given to humans in September

2024-05-28

The world's first human trial of a drug that can regenerate teeth will begin in a few months, less than a year on from news of its success in animals. This paves the way for the medicine to be commercially available as early as 2030.

The trial, which will take place at Kyoto University Hospital from September to August 2025, will treat 30 males aged 30-64 who are missing at least one molar. The intravenous treatment will be tested for its efficacy on human dentition, after it successfully grew new teeth in ferret and mouse models with no significant side effects.

"We want to do something to help those who are suffering from tooth loss or absence," said lead researcher Katsu Takahashi, head of dentistry and oral surgery at Kitano Hospital. "While there has been no treatment to date providing a permanent cure, we feel that people's expectations for tooth growth are high."

Following this 11-month first stage, the researchers will then trial the drug on patients aged 2-7 who are missing at least four teeth due to congenital tooth deficiency, which is estimated to affect 1% of people. The team is recruiting for this Phase IIa trial now.

Researchers are then looking at expanding the trial to those with partial edentulism, or people missing one to five permanent teeth due to environmental factors. The incidence of this varies from country to country, but it's estimated around 5% of Americans are missing teeth, with a much higher incidence among older adults.

The medicine itself deactivates the uterine sensitization-associated gene-1 (USAG-1) protein, which suppresses tooth growth. As we reported in 2023, blocking USAG-1's interaction with other proteins encourages bone morphogenetic protein (BMP) signaling, which triggers new bone to generate.

It resulted in new teeth emerging in the mouths of mice and ferrets, species that share close to the same USAG-1 properties as humans.

"The USAG-1 protein has a high amino acid homology of 97% between different animal species, including humans, mice, and beagles," the researchers noted. However, there's no word on a beagle trial just yet…

Molecular biologist and dentist Takahashi has been working on tooth regeneration since 2005, and hopes this treatment won't just be for congenital dental conditions but for anyone who has lost teeth, at any age.

If successful, this therapy could be available to patients with any permanently missing teeth within six years.

New Atlas, 28 May 2024

https://newatlas.com

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

New Carbon-Capture Batteries Store Renewable Energy, Help Climate

2024-05-17

Researchers at the Department of Energy's Oak Ridge National Laboratory are developing battery technologies to fight climate change in two ways, by expanding the use of renewable energy and capturing airborne carbon dioxide.

This type of battery stores the renewable energy generated by solar panels or wind turbines. Utilizing this energy when wind and sunlight are unavailable requires an electrochemical reaction that, in ORNL's new battery formulation, captures carbon dioxide from industrial emissions and converts it to value-added products.

ORNL researchers recently created and tested two different formulations for batteries that convert carbon dioxide gas, or CO2, into a solid form that has the potential to be used in other products.

One of these new battery types maintained its capacity for 600 hours of use and could store up to 10 hours of electricity. Researchers also identified, studied and overcame the primary challenge, a deactivation caused by chemical buildup, that had been an obstacle for the other battery formulation.

"The Transformation Energy Science and Technology, or TEST, initiative at ORNL is precisely the kind of effort needed to address climate change. We are excited that ORNL is investing in innovative ideas and approaches that can transform the way we think about storing energy beyond lithium-ion batteries and other conventional electrochemical energy storage systems," said Ilias Belharouak, an ORNL Corporate Fellow and initiative director. "What a fantastic scenario: Using free electrons to store CO2 and converting it to revenue-generating products is a concept I never would have imagined 10 years back, but this is just a start."

Batteries operate through electrochemical reactions that move ions between two electrodes through an electrolyte. Unlike cell phone or car batteries, those designed for grid energy storage do not have to function as a portable, closed system. This allowed ORNL researchers to create and test two types of batteries that could convert CO2 from stationary, industrial sources.

For example, CO2 generated by a power plant could be pumped through a tube into the liquid electrolyte, creating bubbles similar to those in a

carbonated soft drink. During battery operation, the gas bubbles turn into a solid powder.

How it works

Each component of a battery can be made of different elements or compounds. These choices determine the battery's operational lifetime, how much energy it can store, how big or heavy it is, and how fast it charges or consumes energy. Of the new ORNL battery formulations, one combines CO2 with sodium from saltwater using an inexpensive iron-nickel catalyst. The second combines the gas with aluminum.

Each approach uses abundant materials and a liquid electrolyte in the form of saltwater, sometimes mixed with other chemicals. The batteries are safer than existing technology because their electrodes are stable in water, said lead researcher Ruhul Amin.

Very little CO2 battery research has been conducted. The previously-tried approach relies on a reversible metal-CO2 reaction that regenerates carbon dioxide, continuing to contribute greenhouse gases to the atmosphere. In addition, solid discharge products tend to clog the surface of the electrode, degrading the battery performance.

However, the CO2 batteries developed at ORNL do not release carbon dioxide. Instead, the carbonate byproduct dissolves in the liquid electrolyte. The byproduct either continuously enriches the liquid to enhance battery performance, or it can be filtered from the bottom of the container without interrupting battery operation. Battery design can even be tuned to create more of these byproducts for use by the pharmaceutical or cement industries. The only gases released are oxygen and hydrogen, which do not contribute to climate change and can even be captured to produce energy or fuel.

ORNL researchers used an almost completely new combination of materials for these CO2 batteries. The few similar previous designs worked for only short periods or incorporated expensive metals.

Pros, cons and challenges overcome

The sodium-carbon dioxide, or Na-CO2, battery was developed first and faced some obstacles. For this system to function, the electrodes must be separated in wet and dry chambers with a solid ion conductor between them. The barrier slows the movement of ions, which in turn slows down battery operation, reducing battery efficiency.

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

One significant challenge for this Na-CO2 battery is that after prolonged use, a film forms on the electrode surface, which eventually causes the battery to deactivate. Amin's research team used highly specialized microscopes and X-ray techniques to examine the battery cell when it failed and at various stages of operation.

Studying how the film formed helped researchers understand how to break it down again. They were intrigued to realize the battery could be reactivated, or prevented from deactivating at all, simply through operational changes in the charge/discharge cycle. Uneven pulses of charging and discharging prevented film buildup on the electrode.

"We are reporting for the first time that the deactivated cell can be reactivated," Amin said. "And we found the origin of the deactivation and activation. If you symmetrically charge-discharge the battery too long, it's dead at one stage. If you use the protocol we established for our cell, the chance of failure is very slim."

A second design for long-term storage

Next, researchers focused on the design of the aluminum-carbon dioxide, or Al-CO2, battery. The team experimented with various electrolyte solutions and three different synthesis processes to identify the best combination. The result was a battery which provides enough storage for more than 10 hours of electricity to be used later.

"That's huge for long-duration storage," Amin said. "This is the first Al-CO2 battery that could run with stability for a long time, which is the goal. Holding just a few hours of stored energy doesn't help."

Testing found that the ORNL battery could operate more than 600 hours without losing capacity, Amin said – far more than the only previously reported Al-CO2 battery, which was only tested for eight hours of cycling.

The cherry on top is that this battery captures almost twice as much carbon dioxide as the Na-CO2 battery. It can be designed for the system to operate in a single chamber, with both electrodes in the same liquid solution, so there is no barrier to ion movement.

The challenge for the Al-CO2 battery is to bring it closer to scale-up, Amin said. Even so, the team will continue systematically studying its properties to extend the operating lifetime and capture CO2 more efficiently. For the Na-CO2 battery to be competitive, the team will focus on developing a

very fine, dense, mechanically stable ceramic membrane to separate the battery chambers.

Technology Networks, 17 May 2024

https://technologynetworks.com

A new Hungarian method may aid protein research

2024-05-29

In a paper recently published in Nature Communications, the HUN-REN-ELTE Protein Modeling Research Group (Institute of Chemistry) has laid the foundations for a mathematical method, allowing the computer-assisted comparison of the three-dimensional structures of proteins. The method is unique in that while the alternatives available so far only took into account the position of the atoms, the new technique, called LoCoHD (Local Composition Hellinger Distance), also includes the chemical information of the atoms.

Proteins are molecular machines that carry out processes necessary for cells to function, acting as molecular switches, transcribing information from DNA, transporting small and large molecules and regulating metabolism related chemical reactions. However, for all this to succeed, the protein in question must have the right spatial conformation, i.e. its own, correct 3D arrangement.

Several experimental methods (X-ray crystallography, nuclear magnetic resonance spectroscopy, cryo-electron microscopy) are available to determine the arrangement of atoms in a protein, and over the last few decades, protein researchers have discovered the shape of nearly 220,000 proteins. These results increasingly demand the development of computational methods capable of analyzing these arrangements.

One such method is the algorithm called LoCoHD, developed by Zsolt Fazekas, a Ph.D. candidate at the ELTE Hevesy György School of Chemistry and a researcher in Dr. András Perczel's research group. The algorithm compares local environments around amino acids in proteins based on their chemical nature (e.g., elemental composition, charge, hydrophobicity, etc.).

The method decides on a simple scale of 0 to 1 how different the structures in question are from each other. Values close to 0 suggest a high similarity between atomic arrangements and chemical properties, while values close to 1 indicate that the proteins being compared may have very

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

different properties. The resulting numerical value (a so-called metric) can thus be used to obtain new information about the system under study.

The algorithm uses a multi-step protocol to generate the number representing the structural differences. In the first step, it converts real atoms in the protein into so-called primitive atoms. These can be represented as virtually labeled positions whose labels tell the chemical nature of the original atom.

So, for example, a primitive atom can be a "positively charged nitrogen," a "negatively charged oxygen," a "neutrally charged oxygen," an "aromatic carbon," etc. The labels are generated according to a so-called primitive typing scheme, which tells us in a tabulated manner how to convert real atoms into primitive atoms. The user can freely specify this table, fixing the chemical resolution of the method.

The second step is to determine the reference points of the comparison by selecting a subset of primitive atoms. These selected special primitive atoms are called the anchor atoms. For each selected anchor atom pair, the algorithm performs a comparison step, the result of which gives the dissimilarity measure we want. These numbers can be used at a local level, or they can be averaged into a single descriptor characterizing the whole protein.

In the study, the researchers highlighted that the method can also be used in the biannual CASP (Critical Assessment of Protein Structure Prediction) competitions, which is a well known competition in the field of protein research. During this event, competitors use different algorithms to model the shape of proteins having yet unpublished structures. CASP judges use a number of structure comparison methods to evaluate the contenders, but none of these take into account the chemistry of the local amino acid environments.

Using data from the 2020 CASP14 competition, the researchers have now performed comparative analysis of several modeled proteins, including the structures predicted by the artificial-intelligence-based AlphaFold2 method. Among these, they highlighted the analysis of a protein from the SARS-CoV-2 virus called ORF8. In the modeled structures of this protein, amino acid environments were identified that differ significantly in their interaction patterns from the environments found in the experimental structure.

In addition to studying static structures, the researchers also tested whether the method is suitable for analyzing the internal motion of

proteins. They used simulations capable of reproducing molecular motions and data extracted from structural ensembles. One of the systems under study was the podocin protein, which performs vital functions in the kidney and whose mutations can cause severe, often fatal conditions.

The LoCoHD method was used to identify amino acids in the protein that undergo major chemical-environmental changes during the movement of podocin, which can affect both its structure and function. Similarly, the LoCoHD method has been applied successfully in the study of the HIV-1 capsid protein, in which an amino acid critical for the formation of the viral envelope has been identified.

These results are not only research curiosities, but by studying protein structures more effectively, we can get closer to better understanding the pathogens causing severe diseases and to developing effective drugs and therapeutics.

Phys Org, 29 May 2024

https://phys.org

Pan-cancer approval shows huge potential for antibody–drug conjugates

2024-05-21

Enhertu (trastuzumab deruxtecan), has become the first antibody—drug conjugate (ADC) to receive US approval for treating cancer based on the molecular profile of the tumour rather than its location of origin. The approval is based on positive results from clinical trials of the drug against a range of cancers expressing human epidermal growth factor receptor 2 (HER2).

'This is a globally important finding because there are many cancers where there is HER2 expression,' says Funda Meric-Bernstam, an oncologist at the University of Texas, US, who coordinated one of the trials that supported pan-tumour approval by the US Food and Drug Administration (FDA).

The drug combines an antibody (trastuzumab – marketed as a cancer therapy on its own as Herceptin) for homing in on the target, with a cell-killing payload of deruxtecan, a topoisomerase 1 inhibitor that interfere with DNA replication during cell division. It was jointly developed by Daiichi Sankyo and AstraZeneca.

Enhertu had already been approved for breast cancer, metastatic lung cancer and stomach cancer. Its recent pan-tumour approval was based on

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

three specially-designed clinical trials where it shrank a variety of tumours in many people with advanced HER2-positive cancers.

There are a small number of other antibody and small-molecule therapies that have some degree of location-agnostic approval based on molecular or gene profiling. More pan-tumour ADC approvals could follow on from Enhertu. 'This has great implications for the field because many other antibody-drug conjugates were being developed based on disease types, but maybe we can look more broadly,' says Meric-Bernstam.

Broad approval

One standout finding with Enhertu was that it was active not only in tumours with high HER2 expression, but also in breast cancer with lower HER2 expression. 'HER2 is an especially compelling target because it is expressed across many tumour types,' says Meric-Bernstam.

The Destiny-PanTumor02 trial was designed to indicate whether the drug could work in cancers that would be too rare to run individual clinical trials for, but that can be tested for HER2. There were positive results in gynaecological cancers, even with lower expression of HER2. And while the results pancreatic and biliary cancer were less dramatic, there were still clear benefits, says Meric-Bernstam. 'Over half the patients had responses, meaning 30% or greater decrease in their tumour burden, and these responses last for a long time,' she adds.

'We can have confidence that if a patient has a disease with HER2 expression, there is a likelihood that trastuzumab deruxtecan will have anti-tumour efficacy,' says Meric-Bernstam, adding that the results make it worthwhile routinely testing patients with advanced metastatic cancer for HER2 expression.

Of the 15 ADCs so far approved to treat cancer, ten gained approval since 2019. Another dozen or so are in late-stage clinical trials. 'There's been a lot of excitement over the past five years with these ADCs that have shown very impressive activity as compared with chemotherapy,' says Aditya Bardia, an oncologist at the University of California, Los Angeles in the US.

Since the first ADCs were developed, there have been major advances in antibody design, target selection, linkers and cell-killing payloads. 'A problem with the first generation of antibody-drug conjugates was that the linker was not stable and resulted in significant off-tumour toxicity,' Bardia explains.

Linkers are crucial for safety and potency. Once the antibody has bound to its target on the cell surface, the whole drug must get inside a cell to release the cytotoxic compounds. If the linker is unstable, the payload can fall off and affect healthy cells. 'Newer ADCs have a more stable linker, which has reduced toxicities,' says Bardia.

Loading up

There have been arguably surprising trends in the types of drugs placed on ADCs. Newer, highly potent agents that bind DNA (such as pyrrolobenzodiazepine) proved mostly too toxic in trials, with only Zynlonta (loncastuximab tesirine) for B-cell lymphoma approved. This had a drug-antibody ratio (DAR) of just two – meaning on average there are two payload molecules attached to each antibody.

If a warhead is extremely potent, then a lower DAR is suitable. To reach an effective dose of a less-toxic payload, a higher DAR is required. But that can mean more payload molecules may fall off, which can kill healthy cells and cause side effects. 'Conventional thinking five to 10 years ago favoured highly toxic payloads, but Enhertu goes the other way,' says Andy Hsieh, market analyst with William Blair.

Higher DARs required advances in linker technology. For example, making linkers more hydrophobic helped overcome problems of hydrophobicity of the payload molecules. This allows the DARs of between seven and eight achieved with less potent topoisomerase 1 inhibitor payloads in in Enhertu and Gilead's Trodelvy (sacituzumab govitecan).

'The DAR of eight allows you to target what were inaccessible tumour cells,' says Hsieh. This is because more cancer-killing molecules are around to spill out of target cancer cells and kill nearby bystander cells. This is useful because tumours are often complex and heterogeneous, with not all cells expressing the same genetic profile.

Trodelvy and Enhertu are believed to also kill cells that lack the target receptor for their antibodies by diffusion of the payload. For example, when Enhertu gets inside a cancer cell, deruxtecan is released and kills the cell. However, because deruxtecan is membrane permeable, it can then enter nearby cells that do not express HER2 and terminate them. However, there is also the possibility of damaging healthy cells around the site of the tumour.

Overall, this has delivered benefits to patients. Trodelvy – which targets tumour-associated calcium signal transducer 2 – was approved for

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

metastatic breast cancer and bladder cancer in the US in 2020 and in the EU in 2021. 'It showed doubling of overall survival, something we had not seen in triple-negative breast cancer [tumours that don't express receptors for either oestrogen, progesterone or HER2],' says Bardia, who led the clinical trials of Trodelvy.

He says ADCs have 'changed the therapeutic landscape for breast cancer.' His group's focus now is to move the drug to early breast cancer to prevent the return of triple-negative breast cancer.

Commercial clamour

For now, commercial interests in ADCs are focused on cancer. 'Most pharma companies want exposure to ADCs as part of their strategy, but some companies really have ADCs as an anchoring strategy,' says Hsieh. Earlier this year, it was reported that Daiichi Sankyo raised its sales forecast for the 12 months ending in March to $2.6 billion (£2 billion) for Enhertu. This success is drawing renewed attention on the commercial potential of ADCs for cancer.

AstraZeneca's partnership with Daiichi Sankyo for its linker-payload technology, which produced Enhertu, positions them as leaders in the field. Meanwhile, Pfizer agreed to pay $43 billion in 2023 for Seattle-based ADC pioneer Seagen. And earlier this year Johnson & Johnson completed its $2 billion acquisition of Ambrx.

In February, AbbVie completed a $10 billion takeover of ImmunoGen, giving it the only ADC approved for ovarian cancer, Elahere (mirvetuximab soravtansine). Genmab agreed to buy ProfoundBio for $1.8 billion to boost its ADCs for solid tumours in April.

'There's a lot of excitement related to ADCs. Every few months, we read about big pharma buying a smaller company for its ADC portfolio,' says Bardia.

Also active in this space are GSK, Roche, Takeda Pharmaceuticals and Bristol Myers Squibb, which signed a $1 billion licensing agreement with Tubulis to develop ADCs. 'For big pharma, decisions are always revenue driven and ADCs are becoming de-risked,' says Hsieh.

Linker letdown

Despite progress, there are still many opportunities to improve linker chemistry. 'The majority of ADCs are attached to an antibody via a

maleimide cysteine linkage,' says David Spring, an organic chemist at the University of Cambridge, UK.

'It's very good for chemical biology and short-term studies,' he says, 'but these are unstable linkages, and the drug can be falling off within a matter of days, leading to systemic toxicity.' This is because it is unstable in blood plasma, at pH 7.3, leading to a retro-Michael addition, a reverse of the reaction that formed the linkage.

His group has reported on arylsulfate-containing ADC linkers that are stable in plasma, but can be cleaved by sulfatase enzymes in the lysosome once inside the cell. The team has also developed a strategy for loading odd-integer DARs (which are harder to produce than even numbers) using disulfide re-bridging. Spring says not enough chemists have been involved in improving linker technology.

This all leaves plenty of room to improve an already commercially successful strategy for treating cancer. And there are moves to attach not just cell-killing molecules to the antibodies of ADCs. For example, Genentech has developed an experimental ADC to eliminate reservoirs of Staphylococcus aureus bacteria inside cells. More recently, Spring and colleagues in Cambridge have been looking into antibodies that target tuberculosis. 'Other strategies are being considered such as adding immune modulators or novel payload to antibodies,' says Meric-Bernstam.

Chemistry World, 21 May 2024

https://chemisteyworld.com

New Gel Breaks Down Alcohol in the Body

2024-05-14

Most alcohol enters the bloodstream via the mucous membrane layer of the stomach and the intestines. These days, the consequences of this are undisputed: even small amounts of alcohol impair people's ability to concentrate and to react, increasing the risk of accidents. Drinking large quantities on a regular basis is detrimental to one's health: common consequences include liver disease, inflammation of the gastrointestinal tract and cancer. According to the World Health Organization, around 3 million people die every year from excessive alcohol consumption.

Researchers at ETH Zurich have now developed a protein gel that breaks down alcohol in the gastrointestinal tract. In a study recently published in the journal Nature Nanotechnology, they show that in mice, the gel converts alcohol quickly, efficiently and directly into harmless acetic acid

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

before it enters the bloodstream, where it would normally develop its intoxicating and harmful effects.

Reducing health damage caused by alcohol

"The gel shifts the breakdown of alcohol from the liver to the digestive tract. In contrast to when alcohol is metabolised in the liver, no harmful acetaldehyde is produced as an intermediate product," explains Professor Raffaele Mezzenga from the Laboratory of Food & Soft Materials at ETH Zurich. Acetaldehyde is toxic and is responsible for many health problems caused by excessive alcohol consumption.

In the future, the gel could be taken orally before or during alcohol consumption to prevent blood alcohol levels from rising and acetaldehyde from damaging the body. In contrast to many products available on the market, the gel combats not only the symptoms of harmful alcohol consumption but also its causes. Yet, the gel is only effective as long as there is still alcohol in the gastrointestinal tract. This means it can do very little to help with alcohol poisoning, once the alcohol has crossed into the bloodstream. Nor does it help to reduce alcohol consumption in general. "It's healthier not to drink alcohol at all. However, the gel could be of particular interest to people who don't want to give up alcohol completely, but don't want to put a strain on their bodies and aren't actively seeking the effects of alcohol," Mezzenga says.

Main ingredients: Whey, iron and gold

The researchers used ordinary whey proteins to produce the gel. They boiled them for several hours to form long, thin fibrils. Adding salt and water as a solvent then causes the fibrils to cross-link and form a gel. The advantage of a gel over other delivery systems is that it is digested very slowly. But to break down the alcohol, the gel needs several catalysts.

The researchers used individual iron atoms as the main catalyst, which they distributed evenly over the surface of the long protein fibrils. "We immersed the fibrils in an iron bath, so to speak, so that they can react effectively with the alcohol and convert it into acetic acid," says ETH researcher Jiaqi Su, the first author of the study. Tiny amounts of hydrogen peroxide are needed to trigger this reaction in the intestine. These are generated by an upstream reaction between glucose and gold nanoparticles. Gold was chosen as a catalyst for hydrogen peroxide because the precious metal is not digested and therefore stays effective for longer in the digestive tract. The researchers packed all these substances – iron, glucose and gold – into the gel. This resulted in a multi-

stage cascade of enzymatic reactions that ultimately converts alcohol into acetic acid.

Gel works in mice

The researchers tested the effectiveness of the new gel on mice that were given alcohol just once as well as on mice that were given alcohol regularly for ten days. Thirty minutes after the single dose of alcohol, the prophylactic application of the gel reduced the alcohol level in the mice by 40 percent. Five hours after alcohol intake, their blood alcohol level had dropped by as much as 56 percent compared to the control group. Harmful acetaldehyde accumulated less in these mice, and they exhibited greatly reduced stress reactions in their livers, which was reflected in better blood values.

In the mice that were given alcohol for ten days, the researchers were able to demonstrate not only a lower alcohol level but also a lasting therapeutic effect of the gel: the mice that were given the gel daily in addition to alcohol showed significantly less weight loss, less liver damage and hence better fat metabolism in the liver as well as better blood values. Other organs in the mice, such as the spleen or the intestine, as well as their tissues also showed much less damage caused by alcohol.

Patent pending

In an earlier study of administering iron through whey protein fibrils, the researchers had discovered that iron reacts with alcohol to form acetic acid. As this process was too slow and too ineffective at the time, they changed the form in which they attached the iron to the protein fibrils. "Instead of using larger nanoparticles, we opted for individual iron atoms, which can be distributed more evenly on the surface of the fibrils and therefore react more effectively and quickly with the alcohol," Mezzenga says.

The researchers have already applied for a patent for the gel. While several clinical tests are still required before it can be authorised for human use, the researchers are confident that this step will also be successful, as they already showed that the whey protein fibrils that make up the gel are edible.

Technology Networks, 14 May 2024

https://technologynetworks.com

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

Novel material shows potential to produce green hydrogen

2024-05-29

An article published in the journal Polymer describes the production of a material with the potential to be used to obtain hydrogen (H2) by solar-driven water splitting (photoelectrocatalysis) instead of the conventional electricity-driven process.

Also known as green hydrogen, H2 produced from renewable sources is a strong candidate for the accolade "fuel of the future."

The article describes the preparation of films comprising polyaniline nanostructures with an underlayer of multi-walled carbon nanotubes and their promising photoelectrocatalysis performance, especially in H2 production, which requires good light absorption and enhanced stability, among other characteristics.

Polyaniline is an organic semiconductor belonging to the flexible polymer family. Although it was discovered over 150 years ago, it has only recently caught the attention of the scientific community owing to its high electrical conductivity.

The research involved groups at the Center for Development of Functional Materials (CDMF) and the Center for Innovation in New Energies (CINE).

Phys Org, 29 May 2024

https://phys.org

Harvard Scientists Discover Quantum Order in Chemical Chaos

2024-05-26

Harvard researchers have shown that quantum coherence can survive chemical reactions at ultracold temperatures. Using advanced techniques, they demonstrated this with 40K87Rb bialkali molecules, suggesting potential applications in quantum information science and broader implications for understanding chemical reactions.

Zoom in on a chemical reaction to the quantum level and you'll notice that particles behave like waves that can ripple and collide. Scientists have long sought to understand quantum coherence, the ability of particles to maintain phase relationships and exist in multiple states simultaneously; this is akin to all parts of a wave being synchronized. It has been an open

question whether quantum coherence can persist through a chemical reaction where bonds dynamically break and form.

Now, for the first time, a team of Harvard scientists has demonstrated the survival of quantum coherence in a chemical reaction involving ultracold molecules. These findings highlight the potential of harnessing chemical reactions for future applications in quantum information science.

Experimental Breakthrough

"I am extremely proud of our work investigating a very fundamental property of a chemical reaction where we really didn't know what the result would be," said senior co-author Kang-Kuen Ni, Theodore William Richards Professor of Chemistry and Professor of Physics. "It was really gratifying to do an experiment to find out what Mother Nature tells us."

In the paper, published in the journal Science, the researchers detailed how they studied a specific atom-exchange chemical reaction in an ultra-cold environment involving 40K87Rb bialkali molecules, where two potassium-rubidium (KRb) molecules react to form potassium (K2) and rubidium (Rb2) products. The team prepared the initial nuclear spins in KRb molecules in an entangled state by manipulating magnetic fields and then examined the outcome with specialized tools. In the ultra-cold environment, the Ni Lab was able to track the nuclear spin degrees of freedom and to observe the intricate quantum dynamics underlying the reaction process and outcome.

Research Team and Techniques

The work was undertaken by several members of Ni's Lab, including Yi-Xiang Liu, Lingbang Zhu, Jeshurun Luke, J.J. Arfor Houwman, Mark C. Babin, and Ming-Guang Hu.

Utilizing laser cooling and magnetic trapping, the team was able to cool their molecules to just a fraction of a degree above Absolute Zero. In this ultracold environment, of just 500 nanoKelvin, molecules slow down, enabling scientists to isolate, manipulate, and detect individual quantum states with remarkable precision. This control facilitates the observation of quantum effects such as superposition, entanglement, and coherence, which play fundamental roles in the behavior of molecules and chemical reactions.

Findings and Implications

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

By employing sophisticated techniques, including coincidence detection where the researchers can pick out the exact pairs of reaction products from individual reaction events, the researchers were able to map and describe the reaction products with precision. Previously, they observed the partitioning of energy between the rotational and translational motion of the product molecules to be chaotic [Nature 593, 379-384 (2021)]. Therefore, it is surprising to find quantum order in the form of coherence in the same underlying reaction dynamics, this time in the nuclear spin degree of freedom.

The results revealed that quantum coherence was preserved within the nuclear spin degree of freedom throughout the reaction. The survival of coherence implied that the product molecules, K2 and Rb2, were in an entangled state, inheriting the entanglement from the reactants. Furthermore, by deliberately inducing decoherence in the reactants, the researchers demonstrated control over the reaction product distribution.

Future Prospects

Going forward, Ni hopes to rigorously prove that the product molecules were entangled, and she is optimistic that quantum coherence can persist in non-ultracold environments.

"We believe the result is general and not necessarily limited to low temperatures and could happen in more warm and wet conditions," Ni said. "That means there is a mechanism for chemical reactions that we just didn't know about before."

First co-author and graduate student Lingbang Zhu sees the experiment as an opportunity to expand people's understanding of chemical reactions in general.

"We are probing phenomena that are possibly occurring in nature," Zhu said. "We can try to broaden our concept to other chemical reactions. Although the electronic structure of KRb might be different, the idea of interference in reactions could be generalized to other chemical systems as well."

Sci Tech Daily, 26 May 2024

https://scitechdaily.com

New molecule found to suppress bacterial antibiotic resistance evolution

2024-05-28

Researchers from the University of Oxford have developed a new small molecule that can suppress the evolution of antibiotic resistance in bacteria and make resistant bacteria more susceptible to antibiotics. The paper, "Development of an inhibitor of the mutagenic SOS response that suppresses the evolution of quinolone antibiotic resistance," has been published in the journal Chemical Science.

The global rise in antibiotic-resistant bacteria is one of the top global public health and development threats, with many common infections becoming increasingly difficult to treat. It is estimated that drug-resistant bacteria are already directly responsible for around 1.27 million global deaths each year and contribute to a further 4.95 million deaths. Without the rapid development of new antibiotics and antimicrobials, this figure is set to rise significantly.

A new study led by researchers at the Ineos Oxford Institute for antimicrobial research (IOI) and the Department of Pharmacology at Oxford University offers hope in the discovery of a small molecule that works alongside antibiotics to suppress the evolution of drug-resistance in bacteria.

One of the ways that bacteria become resistant to antibiotics is due to new mutations in their genetic code. Some antibiotics (such as fluoroquinolones) work by damaging bacterial DNA, causing the cells to die. However, this DNA damage can trigger a process known as the "SOS response" in the affected bacteria.

The SOS response repairs the damaged DNA in bacteria and increases the rate of genetic mutations, which can accelerate the development of resistance to the antibiotics. In the new study, the Oxford scientists identified a molecule capable of suppressing the SOS response, ultimately increasing the effectiveness of antibiotics against these bacteria.

The researchers studied a series of molecules previously reported to increase the sensitivity of methicillin-resistant Staphylococcus aureus (MRSA) to antibiotics, and to prevent the MRSA SOS response. MRSA is a type of bacteria that usually lives harmlessly on the skin. But if it gets inside the body, it can cause a serious infection that needs immediate treatment with antibiotics. MRSA is resistant to all beta-lactam antibiotics such as penicillins and cephalosporins.

CHEMWATCH
Bulletin Board
Curiosities
MAY. 31, 2024

Researchers modified the structure of different parts of the molecule and tested their action against MRSA when given with ciprofloxacin, a fluoroquinolone antibiotic. This identified the most potent SOS inhibitor molecule reported to-date, called OXF-077. When combined with a range of antibiotics from different classes, OXF-077 made these more effective in preventing the visible growth of MRSA bacteria.

In a key result, the team then tested the susceptibility of bacteria treated with ciprofloxacin over a series of days to determine how quickly resistance to the antibiotic was developing, either with or without OXF-077. They found that the emergence of resistance to ciprofloxacin was significantly suppressed in bacteria treated with OXF-077, compared to those not treated with OXF-077.

This is the first study to demonstrate that an inhibitor of the SOS response can suppress the evolution of antibiotic resistance in bacteria. Moreover, when resistant bacteria previously exposed to ciprofloxacin were treated with OXF-077, it restored their sensitivity to the antibiotic to the same level as bacteria that had not developed resistance.

Phys Org, 28 May 2024

https://phys.org

Second Nobel prize medal for partition chromatography to be auctioned

2024-05-29

The 1952 Nobel prize in chemistry medal awarded to British biochemist Richard Synge for his groundbreaking invention of partition chromatography more than a decade earlier will be auctioned off at the end of May.

Partition chromatography can separate chemicals distributed between two liquid phases and it transformed the emerging field of molecular biology in the second half of the 20th century. It was used to demonstrate that purines from DNA were present in the same ratio as their pyrimidine partner, providing important information that helped in the elucidation of the molecule's structure. The technique also allowed the separation and subsequent sequencing of insulin, an achievement that resulted in Frederick Sanger winning the chemistry Nobel Prize in 1958, which later led to a treatment for diabetes.

Curiosities

MAY. 31, 2024

The Nobel prize medal awarded to British chemist Archer Martin, who invented partition chromatography along with Synge, was recently auctioned. It sold for £150,000 to a private collector in Europe in February 2023.

Other chemistry Nobel prize medals that have recently been sold include German chemist Adolf von Baeyer's 1905 award, which recognised his work on organic dyes and hydroaromatic compounds, fetched £203,000 in December 2023, and in the same week Arne Tiselius' medal, won by the Swedish biochemist in 1948 for his electrophoresis research, sold for $125,000 (£98,000). Earlier that year, George Olah's Nobel medal, awarded in 1994 for his work on carbocations, sold at auction for $250,000 and Walter Kohn's award for the development of density functional theory sold in 2022 for nearly $460,000.

Synge's medal, which is made of 23-carat gold, will be auctioned by Nate Sanders on 30 May. It is accompanied by a red leather Nobel presentation case with his name tooled on the lid. The reserve price for the medal has been set at $150,000.

Chemistry World, 29 May 2024

https://chemistryworld.com

CHEMWATCH
Bulletin Board

Technical Notes

MAY. 31, 2024

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

CHEMICAL EFFECTS

AFB1 Toxicity in Human Food and Animal Feed Consumption: A Review of Experimental Treatments and Preventive Measures

Widespread 2013-2020 decreases and reduction challenges of organic aerosol in China

A review on micro- and nanoplastics in humans: Implication for their translocation of barriers and potential health effects

ENVIRONMENTAL RESEARCH

Evaluation of Germicidal Ultraviolet-C disinfection in a Real-World Outpatient Healthcare Environment

Bioaccumulation of polycyclic aromatic hydrocarbons and their human health risks depend on the characteristics of microplastics in marine organisms of Sanggou Bay, China

PHARMACEUTICAL/TOXICOLOGY

Sensitization to Food and Aero-Allergens in Children with Coeliac Disease Assessed with the Use of a Multiplex Molecular Diagnostic Technique

Development and Evaluation of a Novel Antibacterial Wound Dressing: A Powder Preparation Based on Cross-Linked Pullulan with Polyhexamethylene Biguanide for Hydrogel-Transition in Advanced Wound Management and Infection Control

Bloodstream Infection Caused by Erysipelothrix rhusiopathiae in an Immunocompetent Patient

OCCUPATIONAL

Glyphosate contamination of drinking water and the occurrence of oxidative stress: exposure assessment to rural Brazilian populations

Occupational exposure, carcinogenic and non-carcinogenic risk assessment of formaldehyde in the pathology labs of hospitals in Iran