CHEMWATCH

Bulletin Board

Contents

MAY. 17, 2024

(click on page numbers for links)

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CHEMWATCH

Bulletin Board

Contents

MAY. 17, 2024

CHEMWATCH

Bulletin Board

Contents

MAY. 17, 2024

ASIA PACIFIC

Pesticide used in building products first to be approved through new rapid assessment process

2024-04-17

Fletcher Building Products applied to use zinc borate in the manufacture of engineered wood products for the building industry, to control wood-decaying fungi and insects.

The new pathway for hazardous substance applications allows us to approve a substance via a rapid assessment if the same use has been approved by one of our recognised international regulators.

As of October 2023, these regulators are from Australia, Canada, the European Union, United Kingdom, and the United States – all of which regulate hazardous substances in a similar way to our own system.

In deciding to approve the application for zinc borate, we considered the rules for use set by the Australian Pesticides and Veterinary Medicines Authority and the US EPA, alongside information and assessments from the European Union Chemicals Agency.

Each application must still take into account Aotearoa New Zealand's unique environmental, social and cultural context.

"This new process is an important tool to streamline our application and assessment process for new substances that have been approved overseas," says Dr Lauren Fleury, Manager Hazardous Substances Applications.

"The zinc borate application took six working days to decide, and we've now approved another application using this pathway.

"We are proactively looking at whether other existing hazardous substance applications may meet the criteria, and we encourage applicants to contact us if they think their application may be eligible for this pathway."

Read More

17-04-24, NZ EPA

https://www.epa.govt.nz/news-and-alerts/latest-news/pesticide-used-in-building-products-first-to-be-approved-through-new-rapid-assessment-process/

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 17, 2024

Hydrogen cyanamide reassessment

2024-04-12

We are reassessing the use of hydrogen cyanamide, a restricted spray ingredient used in commercial orchards.

Hydrogen cyanamide has been used in Aotearoa New Zealand since 1988. It is used mainly in kiwifruit orchards to promote bud growth. It is also used in some apple, cherry, apricot, and kiwiberry crops, but to a lesser extent.

There are six hydrogen cyanamide products approved for use. They are restricted to commercial use and can only be used by trained professionals.

Latest application update

12 April 2024

The Decision-making Committee has formally closed the hearing as it considers it now has sufficient information to make its decision on the reassessment. The decision will be publicly notified by 27 May 2024, within 30 working days of the hearing being closed.

Direction and Minute WGT026 (PDF, 202KB)

13 March 2024

We've published the interim transcripts for the public hearing held from 26 February to 1 March 2024. The final versions will include transcription of the te reo Māori content.

Transcription for Monday 26 February (PDF, 759KB)

Transcription for Tuesday 27 February (PDF, 608KB)

Transcription for Wednesday 28 February (PDF, 741KB)

Transcription for Thursday 29 February (PDF, 353KB)

Transcription for Friday 1 March (PDF, 330KB)

1 March 2024

The hearing ran for the week of 26 February and was adjourned on 1 March 2024. The transcriptions are being prepared for publication. The hearing will be formally closed once the DMC are satisfied that they have enough information to make a decision on the reassessment.

Read More

NZ EPA, 30-04-24

https://www.epa.govt.nz/public-consultations/in-progress/hydrogen-cyanamide-reassessment/

Importing and exporting hydrofluorocarbon gases (HFCs)

2024-05-06

You need a permit to import or export bulk HFC gases into or out of New Zealand.

Under the law, "bulk HFC" means new or recycled HFC gas in an unprocessed form - alone or in a mixture - in a container used for gas transport or storage. HFCs in manufactured products, such as car air-conditioning systems or fire extinguishers, do not need an import or export permit.

Read More

NZ EPA, 06-05-24

https://www.epa.govt.nz/hazardous-substances/certificates-permits-and-permissions/hydrofluorocarbon-gases-hfcs-import-and-export/

Cutting lead levels in paints: proposed amendments to group standards

2024-05-24

We have published a submissions summary and EPA response document and are preparing for a hearing.

Submissions summary and EPA response

We received 24 submissions, which are available on our website.

See the submissions and all other application documents

We have published a summary of the submissions and our responses to the feedback received.

Submissions summary and EPA response (PDF, 465KB)

Submitters supported most of the proposals, and these remain unchanged.

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 17, 2024

The main proposals that received significant opposition were:

- the proposal to require accredited laboratory testing to show evidence of compliance with the lead limits.
- the proposal to remove the notification requirement from the Graphic Materials Group Standard.

Based on submitter feedback we have updated our proposal to require testing. We now recommend that the individual company should decide what evidence is suitable to meet the maximum lead level requirement. We no longer propose accredited laboratory testing as the only evidence accepted.

However, we maintain that the notification requirement in the Graphic Materials Group Standard should be removed as it is inconsistent and does not reflect the risk.

Read More

NZ EPA, 06-05-24

https://www.epa.govt.nz/public-consultations/in-progress/lead-in-paints/

AMERICA

Companies Legally Use Poison to Make Your Decaf Coffee

2024-05-04

Do you drink decaffeinated coffee? Are you aware that it's often made by applying a chemical so dangerous it was banned for use in paint stripper five years ago? And are you aware that companies think banning this chemical is really, really unfair?

This week the Environmental Protection Agency finalized a rule prohibiting all but "critical" uses of methylene chloride, a highly toxic liquid that is believed to have killed at least 88 people since 1980—mostly workers refinishing bathtubs or doing other home renovations. Methylene chloride can cause liver damage and is linked to multiple cancers, among other health effects. Amazingly, while the EPA banned its sale for paint stripping in 2019 for this reason, it continues to be used for a lot of other purposes. And one of those is decaffeinating coffee, because the Food and Drug Administration decided in the 1980s that the risk to coffee drinkers was low given how the coffee was processed.

The EPA's ban on noncritical use of methylene chloride is one of many rules the Biden administration has announced or finalized ahead of the Congressional Review Act deadline. (The CRA, essentially, makes it easier for an unfriendly Congress to nix any administrative regulations finalized in the last 60 days of a legislative session.) A lot of the recently announced rules ban or curtail toxic substances that have made their way into everyday life and are poisoning people. The EPA has limited long-lasting chemicals called PFAS in drinking water, requiring water utilities within five years to build treatment systems that remove it. The agency has categorized two types of PFAS as hazardous substances under the Superfund law, requiring manufacturers to monitor whether they've been released into the environment and, if so, clean them up. It has also—finally—fully banned asbestos. It's finalized a rule to further restrict fine particulate pollution in the air, which has been linked to heart disease, heart attacks, asthma, low birth weight, Alzheimer's, and other forms of dementia. It's in the process of finalizing a rule reducing lead in drinking water, which would require the replacement of lead pipes throughout the nation.

Read More

New Republic, 04-05-24

https://newrepublic.com/post/181229/companies-poison-decaf-coffee

PFAS in water growing concern, UMES hosts session with stakeholders; lessons learned from Maine

2024-05-05

The University of Maryland Eastern Shore late last month hosted a discussion on PFAS with representatives from federal and state agencies, researchers and Maine stakeholders.

The man-made forever chemicals began getting public attention in 2021 in Maine, which has since become a model for other states as PFAS becomes an emerging concern.

"The focus of this collaborative workshop is a better understanding of PFAS garnered from those who have experienced its challenges and those resolved to finding solutions and ways to move forward," said Dr. Moses T. Kairo, dean of UMES' School of Agricultural and Natural Sciences.

"Our goal as a university is to identify the research, outreach and support we can provide citizens of Maryland in addressing these issues through

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 17, 2024

our Agricultural Experiment Station, UMES Extension and by exploring the establishment of a dedicated center."

Dr. Greg Allen, an environmental scientist with the Environmental Protection Agency's Chesapeake Bay Program Office and UMES alumnus, said the agency is finding that per- and polyfluoroalkyl (PFAS) substances are widely distributed in the environment.

"They have one of the strongest chemical bonds we know of, leading to its persistence and bioaccumulation. This perfect storm will be part of the environmental landscape and for a very long time. It will be in every corner of what EPA does."

There are an estimated 12,000 compounds in this classification, Allen said. They have been used commercially for water-repellent properties in paper goods, food packaging and clothing, stain resistance, non-stick cookware and firefighting foam among them.

The scenario for concern is their leaching into groundwater through effluents and biosolids with the potential to enter agriculture and fisheries.

Read More

Bay To Bay News, 05-05-24

https://baytobaynews.com/stories/pfas-in-water-growing-concern-umes-hosts-session-with-stakeholders-lessons-learned-from-maine,134463

What the Hazardous Substance Designation of PFAS Chemicals Means for Local Governments

2024-05-06

On April 19, the U.S. Environmental Protection Agency (EPA) released a final rule designating perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) as hazardous substances under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), also known as the Superfund law. PFOA and PFOS are two of the most widely used and widely studied PFAS chemicals.

NLC has been tracking this rulemaking since 2022 and sharing local government concerns with the EPA. While the recently finalized EPA drinking water regulation for PFAS creates an unfunded mandate for local governments, this CERCLA rule is likely to have significant economic impacts, as well as unintended consequences, for local governments. As

such, the NLC urges Congress to act to protect local governments and provide additional resources.

What Does a CERCLA Designation Mean?

With this final rule, PFOA and PFOS are added to the list of over 800 hazardous substances regulated by the EPA. As with all the elements, compounds, mixtures, and solutions designated as hazardous substances, any entity that releases a substance over the allowed limit (in the case of PFOA and PFOS: one pound) needs certain notification and reporting steps.

This final rule does not contain any immediate or required actions for investigation or cleanup in the traditional sense.

- CERCLA is a discretionary statute and decisions about whether to pursue enforcement action are made on a site-by-site basis based on whether releases pose an unacceptable risk to human health or the environment.
- CERCLA allows EPA to take action and respond to and clean up contaminated sites without having to first make a separate finding that a release, or a threat of release, "may present an imminent and substantial danger."
- CERCLA enables EPA to pursue parties responsible for significant contamination for enforcement action and costs related to investigation, cleanup, or exposure mitigation, adhering to the "polluter pays" model. Holding polluters accountable and responsible will have benefits for communities.

Read More

NLC, 06-05-24

https://www.nlc.org/article/2024/05/06/what-the-hazardous-substance-designation-of-pfas-chemicals-means-for-local-governments/

Michigan Takes Step to Limit PFAS Through Hazardous Products Act

2024-05-06

The State of Michigan recently took another step aimed at protecting the environment and public health from the impact of per- and polyfluoroalkyl substances (PFAS). Last week, State Rep. Penelope Tsernoglou (D-East Lansing) and Majority Floor Leader Abraham Aiyash (D-Hamtramck) introduced The Hazardous Products Act under House Bill 5657 (the

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 17, 2024

"Legislation"), which would prohibit, the sale and distribution of products containing intentionally added PFAS by Jan. 1, 2027, including, without limitation, cookware, cosmetics, and children's products. The Legislation would also prohibit the discharge or use of PFAS-containing class A or class B firefighting foam by Jan. 1, 2027. The Legislation has roughly 20 co-sponsors and was referred to the Michigan House's Natural Resources Committee.

If enacted, the Legislation would ban the sale of products that contain intentionally added PFAS. The Legislation defines "PFAS" as a "perfluoroalkyl or polyfluoroalkyl substance that includes any member of the class of fluorinated organic chemicals containing at least 1 fully fluorinated carbon atom." Under the Legislation, PFAS is intentionally added if the PFAS added by a manufacturer "has a functional or technical effect on a product, or a component thereof, or the manufacturing process. Intentionally added PFAS includes any PFAS that is a component or a breakdown product of an intentionally added chemical that has a functional or technical effect on the product, or a component thereof, or the manufacturing process."

Beginning Jan. 1, 2027, the Legislation would also require the manufacturer of a product sold in Michigan and containing intentionally added PFAS to submit to Michigan's Department of Environment, Great Lakes, and Energy (EGLE), and any person that will sell, offer, or distribute the product for sale, a notice with the following information: (a) a description of the product; (b) information regarding why PFAS was added to the product; (c) the amount of PFAS used in the product; (d) the name, address, and telephone number of the manufacturer and its agent; and (e) any additional, relevant information.

Similar to Amara's Law in the state of Minnesota, the Legislation would allow EGLE to exempt certain products or components if EGLE determines those products meet the definition of a "currently unavoidable use." The Legislation defines "currently unavoidable use" as a use of PFAS that EGLE has determined by rule to be temporarily essential if all of the following are met:

• There are no reasonably available safer alternatives to the PFAS that are used in the product;

• The PFAS's function in the product is necessary for the product to work; and

• The PFAS is being used in a product that is critical for health, safety, or the function of society.

Read More

Lexology, 06-05-24

https://www.lexology.com/library/detail.aspx?g=a5987141-9a71-4d2e-95dc-025b210d215d

EUROPE

Air pollution measures 'will reduce thousands of premature adult deaths in the UK'

2024-04-06

Existing air pollution regulations will reduce thousands of premature adult deaths in the UK, a study has revealed.

Research by University College London found that air pollution policies could prevent 6,751 early deaths amongst adults in the UK by 2030 compared to if no regulations existed.

That estimate nearly doubles to 13,269 avoided deaths if all possible measures are employed to reduce air pollution and emissions immediately, such as installing more efficient home stoves and boilers and stricter emission standards for vehicles.

For the study, UCL academics looked at a range of pollutants and their effects on people and the environment. They then calculated their projected effects in the coming decade based on current levels of regulation.

The researchers found that the amount of fine particulate matter in the atmosphere, the air pollutant most harmful to human health, can be significantly reduced.

More than 600 premature deaths could be prevented in London if ministers implement the full range of possible environmental policies, the study found. The capital has by far the worst exposure to PM2.5, a harmful pollutant, than any other region in the country.

The study comes months after Mayor of London Sadiq Khan expanded the ultra low emission zone (ULEZ) to all 32 of the capital's boroughs in a bid to reduce air pollution.

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 17, 2024

Read More

News. yahoo, 06-04-24

https://ca.news.yahoo.com/air-pollution-measures-reduce-thousands-130058158.html

INTERNATIONAL

New AI method can detect toxic chemicals

2024-05-04

By utilizing artificial intelligence, researchers at Chalmers University of Technology and the University of Gothenburg in Sweden have developed a method to enhance the identification of toxic chemicals based solely on their molecular structure. This AI method can assist in better regulating the growing number of chemicals used in society, while also reducing reliance on animal testing. Chemicals are prevalent in various products and processes, posing risks to humans and the environment when they enter waterways. PFAS, a group of problematic substances, has been found in alarming concentrations in groundwater and drinking water, highlighting the need for effective toxicity assessments.

Despite existing chemical regulations, negative effects persist, necessitating time-consuming animal testing to establish safety standards. With over two million animals used annually in the EU alone for regulatory compliance, the rapid development of new chemicals presents challenges in determining toxicity. The AI method developed by Swedish researchers offers a cost-effective solution for assessing chemical toxicity early on, minimizing the need for extensive animal testing. By training on large datasets from past laboratory tests, the method accurately predicts toxic properties of previously untested chemicals based on their chemical structures.

Read More

Globe Echo, 04-05-24

https://globeecho.com/new-ai-method-can-detect-toxic-chemicals/

Peru continues to give permits for Europe's banned pesticides

2024-05-06

Flexible laws and limited controls have enabled Europe-based agrochemical company Syngenta to register 42 pesticides banned at home for use in Peru

worn cloth rag was the only protection used by a young Lorgio Ñaupas during his early years spraying pesticides in cotton fields. Looking back decades later, he recalls unpleasant memories.

"I almost died once. I was spraying for a whole week, I had a headache and was vomiting," says the 57-year-old, who now works on a farm in the Chillón Valley, north of Peru's capital, Lima. He also remembers the day he accidentally spilled paraquat, a herbicide, on the leg of one of his sons, wounding him and leaving a scar that remains to this day.

Ñaupas says his bad experiences were a reminder that pesticides are not only a potent poison for pests and weeds, but also potentially dangerous chemicals that can have damaging impacts on health and the land. They motivated him to dedicate his work to agroecology, which promotes more sustainable practices that encourage reductions in pesticide use.

"Why do we allow dangerous agrochemicals, and aren't there other ways to avoid poisoning ourselves?" Ñaupas asks.

For this investigation, led by Salud Con Lupa in collaboration with Dialogue Earth, we began by analysing the pesticide market in Peru. What was most striking is that the system for evaluating and authorising pesticides in many countries allows large companies, such as the Switzerland-based, Chinese-owned company Syngenta, to register and sell pesticides that are otherwise banned in their home countries, taking advantage of more permissive regulations such as those in Peru.

Unlike countries such as Chile and Costa Rica, or the European Union, Peru does not issue authorisations for the use of individual pesticides for ten-year periods; rather, many of its pesticide registrations have been valid indefinitely since the 1990s.

This means that after a company receives authorisation to sell a product, its impacts will not be re-evaluated with more recent scientific information or studies, unless extraordinary initiatives to do so are launched by regulatory bodies. Under these regulations, Syngenta currently has

CHEMWATCH
Bulletin Board
Regulatory Update
MAY. 17, 2024

registrations in Peru for the sale of 42 pesticides that are banned in the EU and Switzerland.

Read More

Dialogue Earth, 06-05-24

https://dialogue.earth/en/business/peru-continues-to-give-permits-for-europes-banned-pesticides/

New research on flavoured vapes shows potential for 'a new wave of chronic diseases'

2024-05-08

NEW VAPING RESEARCH highlights the need for urgent public health policies, according to a study by the Royal College of Surgeons in Ireland (RCSI).

The study found that many of the chemicals used to flavour vapes are harmful once heated for inhalation.

127 hazardous chemicals formed were classed as 'acute toxic', while 153 are 'health hazards'. A further 225 were classed as 'irritants'.

Lead author of the report Professor Donal O'Shea said that the findings were very concerning.

"We wanted to understand, before it's too late, the likely impact flavoured vapes are having on the health of the growing number of vapers." He said that the findings show a different profile of chemical hazards compared to traditional tobacco smoking.

"It is plausible that we are on the cusp of a new wave of chronic diseases that will emerge 15 to 20 years from now due to these exposures." Speaking to The Journal, he said, "I think we need to dramatically reduce the number of different chemicals that are in the vaping solutions.

"I think we need regulation on the vaping devices themselves, in terms of disposable vapes and reusable vapes and that they are regulated into what type of temperatures they can reach and the correct disposal of them." He said that he hopes the new research will help people make more informed choices, and contribute to the conversation surrounding the regulation of vaping. In the UK, Prime Minister Rishi Sunak announced a ban on a single-use vapes from April 2025 as part of his plan to create the UK's first smoke-free generation.

However, O'Shea doesn't believe that an overall ban would work in Ireland. "They could be through a more controlled environment like a pharmacy, for those who may feel like they may help them with quitting tobacco smoking.

Read More

The Journal, 08-05-24

https://www.thejournal.ie/vaping-research-regulation-6373898-May2024/

CHEMWATCH
Bulletin Board

Restriction proposal on chromium (VI) to cover more substances

2024-05-08

The European Commission has requested ECHA to broaden the scope of the REACH restriction proposal to cover at least 12 chromium (VI) substances.

Helsinki, 8 May 2024 – ECHA has received an updated mandate from the Commission to prepare a proposal for a possible restriction on chromium (VI) substances. This update complements the original request from September 2023, which focused on two entries currently listed on the REACH Authorisation List, namely chromium trioxide (entry 16) and chromic acids (entry 17).

The updated mandate now includes the chromium (VI) substances specified in entries 16 to 22 and 28 to 31 of the REACH Authorisation List. In addition, ECHA has been requested to consider in the restriction proposal other chromium (VI) substances not listed on the Authorisation List, in particular barium chromate (EC number 233-660-5). These substances may pose risks to workers and the public if used as substitutes for chromium (VI) substances subject to authorisation.

Given the wider scope, ECHA will submit the restriction proposal by 11 April 2025, instead of the originally planned date of 4 October 2024.

ECHA will launch a second call for evidence to support the preparation of the proposal in June. Questions will cover a broad range of topics such as alternatives to chromium (VI) substances and how chromium (VI) is used in spraying applications. Any information provided by stakeholders during the first call for evidence will be considered and does not need to be resubmitted. ECHA will organise a webinar on 6 June 2024 to discuss the main outcomes of the first call for evidence and highlight the additional data requested in the second call.

The preparation of the restriction proposal and its evaluation by RAC and SEAC will follow the standard REACH restrictions process. In preparing the proposal, ECHA will consider the knowledge and experience it has gained from processing applications for authorisation for these substances.

Read More

ECHA, 08-05-24

https://echa.europa.eu/-/restriction-proposal-on-chromium-vi-to-cover-more-substances

One Health: joint framework for action published by five EU agencies

2024-05-07

Today, the European Centre for Disease Prevention and Control (ECDC), European Chemicals Agency (ECHA), European Environment Agency (EEA), European Food Safety Authority (EFSA), and European Medicines Agency (EMA) published a joint framework for action to strengthen cooperation to support the implementation of the One Health agenda in the European Union (EU).

One Health recognises the complex interplay between human, animal and plant health, food safety, the climate crisis, and environmental sustainability. Implementing this approach across different sectors will be key to make the EU and its Member States better equipped to prevent, predict, detect, and respond to health threats. It will mitigate the impact and societal cost of such threats, or even prevent their emergence, while also helping to reduce human pressures on the environment and safeguarding key societal needs such as food security and access to clean air and water.

A cross-agency task force will work on implementing the joint framework for action over the next three years (2024-2026), focusing on five strategic objectives: strategic coordination, research coordination, capacity building, stakeholder engagement, and joint inter-agency activities. This will ensure that the scientific advice provided by the agencies is increasingly integrated, that the evidence base for One Health is strengthened, and that the agencies are able to contribute with a common voice to the One Health agenda in the EU.

In November 2023, the five EU agencies that provide scientific advice on the environment, public health, and food safety topics issued a joint statement expressing their shared commitment to supporting the One Health agenda in Europe.

CHEMWATCH
Bulletin Board
REACH Update
MAY. 17, 2024

On the occasion of the launch of the joint framework for action the Executive Directors of the five EU Agencies reinforced their commitment to the One Health approach in a joint video statement.

Read More

ECHA, 07-05-24

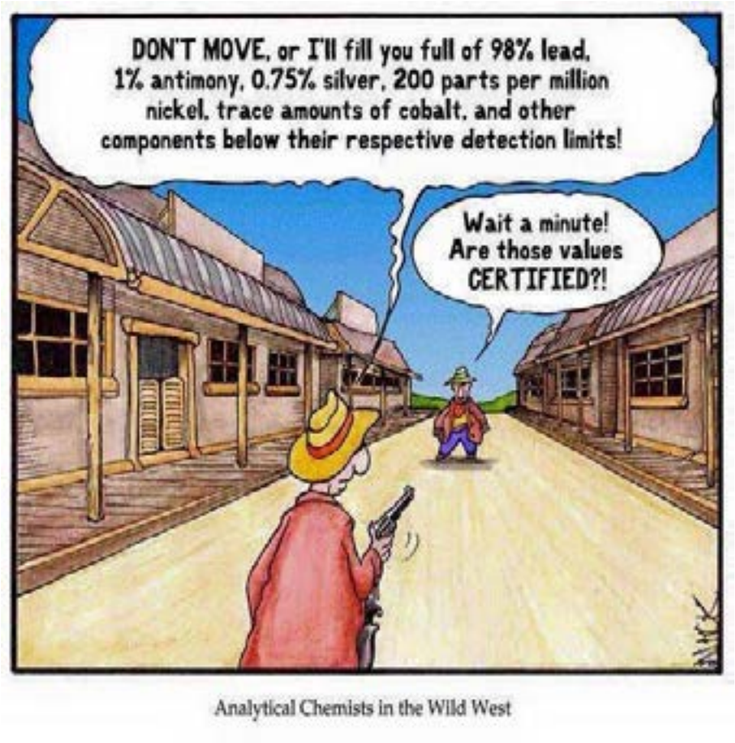
https://echa.europa.eu/-/one-health-a-joint-framework-for-action-published-by-five-eu-agencies

Janet's Corner

MAY. 17, 2024

Analytical Chemists in the Wild West

2024-05-17



Analytical Chemists in the Wild West

https://mobile.twitter.com/chemistryjokes

CHEMWATCH
Bulletin Board

Hazard Alert

MAY. 17, 2024

Beryllium

2024-05-17

lightweight, primarily used as hardening agent in alloys. Beryllium has one of the highest melting points of the light metals. It has excellent thermal conductivity, is nonmagnetic, it resists attack by concentrated nitric acid and at standard temperature and pressures beryllium resist oxidation when exposed to air. Beryllium is a naturally occurring element that is present in rocks, coal, oil, soil, and volcanic dust. Some beryllium compounds are soluble in water. Two kinds of minerals, bertrandite and beryl, are commercially mined for the recovery of beryllium. The majority of beryllium that is mined is converted into alloys. [1,2]

USES [2,3]

Industrial grade beryl is used as a feedstock for beryllium metal, alloys and oxide, all of which have many high-tech applications particularly in the nuclear, electronic and ceramic industries. Beryllium is a structural material in space technology, inertial guidance systems, additive in rocket fuels, moderator and reflector of neutrons in nuclear reactors (e.g. at ANSTO, Lucas Heights). Pure beryllium metal is used to make aircraft disc brakes, nuclear weapons and reactors, aircraft-satellite-space vehicle structures and instruments, X-ray transmission windows, missile parts, fuel containers, precision instruments, rocket propellants, navigational systems, heat shields, and mirrors. Beryllium alloys such as beryllium-copper are used in electrical connectors and relays, springs, precision instruments, aircraft engine parts, non-sparking tools, submarine cable housings and pivots, wheels, and pinions. More specifically, beryllium oxide is used in the manufacture of specialty electrical and high-technology ceramics, special glass, electronic heat sinks, electron tubes, electrical insulators, electronics components, microwave oven components, nuclear fuels and nuclear moderators, gyroscopes, military vehicle armour, rocket nozzles, and laser structural components. Beryllium chloride is used in refining beryllium ores and as a chemical reagent. Beryllium fluoride is used in refining beryllium and manufacturing beryllium alloys, and as a chemical reagent. Beryllium nitrate is used as a chemical reagent, a gas mantle hardener and in refining beryllium ores.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Exposure Sources

- **Industry sources:** Mining of ores containing beryllium can contribute to higher levels in air, soil and water, i.e. small quantities of beryl are produced as a by-product of feldspar mining at Broken Hill (NSW). Emissions to air can result from combustion of coal and oil in power plants.
- **Diffuse sources:** Some hazardous waste sites and tobacco smoke.
- **Natural sources:** Pure beryllium is not found in nature. Beryllium compounds can be found in mineral rocks, soil, coal, oil, and volcanic dust.
- **Transport sources:** Beryllium emissions are normally not associated with mobile sources.
- **Consumer products:** Small quantities can be found in products such as personal computers, televisions, calculators, and microwave ovens.

Routes of Exposure

- **Inhalation** – Predominant route of exposure for the general and occupational populations.
- **Oral** – Major route of exposure for the general populations.
- **Dermal** – Minor route of exposure for general and occupational populations.

HEALTH EFFECTS [4]

Acute Health Effects

Acute inhalation exposure to high levels of beryllium has been observed to cause inflammation of the lungs and acute pneumonitis (reddening and swelling of the lungs) in humans; after exposure ends, these symptoms may be reversible. Acute animal tests have demonstrated beryllium compounds to vary in acute toxicity, ranging from high to extreme acute toxicity from oral exposure.

Carcinogenicity

Several human epidemiological studies have investigated the relationship between beryllium exposure in workers and lung cancer deaths. Although there are shortcomings in all the studies, the results are suggestive of a causal relationship between beryllium exposure and an increased risk of lung cancer. Beryllium compounds have been shown to cause lung cancer

CHEMWATCH
Bulletin Board
Hazard Alert
MAY. 17, 2024

from inhalation exposure in rats and monkeys. EPA has classified beryllium as a Group B1, probable human carcinogen.

Other Effects

The potential for beryllium to induce developmental or reproductive effects has not been adequately assessed. Limited information is available on the reproductive or developmental effects of beryllium in humans following inhalation exposure. A case control study found no association between paternal occupational exposure and the risk of stillbirth, pre-term delivery, or small-for-gestational-age infants, although this study has limited sensitivity. No data are available on reproductive or developmental effects in animals following inhalation.

SAFETY

First Aid Measures [5]

- **Inhalation:** Breathing difficulty caused by inhalation of particulate requires immediate removal to fresh air. If breathing has stopped, perform artificial respiration and obtain medical help.
- **Ingestion:** Induce vomiting immediately as directed by medical personnel. Never give anything by mouth to an unconscious person.
- **Skin:** Thoroughly wash skin cuts or wounds to remove all particulate debris from the wound. Seek medical attention for wounds that cannot be thoroughly cleansed. Treat skin cuts and wounds with standard first air practices such as cleansing, disinfecting and covering to prevent wound infection and contamination before continuing work. Obtain medical help for persistent irritation. Material accidentally implanted or lodged under the skin must be removed.
- **Eyes:** Immediately flush eyes with plenty of water for at least 15 minutes, lifting lower and upper eyelids occasionally. Get medical attention immediately.

Treatment of Chronic Beryllium Disease: There is no known treatment that will cure chronic beryllium disease. Prednisone or other corticosteroids are the most specific treatment current available. They are directed at suppressing the immunological reaction and can be effective in diminishing signs and symptoms of chronic beryllium disease. In cases where steroid therapy has had only partial or minimal effectiveness, other immunosuppressive agents, such as cyclophosphamide, cyclosporine, or methotrexate, have been used. These latter agents remain investigational. Further, in view of the potential side effects of all the immunosuppressive

medications, including steroids such as prednisone, they should be used only under the direct care of a physician. In general, these medications should be reserved for cases with significant symptoms and/or significant loss of lung function. Other symptomatic treatment, such as oxygen, inhaled steroids, or bronchodilators, may be prescribed by some physicians and can be effective in selected cases.

Workplace Controls & Practices [4]

- Whenever possible, the use of local exhaust ventilation or other engineering controls is the preferred method of controlling exposure to airborne particulate. Where utilised, exhaust inlets to the ventilation system must be positioned as close as possible to the source of airborne generation. Avoid disruption of the airflow in the area of a local exhaust inlet by equipment such as a man-cooling fan. Check ventilation equipment regularly to ensure it is functioning properly. Provide training on the use and operation of ventilation to all users. Use qualified professionals to design and install ventilation systems.
- Machining operations conducted under a flow of liquid coolant require compete hooded containment and local exhaust ventilation. Openings into the hood must be baffled to prevent release of fast moving particulate. The cycling through a machine of liquid lubricant/coolant containing finely divided beryllium particulate in suspension can result in the concentration building to a point where the particulate may become airborne during use. Prevent coolant from splashing onto floor areas, external structures or operators' clothing. Utilise a coolant filtering system to remove particulate from the coolant.

Personal Protective Equipment [5]

Respiratory Protection

- When airborne exposures exceed or have the potential to exceed the occupational limits, approved respirators must be used as specified by an Industrial Hygienist or other qualified professional.
- Exposure to unknown concentrations of particulate requires the wearing of a pressure-demand airline respirator or pressure-demand self-contained breathing apparatus (SCBA). Use pressure-demand airline respirators when performing jobs with high potential exposures such as changing filters in a baghouse air cleaning device.

CHEMWATCH
Bulletin Board
Hazard Alert
MAY. 17, 2024

REGULATION

United States

- ACGIH has set a time weighted average (TWA) of 0.05 µg/m3 and a short-term exposure limit (STEL) of 0.2 µg/m3
- NIOSH has established a 10-hour TWA of 0.5 µg/m3
- OSHA regulation for beryllium and its compounds is an 8-hour time-weighted average (TWA) of 2 micrograms (as beryllium) per cubic metre of air (2 µg/m3). An employee should not be exposed to a concentration of beryllium and beryllium compounds exceeding 5 µg/m3. The 30-minute maximum peak level is 25 µg/m3.
- EPA has designated beryllium a hazardous air pollutant under the Clean Air Act. Accordingly, beryllium emissions from stationary sources cannot exceed 10 g (0.022 lbs) over a 24-hour period. Ambient air concentrations averaged over a 30-day period near stationary sources must not exceed 0.01 µg/m3. In water, the EPA has set an advisory of less than 68 nanograms of beryllium per litre (ng/L) for consumption of 2 L of ambient water per day.

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UV Method Helps To Clean Up Harmful PFAS

2024-05-13

Aqueous film-forming foam (AFFF) is incredibly efficient at putting out fires. These foams form an aqueous film over burning gasoline, fuels and other flammable liquids, which quickly deprives the blaze of oxygen and extinguishes it. For this reason, AFFF is often used for rapid fire suppression on military bases and at commercial airports.

But, while lifesaving in one way, AFFF also comes with significant health risks of its own; the foam is full of per- and polyfluoroalkyl substances (PFAS). Sustained exposure to these chemicals has been linked to serious health problems, including reproductive issues and an increased risk of some cancers. Recent assessments of 715 military sites carried out by the US Department of Defense have found concerningly high levels of PFAS at 574 sites due to the use of AFFF, with the federal government now requiring cleanups or further investigations.

But how exactly do you clean up PFAS contamination? Researchers at the University of California Riverside (UCR) and Clarkson University think they have an answer. Published in Nature Water, the researchers' new method promises to destroy nearly all the PFAS compounds present in AFFF-contaminated water.

Using light to tackle PFAS contamination

The new treatment method involves using ultraviolet (UV) light in conjunction with a sulfite–electrochemical oxidation process to degrade PFAS and other organic chemicals present in AFFF.

"In this work, we continued our research on the UV-based treatment, but this time, we had a collaboration with an electrochemical oxidation expert at Clarkson University," said Jinyong Liu, an associate professor of chemical environmental engineering at UCR, who has published nearly 20 papers on treating PFAS pollutants in contaminated water. "We put these two steps together and we achieved near-complete destruction of PFAS in various water samples contaminated by the foams."

Water contamination by AFFF foams is a surprisingly tricky nut to crack. In addition to PFAS, these foams can also release other unwanted organic compounds into the water, which can hinder attempts to break the strong carbon–fluorine bonds in PFAS and make their remediation even more difficult.

CHEMWATCH
Bulletin Board
Gossip
MAY. 17, 2024

Liu's team had previously worked on a PFAS eradication method using UV light and sulfite that was able to destroy up to 90% of these carbon–fluorine bonds. Now, by incorporating the expertise from the Clarkson University electrochemical oxidation group, the team's hybrid method promises to realize the "near-complete defluorination and mineralization of most PFAS and organics in AFFF" by targeting the organics too.

Cleansing highly contaminated groundwater

The team said that their new decontamination method is well suited for cleansing the highly contaminated water that results from flushing out used tanks, containers, hoses and other firefighting equipment.

They also believe that the method could help water utilities deal with polluted groundwater. One common method for tackling PFAS-contaminated groundwater is the use of ion exchange resin beads, which "grab" onto PFAS molecules and help with their removal. By combining this with the new photo-electrochemical process, Liu hopes that it should be possible to regenerate and recycle these beads, making the water treatment process more sustainable overall.

"We want to have sustainable management of the resin," Liu said. "We want to reuse it."

Technology Networks, 13 May 2024

https://technologynetworks.com

Chemists succeed in synthesizing a molecule first predicted 20 years ago

2024-05-14

The first and the best-known metallocene is "ferrocene," which contains a single iron atom. Today, sandwich complexes can be found in many inorganic chemistry textbooks, and the bonding and electronic structure of metallocenes is taught in undergraduate chemistry lecture courses. Sandwich molecules also play an important role in industry, where they are used as catalysts and in the synthesis of special metallopolymers.

Nobody knows exactly how many sandwich molecules there are today, but the number is certainly in the thousands. And they all have one thing in common: a single metal atom located between two flat rings of carbon atoms.

At least that was what was thought up until 2004, when a research group from the University of Seville made a startling discovery. The Spanish research team succeeded in synthesizing a sandwich molecule that contained not one but two metal atoms. For a long time, this "dimetallocene" containing two zinc atoms remained the only example of its kind until a group in the UK succeeded last year in synthesizing a very similar molecule that contained two beryllium atoms.

But now, Inga Bischoff, a doctoral student in Dr. André Schäfer's research team at Saarland University, has taken things one big step further. She has managed to synthesize in the laboratory the world's first 'heterobimetallic' sandwich complex—a dimetallocene that contains two different metal atoms.

Shortly after the discovery of the first dimetallocene in 2004, theoretical work indicated that dimetallocenes do not necessarily have to contain two identical metal atoms, and that a complex with two different metal atoms should also be stable. These predictions were made on the basis of quantum-chemical modeling calculations using powerful computers. Despite this predicted stability, all attempts to create such a molecule in the lab were unsuccessful until Bischoff's current breakthrough.

"It is really exciting and special when you realize what you're holding in your hands. To the naked eye, it just looks like another white powder. But I can still clearly remember the moment when we first saw the experimentally determined molecular structure on the computer screen and we knew that we had a sandwich molecule with two different metal atoms," said Dr. Schäfer.

"Which carbon rings you choose is just as important as which metal atoms you want to enclose between them. This is critical because the electronic structures of the cyclic carbon rings and the metal atoms have to match one another," explained Bischoff.

"The metals contained in our 'heterobimetallic dimetallocene' are lithium and aluminum. Calculations predicted that these two metals would be suitable candidates because their electronic structure is in some senses similar to that of two zinc atoms, which we knew could form a stable dimetallocene."

But what sounds so simple and straightforward took months to achieve. The molecule turns out to be so reactive that it can only be synthesized, stored and analyzed under an inert nitrogen or argon blanket. If it came into contact with air, it would simply decompose.

CHEMWATCH
Bulletin Board
Gossip
MAY. 17, 2024

Once it had been synthesized, the molecule needed to be characterized, which involved a whole team of scientists from Saarland University. The results of their work have now been published in Nature Chemistry.

"Our heterobimetallic dimetallocene represents what is effectively a whole new class of sandwich molecules," said group lead Dr. Schäfer. "Who knows, maybe it will also be included in a student textbook one day. But first of all, we need to study it further.

"At the moment, we have a pretty good understanding of its structure, but still know very little about its reactivity. If we find other suitable combinations of metal atoms, it may well prove possible in future to synthesize other heterobimetallic dimetallocenes."

Phys Org, 14 May 2024

https://phys.org

Research explores ways to mitigate the environmental toxicity of ubiquitous silver nanoparticles

2024-05-10

Nanoparticles are tiny pieces of material ranging in size from one- to 100-billionths of a meter. In addition to their antimicrobial properties, silver nanoparticles are industrially important as catalysts and in electronics applications.

Despite their ubiquity, little is known about their environmental toxicity or how it might be mitigated.

Researchers at Oregon State University have taken a key step toward closing the knowledge gap with a study that indicates the particles' shape and surface chemistry play key roles in how they affect aquatic ecosystems.

The findings, published in Nanomaterials, are important because they suggest silver nanoparticles can be produced in formats that preserve their beneficial properties while limiting environmentally negative ones.

Scientists led by Marilyn Rampersad Mackiewicz and Stacey L. Harper assessed how spherical and triangular-shaped silver nanoparticles with five different surface chemistries affected their uptake and toxicity in a laboratory microcosm of bacteria, algae, Daphnia and embryonic zebrafish.

Daphnia are tiny crustaceans, and zebrafish are a small freshwater species that go from a cell to a swimming fish in about five days.

Zebrafish are particularly useful for studying the development and genetics of vertebrates, including the effects of environmental contaminants and pharmaceuticals on early embryonic development. They share a remarkable similarity to humans at the molecular, genetic and cellular levels; embryonic zebrafish are of special interest because in addition to developing quickly, they are transparent and can be easily maintained in small amounts of water.

The authors note that hundreds of tons of silver nanoparticles are produced every year for commercial uses, meaning it's inevitable some will end up in aquatic environments.

"Silver nanoparticles are not regulated by the Food and Drug Administration and not much is known about their toxicity except for the free silver ions that can result from surface oxidation of the nanoparticles," said Mackiewicz, assistant professor of chemistry. "Free silver ions are known to be toxic and in this paper we found a way to study the toxicity of silver nanoparticles and how they impact the environment irrespective of poisonous silver ions."

Mackiewicz, Harper and collaborators in the OSU colleges of Science, Engineering and Agricultural Sciences found silver nanoparticles negatively affect some species but not others.

"For example, there is a decrease in bacterial and Daphnia growth, and the size and shape of the particles can contribute to that, but the nanoparticles didn't affect zebrafish," she said. "And nanoparticles coated in lipids, organic compounds found in many natural oils and waxes, did not release significant amounts of silver ions -- but they exhibited the greatest toxicity to Daphnia magna, the most sensitive species in the microcosm."

Overall, Mackiewicz said, the study showed that silver nanoparticles' shape and surface chemistry can be manipulated to achieve specific objectives necessary for better understanding and mitigating the risks associated with silver nanoparticles. A related study awaiting publication, she added, shows that small, spherical nanoparticles are more toxic than triangles or cubes.

Nanoparticles are the latest format, Mackiewicz notes, for an element that throughout history has been used to restrict the spread of human disease

CHEMWATCH
Bulletin Board
Gossip
MAY. 17, 2024

via incorporation into items used in everyday life. Its earliest recorded use for therapeutic purposes dates back 3,500 years.

During the Middle Ages, wealthy families used so many silver vessels, plates and other products that they developed bluish skin discolorations known as argyria, a condition believed to have led to the term "blue blood" as a description for members of the aristocracy.

Collaborating with Mackiewicz and Harper on the study were OSU researchers Bryan Harper and Arek Engstrom.

The National Science Foundation and the National Institutes of Health provided funding for the research.

Science Daily, 10 May 2024

https://sciencedaily.com

Psilocybin Looking "Rather Good" as an Anti-Depressant, Trial Data Shows

2024-05-13

When the psychedelic compound psilocybin was subject to federal regulation in the US during the 1960s, it swiftly brought any "above ground" research working to deduce its therapeutic potential to a grinding halt.

During the psychedelic renaissance of recent years, there has been a revival of work exploring psilocybin's utility for treating psychiatric conditions. Legal restrictions have eased, enabling this work to be conducted ethically across research institutions and private practice sites.

A new meta-analysis by UK researchers analyzed data from a collection of such studies to further address the question: is psilocybin effective as an anti-depressant? The research – published in the BMJ – reports "encouraging findings" according to the research team. [Updated May 13, 2024].

An estimated five percent of the global population suffer from depression, also referred to as major depressive disorder (MDD) or clinical depression. While anti-depressant medications are available and can offer some individuals relief, they are not universally effective, and alternative treatment options are desperately sought.

"Psilocybin would hopefully provide a more quick-acting and tolerable (in terms of side effects) treatment," Athina-Marina Metaxa, a former researcher in the Nuffield Department of Medicine at the University Oxford who now works in the pharmaceutical industry, told Technology Networks. Metaxa is a co-author of the BMJ study, along with Professor Mike Clarke from the School of Medicine, Dentistry and Biomedical Sciences at Queen's University Belfast.

Metaxa and Clarke searched through databases looking for randomized controlled trials that compared psilocybin as a treatment for symptoms of depression with controls, including placebo, niacin (vitamin B) or microdoses of psychedelics. They found 7 trials, recruiting a total of 436 participants with an average age of 36–60 years, that met their inclusion criteria. The participants were roughly 50/50 male and female but were 90% white. This lack of diversity, Metaxa says, is common across psychedelic studies, and makes it challenging to generalize results.

The effects of psilocybin on depressive symptoms were measured using the statistical method Hedges' g. Using this method, a score of 0.9 or more indicates a large effect.

Across the seven trials analyzed, Metaxa and Clarke found that psilocybin induced a significantly greater improvement in depressive scores compared to placebo or alternative treatments, with a Hedge's g score of 1.64.

There were, however, several factors that influenced the level of a participant's improvement after psilocybin treatment, including whether an individual was experiencing secondary depression, the type of assessment used in their style and their age.

Metaxa expanded on these findings: "It has been proposed that patients with secondary depression benefit more because they tend to be older or because they have more severe depression, so improvements are more pronounced," she said. "However, patients with secondary depression did not differ in average age or symptom severity than primary depression patients in this study. It would be interesting to look at the neural correlation of psilocybin treatment for each patient group – maybe that could tell us more about psilocybin's specific effects in each patient type."

"Self-assessment scales have shown larger treatment effects compared to clinician-assessed scales across psychological literature, so this is not unique to psilocybin interventions. This may be because clinicians tend to underestimate the severity of depression symptoms at baseline

CHEMWATCH
Bulletin Board
Gossip
MAY. 17, 2024

assessment, leading to less pronounced pre- vs post-treatment differences identified in clinician-assessed scales," she continued. In other words, a patient is more likely to rate their initial symptoms as "more severe" than a doctor would when making the same assessment.

"When it comes to older age, it could be because older people have more experience in managing negative emotions. Additionally, some studies have shown that older patients' cognitive performance improves significantly more than that of younger patients following psilocybin treatment – thus, the higher decrease in depressive symptoms associated with older age could be attributed to a decrease in the cognitive difficulties experienced by older participants," Metaxa added.

Combined, do these findings imply that creating and implementing a "one-size-fits-all" psilocybin treatment approach for depression would be challenging? "The findings are encouraging in that they showed that psilocybin is overall effective when we pool all the data together. This means that while it may be more effective for some patient 'types' it can still be overall beneficial across patients," Metaxa explained. "It would also be interesting to consider that the 'individualized' component of psilocybin treatment comes from the therapeutic support the patient receives along the treatment, and not the drug itself."

Implementing psilocybin-based treatments: Opportunities and challenges

Unfortunately, Metaxa and Clarke could not measure pre-treatment expectations and the extent to which participants knew they were being treated with psilocybin or placebo. This data was not collected in the majority of studies analyzed by the duo, Metaxa explained to Technology Networks. Dr. Paul Keedwell, consultant psychiatrist and fellow of the Royal College of Psychiatrists, said that concerns surrounding this limitation are "tempered by the fact that improvements were maintained for up to 12 weeks in one study." Regardless, Metaxa suggests that future research measures pre-treatment expectations, as they would provide "invaluable" insight into how the patient's mindset might affect treatment outcomes.

Metaxa and Clarke are encouraged both encouraged by their findings but also realistic in their expectations. "We argue that the complexity of psilocybin-based interventions would be a significant barrier to implementation – the patient needs to go to the clinic and remain there for hours while the treatment is administered, a specially designed room is required to ensure the patient is calm and comfortable, and a trained therapist must be present to assist," Metaxa said.

This makes the intervention costly and challenging to implement in a standardized way. "Also, due to its high cost, such an intervention may not be readily reimbursed, so it would be difficult for most patients to access," Metaxa added.

She is, however, optimistic: "I want to believe that if a treatment is effective, it will end up being used in practice. While there are barriers to treatment implementation, there are also many brilliant researchers working across academia and industry who are trying to find ways to make psilocybin treatment more cost-effective and easier to implement in clinical practice."

"I hope this work will encourage researchers to examine patient- and study design-related factors that could modify psilocybin's antidepressant effectiveness," Metaxa concluded. "Additionally, this study would hopefully stimulate more interest in psilocybin research across research organizations and patient groups and would encourage participation in such trials."

Technology Networks, 04 May 2024

https://technologynetworks.com

Scientists develop an affordable sensor for lead contamination

2024-05-14

Engineers at MIT, Nanytang Technological University, and several companies have developed a compact and inexpensive technology for detecting and measuring lead concentrations in water, potentially enabling a significant advance in tackling this persistent global health issue.

The World Health Organization estimates that 240 million people worldwide are exposed to drinking water that contains unsafe amounts of toxic lead, which can affect brain development in children, cause birth defects, and produce a variety of neurological, cardiac, and other damaging effects. In the United States alone, an estimated 10 million households still get drinking water delivered through lead pipes.

"It's an unaddressed public health crisis that leads to over 1 million deaths annually," says Jia Xu Brian Sia, an MIT postdoc and the senior author of the paper describing the new technology.

But testing for lead in water requires expensive, cumbersome equipment and typically requires days to get results. Or, it uses simple test strips

CHEMWATCH
Bulletin Board
Gossip
MAY. 17, 2024

that simply reveal a yes-or-no answer about the presence of lead but no information about its concentration. Current EPA regulations require drinking water to contain no more that 15 parts per billion of lead, a concentration so low it is difficult to detect.

The new system, which could be ready for commercial deployment within two or three years, could detect lead concentrations as low as 1 part per billion, with high accuracy, using a simple chip-based detector housed in a handheld device. The technology gives nearly instant quantitative measurements and requires just a droplet of water.

The findings are described in a paper appearing today in the journal Nature Communications, by Sia, MIT graduate student and lead author Luigi Ranno, Professor Juejun Hu, and 12 others at MIT and other institutions in academia and industry.

The team set out to find a simple detection method based on the use of photonic chips, which use light to perform measurements. The challenging part was finding a way to attach to the photonic chip surface certain ring-shaped molecules known as crown ethers, which can capture specific ions such as lead.

After years of effort, they were able to achieve that attachment via a chemical process known as Fischer esterification. "That is one of the essential breakthroughs we have made in this technology," Sia says.

In testing the new chip, the researchers showed that it can detect lead in water at concentrations as low as one part per billion. At much higher concentrations, which may be relevant for testing environmental contamination such as mine tailings, the accuracy is within 4 percent.

The device works in water with varying levels of acidity, ranging from pH values of 6 to 8, "which covers most environmental samples," Sia says. They have tested the device with seawater as well as tap water, and verified the accuracy of the measurements.

In order to achieve such levels of accuracy, current testing requires a device called an inductive coupled plasma mass spectrometer. "These setups can be big and expensive," Sia says. The sample processing can take days and requires experienced technical personnel.

While the new chip system they developed is "the core part of the innovation," Ranno says, further work will be needed to develop this into an integrated, handheld device for practical use. "For making an actual product, you would need to package it into a usable form factor," he

explains. This would involve having a small chip-based laser coupled to the photonic chip.

"It's a matter of mechanical design, some optical design, some chemistry, and figuring out the supply chain," he says. While that takes time, he says, the underlying concepts are straightforward.

The system can be adapted to detect other similar contaminants in water, including cadmium, copper, lithium, barium, cesium, and radium, Ranno says. The device could be used with simple cartridges that can be swapped out to detect different elements, each using slightly different crown ethers that can bind to a specific ion.

"There's this problem that people don't measure their water enough, especially in the developing countries," Ranno says. "And that's because they need to collect the water, prepare the sample, and bring it to these huge instruments that are extremely expensive."

Instead, "having this handheld device, something compact that even untrained personnel can just bring to the source for on-site monitoring, at low costs," could make regular, ongoing widespread testing feasible.

Hu, who is the John F. Elliott Professor of Materials Science and Engineering, says, "I'm hoping this will be quickly implemented, so we can benefit human society. This is a good example of a technology coming from a lab innovation where it may actually make a very tangible impact on society, which is of course very fulfilling."

"If this study can be extended to simultaneous detection of multiple metal elements, especially the presently concerning radioactive elements, its potential would be immense," says Hou Wang, an associate professor of environmental science and engineering at Hunan University in China, who was not associated with this work.

Wang adds, "This research has engineered a sensor capable of instantaneously detecting lead concentration in water. This can be utilized in real-time to monitor the lead pollution concentration in wastewater discharged from industries such as battery manufacturing and lead smelting, facilitating the establishment of industrial wastewater monitoring systems. I think the innovative aspects and developmental potential of this research are quite commendable."

Wang Qian, a principal research scientist at the Institute of Materials Research in Singapore, who also was not affiliated with this work, says, "The ability for the pervasive, portable, and quantitative detection of lead

CHEMWATCH
Bulletin Board
Gossip
MAY. 17, 2024

has proved to be challenging primarily due to cost concerns. This work demonstrates the potential to do so in a highly integrated form factor and is compatible with large-scale, low-cost manufacturing."

The team included researchers at MIT, at Nanyang Technological University and Temasek Laboratories in Singapore, at the University of Southampton in the U.K., and at companies Fingate Technologies, in Singapore, and Vulcan Photonics, headquartered in Malaysia. The work used facilities at MIT.nano, the Harvard University Center for Nanoscale Systems, NTU's Center for Micro- and Nano-Electronics, and the Nanyang Nanofabrication Center.

Phys Org, 14 May 2024

https://phys.org

AI predicts vape flavours can break down into potentially harmful compounds when heated

2024-05-14

An artificial intelligence-based approach has predicted hundreds of harmful compounds that could form when e-cigarette flavour chemicals are heated in vaping devices. The research adds to mounting evidence concerning the safety of vaping, finding that many of the predicted pyrolysis products from flavours are classed as either acutely toxic, health hazards or irritants. What's more, their impact on health might take years to emerge, say the researchers.

E-cigarettes work by heating up an e-liquid, or e-juice, to produce an aerosol that comprises nicotine, solvents – including propylene glycol and glycerol – and flavourings, which a user then inhales. There are tens of thousands of different flavour e-liquids on the market and ingredients are picked from at least 180 commercially available flavour compounds, which were originally developed for the food industry and deemed safe for consumption. However, the long-term health risks of heating and inhaling these chemicals remain unknown.

'As the flavours being used in vapes have never been clinically tested for heating to high temperatures with lung inhalation, it is important to quickly get an understanding of the cocktail of chemicals that vape-users' lungs are being exposed to,' says Donal O'Shea, who led the new work at the Royal College of Surgeons in Ireland, Dublin. 'Our approach may reveal the longer-term health risks of vaping in advance of clinical diseases emerging in the general population.'

In 2019, O'Shea and co-workers determined that the pyrolysis, or thermal decomposition, of vitamin E acetate, an additive present in some unregulated vaping mixtures, can create highly reactive and toxic ketene gas. This offered the likely chemical basis of a mysterious outbreak of vaping-related lung injuries and deaths in the US at the time and highlighted the need to investigate the pyrolysis products of other components of e-liquids, including flavour ingredients.

Flavour chemistry

The team trained a neural network – a machine-learning model that mimics the human brain – on over 300,000 reactions. It then used this to predict 7307 pyrolysis breakdown products of 180 compounds known to be used as e-liquid flavourings. Next, using mass spectrometry data, the molecular weights of predicted products were compared with a database of known breakdown products, identifying 1169 matches. These were then cross correlated against the PubChem database, revealing that 127 acutely toxic, 153 health hazards and 225 irritant compounds were predicted.

'From the compounds predicted, chronic obstructive pulmonary disease, cardiovascular disease and cancers could be expected to arise from prolonged exposures,' says O'Shea. He was particularly surprised by the structural diversity of compounds that can be produced. 'While many are similar to those found in tobacco smoke, many are not, indicating that the health impacts may ultimately differ,' he explains. 'The ester flavours are particularly concerning as they produce many reactive carbonyls, alkenes and aromatics and are most popular with a younger demographic.' Among the e-liquid flavours that have esters in their ingredients are bubblegum, fruit and citrus-based ones.

Irfan Rahman, who investigates the health impacts of tobacco and e-cigarettes at the University of Rochester Medical Center, says that these are 'interesting chemical analyses'. 'We see aldehydes are predicted which become highly toxic to functional proteins.' He encourages further work to explore the biological effects of the predicted compounds.

Next steps

O'Shea agrees that this is an essential next step. 'Using our dataset of predicted compounds, biomarkers of exposure to these chemicals could now be investigated in vape users and the results compared to non-vape users,' he explains.

CHEMWATCH
Bulletin Board
Gossip
MAY. 17, 2024

'It is so crucially important to understand flavourings' health effects, especially given that users essentially inhale these at a high daily frequency, often for years,' comments Hanno Erythropel, an analytical chemist who studies e-liquid flavours at Yale University, US. 'This approach is very interesting and produces results that would never be possible to realise experimentally due to the sheer volume.'

However, Erythropel notes that it remains to be proven that the predicted compounds will actually form from vaping because of heating and catalytic variables in the many available e-cigarette devices. 'But this might be helpful in pointing researchers in the right direction to look for specific, problematic compounds to be tested experimentally – any approach that will help us to better understand the impact of flavours in e-cigarettes is useful.'

O'Shea envisages further work to confirm the predictions by comparing them with those of other AI training sets, as well as experimental analysis of vape plumes. 'We would also like to expand the chemical reactions to include combustion products and predict the potential for catalysis from the metal components found within vaping devices,' he says.

Chemistry World, 14 May 2024

https://chemistryworld.com

A new method of making diamonds doesn't require extreme pressure

2024-04-24

Diamonds in nature famously form under immense pressure in Earth's mantle. But a new laboratory technique allows diamonds to skip the squeeze.

The most common method for producing synthetic diamonds, known as high-pressure and high-temperature growth, or HPHT, requires around 5 gigapascals of pressure, similar to that in the upper mantle where diamonds form naturally. With this technique, carbon dissolved in liquid metal forms diamonds at temperatures around 1400° Celsius.

But diamonds can be grown at atmospheric pressure in a liquid of gallium, iron, nickel and silicon exposed to a gas of carbon-rich methane as well as hydrogen, scientists report April 24 in Nature. The technique also required lower temperatures than HPHT: 1025° C. The addition of silicon in particular seems to kick off the initial stages of growth, allowing a tiny bit

of diamond to nucleate, says physical chemist Rodney Ruoff. From there, the rest of the crystal can grow.

The demand for diamonds isn't just about gemstones. Scientists can use diamonds for everything from sensing magnetic fields to searching for new subatomic particles (SN: 9/19/22; SN: 6/17/19). The new method could make generating such materials easier. "The syntheses need not depend on expensive or complicated equipment," says Ruoff, of the Institute for Basic Science Center for Multidimensional Carbon Materials in Ulsan, South Korea.

Another technique to produce diamonds in the lab, called chemical vapor deposition, or CVD, takes place at low pressures, with a vapor of carbon-rich gas being deposited on a surface. Unlike CVD and HPHT, the new technique doesn't make use of a diamond "seed," an initial bit of diamond to kick off the growth.

CVD and HPHT are widely used in the jewelry industry. It remains to be seen whether the new technique will make diamonds destined for bling.

Science News, 24 April 2024

https://sciencenews.com

DeepMind AI can predict how drugs interact with proteins

2024-05-08

An artificial intelligence system can now determine not only how proteins fold but also how they interact with other proteins, drug molecules or DNA. Biochemists and pharmaceutical researchers say the tool has the potential to vastly speed up their work, such as helping to discover new drugs.

Proteins, which play many important roles in living things, are made up of chains of amino acids, but their complex 3D shapes are difficult to predict.

The AI company DeepMind first announced in 2020 that its AlphaFold AI could accurately predict protein structure from amino acid sequences, solving one of the biggest challenges in biology. By the middle of 2021, the company said that it had mapped 98.5 per cent of the proteins in the human body.

Now the latest version, AlphaFold 3, is able to model how proteins, including antibodies, interact with each other, as well as with other

CHEMWATCH
Bulletin Board
Gossip
MAY. 17, 2024

biomolecules such as DNA and RNA strands. DeepMind says the accuracy of its predictions is at least 50 per cent higher than existing methods.

Most drug molecules function by binding to specific sites on proteins. AlphaFold 3 could rapidly speed up the development of new drugs by creating a fast way to test how candidate drug molecules interact with proteins in a computer before running lengthy and expensive laboratory tests.

Like earlier versions of AlphaFold, models of proteins or their interactions generated by the latest update aren't experimentally validated. DeepMind's chief executive, Demis Hassabis, says AlphaFold 3 only offers predictions, so validation in the lab remains vital – but that research will now be "massively accelerated".

Julien Bergeron at King's College London, who wasn't involved in developing AlphaFold 3 but has been testing it for several months, says it has changed the way his experiments are run. "We can start testing hypotheses before we even go to the lab, and this will really be transformative. I'm pretty much certain that every single structural biology or protein biochemistry research group in the world will immediately adopt this system," he says.

Keith Willison at Imperial College London says the tool has the potential to streamline large portions of drug discovery and biological research, allowing researchers to focus in on useful molecules that they may never have been able to discover previously.

"Organic chemists used to say the chemical space is larger than the number of atoms in the universe, and we'll never be able to access even the remotest, tiniest portion of it. But I think these AI techniques are going to be able to access a huge amount of relevant chemical space," he says.

Matt Higgins at the University of Oxford says the new features in DeepMind's AI will make a huge difference to biomedical researchers, including in his own work studying host-parasite interactions in malaria.

"While AlphaFold transformed our ability to predict the structures of protein molecules, the protein machines used by our cells rarely work alone," he says. "AlphaFold 3 brings the new and exciting ability to modify protein molecules with the most common additions or bind them to the

most common binding partners found in our bodies and to see what happens."

new Scientist, 08 May 2024

https://newscientist.com

https://www.newscientist.com/article/2429520-deepmind-ai-can-predict-how-drugs-interact-with-proteins/

2024-04-14

A new technique for 3D printing medication has enabled the printing of multiple drugs in a single tablet, paving the way for personalized pills that can deliver timed doses.

Researchers from the University of Nottingham's, Centre for Additive Manufacturing have led research alongside the School of Pharmacy that has fabricated personalized medicine using Multi-Material InkJet 3D Printing (MM-IJ3DP). The research has been published in Materials Today Advances.

The team have developed a cutting-edge method that enables the fabrication of customized pharmaceutical tablets with tailored drug release profiles, ensuring more precise and effective treatment options for patients.

Using Multi-Material InkJet 3D Printing (MM-IJ3DP), tablets can be printed that release drugs at a controlled rate, determined by the tablet's design. This is made possible by a novel ink formulation based on molecules that are sensitive to ultraviolet light. When printed, these molecules form a water-soluble structure.

The drug release rate is controlled by the unique interior structure of the tablet, allowing for timing the dosage release. This method can print multiple drugs in a single tablet, allowing for complex medication regimens to be simplified into a single dose.

Dr. Yinfeng He, Assistant Professor in the Faculty of Engineering's Centre for Additive Manufacturing led the research, he said, "This is an exciting step forwards in the development of personalized medication. This breakthrough not only highlights the potential of 3D printing in revolutionizing drug delivery but also opens up new avenues for the development of next-generation personalized medicines."

CHEMWATCH
Bulletin Board
Gossip
MAY. 17, 2024

"While promising, the technology faces challenges, including the need for more formulations that support a wider range of materials. The ongoing research aims to refine these aspects, enhancing the feasibility of MM-IJ3DP for widespread application," Professor Ricky Wildman added.

This technology will be particularly beneficial in creating medication that needs to release drugs at specific times, making it ideal for treating diseases, where timing and dosage accuracy are crucial. The ability to print 56 pills in a single batch demonstrates the scalability of this technology, providing a strong potential for the production of personalized medicines.

Professor Felicity Rose at the University of Nottingham's School of Pharmacy was one of the co-authors on the research, she says, "The future of prescribed medication lies in a personalized approach, and we know that up 50% of people in the UK alone don't take their medicines correctly and this has an impact on poorer health outcomes with conditions not being controlled or properly treated. A single pill approach would simplify taking multiple medications at different times and this research is an exciting step towards that."

Phys Org, 14 May 2024

https://phys.org

'Mechanochemistry strikes again' – this time for deoxygenating phosphine oxides

2024-05-15

Mechanochemistry can regenerate phosphine oxide waste into phosphine reagents by deoxygenating it under air, new research shows. 'This method circumvents the need for hazardous organic solvents … and does not require complicated synthetic procedures involving inert gases,' notes Koji Kubota from Hokkaido University in Japan, who co-led the study with Hajime Ito.

Phosphine oxide deoxygenation is usually performed in solution using highly reactive metal hydrides or low-valent reducing agents. 'While methods have been developed for this reaction in solution, they are difficult to render operational for three main reasons: reaction length, need for oxygen free conditions and use of large amounts of solvent,' says Audrey Moores, an expert in mechanochemistry and green chemistry at McGill University in Canada. Despite the importance of organophosphine compounds as synthetic building blocks, easy access to these compounds remains challenging. 'I was training as an organometallic chemist in a

phosphorus chemistry lab at École Polytechnique, France, and back then the question of phosphine deoxygenation was a central conundrum, affecting virtually any aspect of our work,' adds Moores.

The mechanochemical process developed by Kubota and Ito uses ball milling and a hydrosilane in the presence of a phosphoric acid additive. It takes 30 minutes – a significant timesaving compared to traditional methods that take over 24 hours. While mechanochemistry inherently omits the need for organic solvents, this proved particularly useful for handling phosphine oxides. 'Since the mechanochemical method does not require substrates to be dissolved in organic solvent, this approach is effective for reactions of poorly soluble compounds. Many phosphine oxides are poorly soluble in organic solvents, and thus their organic transformations in solution are often inefficient,' explains Kubota.

Moores says she's 'truly amazed' that a reaction typically known to require inert conditions, can be performed under air. 'It's a real advantage of this method. Here mechanochemistry strikes again.'

The Hokkaido team tested their mechanochemical deoxygenation process on phosphine oxide byproducts from a Wittig reaction. It successfully recycled the byproducts in situ into organophosphine for the Wittig reaction to use again – 'a really interesting feature in terms of applicability,' according to Moores.

However, as is the case for solution-based phosphine oxide deoxygenation, the mechanical process still needs heat – in this case 120°C. Kubota says the team hope to improve the mechanochemical conditions: 'If we can find conditions that allow deoxygenation of phosphine oxides at room temperature, it would be a breakthrough.'

Chemistry World, 15 May 2024

https://chemistryworld.com

CHEMWATCH
Bulletin Board

Experimental Drug "Hides" Pancreas Cells in Type 1 Diabetes Mouse Models

2024-04-30

Scientists at Johns Hopkins Medicine say that an experimental monoclonal antibody drug called mAb43 appears to prevent and reverse the onset of clinical type 1 diabetes in mice, and in some cases, to lengthen the animals' lifespan.

The drug is unique, according to the researchers, because it targets insulin-making beta cells in the pancreas directly and is designed to shield those cells from attacks by the body's own immune system cells. The drug's specificity for such cells may enable long-term use in humans with few side effects, say the researchers. Monoclonal antibodies are made by cloning, or making identical replicas of, an animal (including human) cell line.

The findings, reported online recently and in the May issue of Diabetes, raise the possibility of a new drug for type 1 diabetes, an autoimmune condition that affects about 2 million American children and adults and has no cure or means of prevention. Unlike type 2 diabetes, in which the pancreas makes too little insulin, in type 1 diabetes, the pancreas makes no insulin because the immune system attacks the pancreatic cells that make it.

The lack of insulin interferes with the body's ability to regulate blood sugar levels.

"People with type 1 diabetes face lifelong injections of insulin and many complications, including stroke and eyesight problems if the condition is not managed properly," says Dax Fu, Ph.D., associate professor of physiology at the Johns Hopkins University School of Medicine and leader of the research team.

Fu says mAb43 binds to a small protein on the surface of beta cells, which dwell in clusters called islets. The drug was designed to provide a kind of shield or cloak to hide beta cells from immune system cells that attack them as "invaders." The researchers used a mouse version of the monoclonal antibody, and will need to develop a humanized version for studies in people.

For the current study, the researchers gave 64 non-obese mice bred to develop type 1 diabetes a weekly dose of mAb43 via intravenous injection when they were 10 weeks old. After 35 weeks, all mice were non-diabetic.

One of the mice developed diabetes for a period of time, but it recovered at 35 weeks, and that mouse had early signs of diabetes before the antibody was administered.

In five of the same type of diabetes-prone mice, the researchers held off giving weekly mAb43 doses until they were 14 weeks old, and then continued dosages and monitoring for up to 75 weeks. One of the five in the group developed diabetes, but no adverse events were found, say the researchers.

In the experiments in which mAb43 was given early on, the mice lived for the duration of the monitoring period of 75 weeks, compared with the control group of mice that did not receive the drug and lived about 18–40 weeks.

Next, the researchers, including postdoctoral fellows Devi Kasinathan and Zheng Guo, looked more closely at the mice that received mAb43 and used a biological marker called Ki67 to see if beta cells were multiplying in the pancreas. They said, after treatment with the antibody, immune cells retreated from beta cells, reducing the amount of inflammation in the area. In addition, beta cells slowly began reproducing.

"mAb43 in combination with insulin therapy may have the potential to gradually reduce insulin use while beta cells regenerate, ultimately eliminating the need to use insulin supplementation for glycemic control," says Kasinathan.

The research team found that mAb43 specifically bound to beta cells, which make up about 1% or 2% of pancreas cells.

Another monoclonal antibody drug, teplizumab, was approved by the U.S. Food and Drug Administration in 2022. Teplizumab binds to T cells, making them less harmful to insulin-producing beta cells. The drug has been shown to delay the onset of clinical (stage 3) type 1 diabetes by about two years, giving young children who get the disease time to mature and learn to manage lifelong insulin injections and dietary restrictions.

"It's possible that mAb43 could be used for longer than teplizumab and delay diabetes onset for a much longer time, potentially for as long as it's administered," says Fu.

CHEMWATCH
Bulletin Board
Curiosities
MAY. 17, 2024

"In an ongoing effort, we aim to develop a humanized version of the antibody and conduct clinical trials to test its ability to prevent type 1 diabetes, and to learn whether it has any off-target side effects," says Guo.

Technology Networks, 30 April 2024

https://technologynetworks.com

Researchers find new approach for antibiotic development

2024-04-13

The opportunistic bacterial pathogen Pseudomonas aeruginosa is dangerous due to its resistance to multiple antibiotics. A research team from Heinrich Heine University Düsseldorf (HHU) and Jülich Research Center (Forschungszentrum Jülich—FZJ) has now found a mechanism that makes it possible to weaken the virulence of the pathogen.

Based on this knowledge, a new approach for antibiotics can be developed, as the authors explain in JACS Au. The editors of the journal have dedicated a cover story to this discovery.

The bacterium Pseudomonas aeruginosa often causes a so-called "nosocomial infection" in humans. It is therefore one of the dangerous hospital bacteria that is resistant to several antibiotics. Immunocompromised patients are particularly affected. The World Health Organization (WHO) has placed P. aeruginosa on the list of "priority pathogens" on which research efforts should focus to find new treatment options.

The bacterium has a broad spectrum of disease-causing virulence factors. These include the "type A phospholipases" (PLA1): Enzymes that can damage the membrane of the host cell and also disrupt various signaling networks in the infected cells. Preliminary work has shown that the enzyme PlaF from P. aeruginosa is a PLA1 that also alters the membrane profile and thus contributes to the virulence of the bacterium.

The research groups of Professor Dr. Holger Gohlke (HHU Institute of Pharmaceutical and Medicinal Chemistry and IBG-4: Bioinformatics at FZJ) and Professor Dr. Karl-Erich Jaeger (HHU Institute of Molecular Enzyme Technology at FZJ) have now identified molecular mechanisms in which medium-chain free fatty acids regulate the activity of PlaF.

The researchers carried out molecular simulations as well as laboratory studies and in vivo assays. All of these research approaches showed an

indirect effect of the fatty acids on the location of PlaF in the bacterial membrane as well as a direct effect by blocking the active center of the enzyme. In both ways, the activity of PlaF is reduced.

On the one hand, the results provide evidence that the interplay of mechanisms is a regulatory factor for PlaF function. Professor Gohlke, "We were only able to unravel these complex relationships through the interaction of computer-aided and experimental techniques within the framework of the projects funded by the CRC 1208."

On the other hand, the results contribute to understanding the regulatory role of fatty acids. It may be possible to transfer the results to other membrane proteins that have a similar structure to PlaF.

Finally, they also open up new perspectives on how PlaF can be inhibited. Professor Jaeger, "This is a promising approach for developing new antibiotics against P. aeruginosa. These are urgently needed to combat the dangerous pathogens in hospitals."

Phys Org, 13 MAY 2024

https://phys.org

Is Vitamin D Supplementation Really One-Size-Fits-All?

2024-05-10

A new study has shed light on factors surrounding vitamin D supplementation across diverse populations. The research suggests the need for personalized approaches to supplementation to help reduce vitamin D deficiency, which remains widespread despite extensive research.

The study is published in Clinical Nutrition.

Vitamin D is incredibly important for our bodies, helping to keep our bones, teeth and muscles healthy – yet deficiency is incredibly common.

Vitamin D is produced in the skin following exposure to ultraviolet-B (UVB) radiation from the sun. Skin pigment, such as melanin, limits UVB penetration and vitamin D synthesis in the skin. Consequently, in places like Europe, the prevalence of vitamin D deficiency varies from 13–40% but can be as much as 3- to 71-fold higher in darker-skinned individuals compared to white ethnicities.

Many health agencies recommend supplementing vitamin D, especially during the darker winter months. However, these recommendations

CHEMWATCH
Bulletin Board
Curiosities
MAY. 17, 2024

typically follow a one-size-fits-all approach, despite many factors influencing vitamin D synthesis in the skin including ambient sunlight intensity, age and skin tone.

Studies have found profound differences in vitamin D status between and within populations. In a new study, researchers hypothesized that predicting vitamin D status could be improved by accounting for ambient UVB radiation and interaction with other key determinants of vitamin D.

Not as simple as one-size-fits-all?

The researchers harnessed data from half a million Asian, Black and White participants from the UK Biobank – specifically, data on vitamin D levels obtained from participants' blood samples. The researchers then estimated the ambient UVB doses for each person depending on their place of residence in the 135 days leading up to their blood draw.

The researchers found that ambient UVB was a key predictor for vitamin D levels for all ethnicities, even in places that – like the UK – receive relatively little sunlight. Vitamin D deficiency was common, particularly among non-White participants.

Other factors were also found to influence how people's bodies responded to UVB, such as age, sex, body mass index (BMI), cholesterol levels and vitamin D supplementation. For example, with increasing age and BMI, vitamin D production in response to UVB was found to decrease.

"We hope this work can highlight the significant differences in vitamin D levels among different ethnic groups at northern latitudes and contribute to efforts to address the long-standing population health issue of vitamin D deficiency," said the study's lead author Dr. Margaret M. Brennan, a research assistant in the Department of Public Health and Primary Care in Trinity College Dublin's School of Medicine.

The authors also highlight that improved methods of predicting vitamin D levels could help develop more nuanced approaches to supplementation, helping to limit deficiency in a range of populations.

"Our study also highlights the effect that natural environmental factors, like sunlight, can have on our health," explained study co-author and PhD candidate Rasha Shraim. "We hope that our approach encourages future

researchers and public health bodies to integrate these factors into their health and disease work."

Technology Networks, 10 May 2024

https://technologynetworks.com

Precious metal-free catalyst conjured using sugar can turn CO2 into chemical feedstock

2024-05-11

A stable, selective and precious metal-free catalyst for the conversion of waste carbon dioxide into synthesis gas has been developed by researchers in the US and Canada.1 The work potentially provides a step towards the production of valuable industrial chemicals from captured carbon in future chemical refineries.

Synthesis gas, or syngas – a mixture of carbon monoxide and hydrogen – is crucial for producing numerous industrial chemicals such as ammonia, methanol and larger hydrocarbons. Today it is most commonly made either from steam reforming of methane or from gasification of coal or heavy hydrocarbons, both of which are highly endothermic processes and have large carbon footprints. An alternative is the reverse water–gas shift, in which carbon dioxide is reduced to carbon monoxide by hydrogen, while the hydrogen is oxidised to water. Using an excess of hydrogen can produce syngas.

Most industrial hydrogen is actually the product of steam reforming of methane followed by the forward water–gas shift reaction to produce more hydrogen from the carbon monoxide. Interest in renewable hydrogen produced by the electrolysis of water is growing, however. 'Dozens of sources of CO2 like steel companies and cement companies are going to keep producing CO2 regardless of the hydrogen production cycle and somebody needs to address that,' says Milad Ahmadi Khoshooei at Northwestern University, US. 'The capture part is much more advanced than the conversion part, so let's assume we capture the CO2. We need to use it instead of just sticking it underground.'

Khoshooei and colleagues at Northwestern and the University of Calgary in Canada, led by Northwestern's Omar Farha, sought an efficient catalyst that was selective for carbon monoxide, rather than methane, under an excess of hydrogen. Previously, molybdenum carbide catalysts have shown promise, but they have often either shown insufficient initial selectivity or decayed rapidly at the high temperatures the reaction uses.

CHEMWATCH
Bulletin Board
Curiosities
MAY. 17, 2024

The researchers discovered from spectroscopic analysis and density functional theory simulations that the metastable cubic phase of molybdenum carbide was more active and selective than the stable hexagonal close-packed phase. They found that, simply by carburising table sugar with ammonium molybdate, they created a catalyst comprising phase-pure nano-crystallites of cubic molybdenum carbide protected by a carbonaceous layer and interstitial atoms that prevented recrystallisation. At 500°C, the catalyst showed rapid, near-equilibrium conversion and 100% selectivity to carbon monoxide. It retained this for 500 hours on stream. The researchers are further developing the catalyst towards commercialisation.

Bert Weckhuysen at the Inorganic Chemistry and Catalysis Group at Utrecht University in the Netherlands, together with colleague Eelco Vogt, this week published a detailed analysis of the challenges of creating fossil-fuel free refineries by 2050.2 Weckhuysen says the present work is 'a mechanistically thorough study on a specially derived catalyst for an important reaction, which in future reaction scenarios could lead to carbon neutrality – or a reduced carbon footprint – in CO2 conversion processes.'

He is especially impressed by the mechanistic explanation underpinning the stability of this particular molybdenum catalyst and the researchers' validation of it through experiment and theory. 'I think they need to look at the influence of impurities, because many of the CO2 point sources from things like metallurgy are not just CO2: they contain other elements – metals and others. The question is if a real, stable operation can be maintained under harsh, true operating conditions.'

Chemistry World, 11 May 2024

https://chemistryworld.com

New database aims to accelerate electrocatalyst development through atomic-scale insights

2024-04-13

The quest for more productive catalysts for the creation of sustainable fuels and commodity chemicals via electrochemical reactions just became easier.

Powered by renewable electricity, electrocatalysts producing fuels and chemicals from water, carbon dioxide, or nitrogen have the potential to decarbonize the heavy transport and chemical industries. This

decarbonization can be achieved by direct replacement of fossil fuels or lower-energy production of fuels and chemicals.

A new open-source electrocatalysis database, developed by the National Renewable Energy Laboratory (NREL) and its partners, provides researchers with a comprehensive view of electrochemical energy conversion. The extensive data enable insight into the fundamental factors that govern changes in catalyst performance and can expedite the design of electrocatalysts.

The new database was developed by the Beyond-Density Functional Theory Electrochemistry with Accelerated and Solvated Techniques (BEAST) team. The BEAST consortium, led by Ravishankar Sundararaman from the Rensselaer Polytechnic Institute, includes collaborators at NREL, Lawrence Berkeley National Laboratory, the University of Colorado Boulder, and the University of South Carolina.

A database for atomistic insights into electrochemistry

The BEAST database, or BEAST DB, allows experimental and theoretical electrochemists to explore atomic-scale catalytic reactions and view numerous properties on catalyst performance.

Examples of critical electrochemical reactions include converting water, carbon dioxide, or nitrogen to hydrogen, formic acid or other reduced carbon-based molecules, and ammonia, respectively, using electrocatalysts. Understanding the fundamental properties during electrocatalysis can lead to advancements in catalyst efficiency and productivity.

Derek Vigil-Fowler, the computational science researcher at NREL who conceptualized BEAST DB, believes that this data can enable a holistic understanding of these catalysts.

"Having standardized baseline results for the most widely studied electrocatalytic reactions in one place allows researchers to have a one-stop shop for acquiring a basic understanding of how their catalyst works at the atomic scale.

"They can visualize molecular adsorption on the surface and the charge transfer that drives electrocatalytic reactions and understand how that varies across catalysts and applied potential ranges. Others can build upon these calculations with new calculations and experiments and make advancements in the field," Vigil-Fowler said.

CHEMWATCH
Bulletin Board
Curiosities
MAY. 17, 2024

"The ultimate goal of BEAST DB is to make it easier to explore catalyst performance and develop new catalysts for different chemical reactions."

The diversity of conditions in published electrochemical experiments and theoretical calculations hinders a complete understanding of electrochemical systems. While density functional theory (DFT) can predict catalytic behavior, DFT methods inadequately represent the length and time scales in electrochemical reactions, especially at the dynamic electrode-electrolyte interface.

BEAST DB employs a systematic framework that overcomes DFT deficiencies and accurately models electrochemical systems, providing clear baselines for electrocatalyst performance and serving as a building block for further theoretical developments.

The database also uses uniform calculation settings, a crucial piece missing in the literature that will allow for easier comparison of catalytic activity and productivity across different electrocatalysts and under different conditions.

A detailed window into thousands of catalytic reactions

BEAST DB utilizes grand-canonical methods to model ab initio electrochemical solvation for electrolytes to generate performance data on more than 24,000 molecule-catalyst combinations, where researchers can explore the reaction energetics for different transformations on catalytic surfaces.

The database includes promising electrocatalysts for the carbon dioxide reduction reaction, oxygen reduction reaction, oxygen evolution reaction, nitrogen reduction reaction, and hydrogen evolution reaction. Users can sort and view by calculation types, including absorbate formula, catalyst composition, and catalyst facet.

Each reaction type links to a dedicated calculation page that provides more reaction data, including an interactive 3D plot of the calculation to visualize the physical structure and plots of the charge on the molecule and the catalyst active site.

Users can also download a POSCAR structure file for ease of use with other visualization and analysis tools standard to the materials and catalysis communities.

The BEAST team provides conversion scripts to the format needed for the software packages powering BEAST DB—JDFTx and BerkeleyGW—to

reproduce the database results and perform additional calculations to provide further scientific insight.

Each of the above database properties can help researchers rationalize why catalysts are as effective as they are during electrocatalysis, while the data itself and the ability to build on it enable the creation of machine learning models that help inform the construction of new catalysts.

Accelerating a decarbonized future with electrocatalysis

Jacob Clary, an applied researcher at NREL working on the BEAST team who was instrumental in developing BEAST DB, is hopeful that the database will become an important tool to the electrocatalysis research community.

"I think the BEAST consortium overall is exciting because we're developing state-of-the-art tools to model electrocatalytic systems at higher fidelity and lower computational cost than existing approaches," Clary said.

Taylor Aubry, a computational science researcher at NREL and contributor of data to BEAST DB, is also looking forward to the value the database will bring.

"I anticipate that studies enabled by BEAST DB will provide invaluable insights into the myriad processes necessary for realizing a sustainable, decarbonized future, wherein electrochemical catalysis assumes a central role," Aubry said.

Bill Tumas, associate laboratory director of NREL's Materials, Chemical, and Computational Science directorate, said, "The versatility and amount of data in BEAST DB will go a long way toward helping researchers understand, predict, and control the design of electrocatalysts.

"Discovery of innovative electrocatalysts that enable the production of sustainable fuels and commodity chemicals has just become easier with this valuable tool."

The BEAST team will collaborate with electrocatalysis researchers on their next round of data generation and encourages input and collaborations from users of the database. The next version will include more complex representations of catalyst surfaces and reactions, e.g., defects, surface coverage, and lattice oxygen mechanisms.

Phys Org, 13 May 2024

https://phys.org

CHEMWATCH
Bulletin Board
Curiosities
MAY. 17, 2024

Researchers create new chemical compound to solve 120-year-old problem

2024-05-02

For the first time, researchers in the University of Minnesota College of Science and Engineering (CSE) created a highly reactive chemical compound that eluded scientists for more than 120 years. The discovery, published in Science, could lead to new drug treatments, safer agricultural products and better electronics.

For decades, researchers investigated molecules called N-heteroarenes, which are ring-shaped chemical compounds containing one or more nitrogen atoms. Molecules with a N-heteroarene core are widely used for medicinal applications, lifesaving pharmaceuticals, pesticides, herbicides and electronics, but they are extremely challenging for chemists to make.

"While the average person does not think about heterocycles on a daily basis, these unique nitrogen-containing molecules are widely applied across all facets of human life," said Courtney Roberts, senior author of the study and an assistant professor in CSE.

The team's experiments were accomplished using organometallic catalysis — the interaction between metals and organic molecules. The research also required collaboration between organic and inorganic chemists, a common practice at the University of Minnesota.

"We were able to run these chemical reactions with specialized equipment while getting rid of elements commonly found in our atmosphere," said Jenna Humke, a graduate student and lead author of the study. "Luckily, we have the tools to do that at the University of Minnesota, including a team of experts in all fields of chemistry — a vital component in solving this long-standing challenge."

After introducing the chemical compound in this study, the next step is to make it widely available to chemists across multiple fields to streamline the creation process. This could help solve important problems like preventing food scarcity and treating illnesses.

This work was primarily funded by the National Institutes of Health and the National Science Foundation. Funding was also provided by four

University of Minnesota-sponsored graduate research fellowships and start-up funding provided by the Department of Chemistry.

News & Events, 02 May 2024

https://twin-cities.umn.edu

Psilocybin Shows Promise as a Treatment for Anorexia Nervosa

2024-05-13

Characterised by pathological weight loss driven by restrictive feeding and excessive exercise behaviours, anorexia nervosa (AN) has one of the highest mortality rates of any psychiatric disease.

Some small clinical trials have shown that psilocybin, the active ingredient in magic mushrooms, may be a potential treatment for anorexia nervosa. The condition is characterised by cognitive inflexibility, or rigid thinking and there is evidence that psilocybin acts to increase this flexibility.

However – crucial to the use of the drug as a recognised treatment for anorexia – is the need to understand how psilocybin actually works in the brain. Now, a study led by Dr Claire Foldi from the Monash University Biomedicine Discovery Institute and published in the journal Molecular Psychiatry, has studied psilocybin in an animal model of anorexia nervosa – revealing that it improves body weight maintenance in female rats and facilitates cognitive flexibility.

Importantly, the Monash researchers found a specific mechanism within the brain by which psilocybin works to make "anorexic thinking" more pliable, opening the way for targeted therapies.

According to Dr Foldi, while selective serotonin reuptake inhibitors (antidepressants) are the leading pharmacological treatment, they are used off-label and "they do not improve clinical symptoms in underweight individuals with anorexia," she said.

"Cognitive inflexibility is a hallmark of the condition often arising before symptoms of anorexia nervosa are obvious, and persisting after weight recovery – making this symptom a primary target for therapeutic intervention."

Technology Networks, 13 May 2024

https://technologynetworks.com

CHEMWATCH
Bulletin Board
Curiosities
MAY. 17, 2024

Metalens expands Its reach from light to sound

2024-04-14

Sound waves, originating from vibrations in mediums like gases and liquids, are omnipresent in our daily experiences. Notably, high-frequency ultrasound waves, imperceptible to the human ear, are utilized in medical ultrasound examinations for diagnosing tissues or organs within the body. Consequently, sound waves serve as a vital energy source not only in medicine but also in telecommunications, energy harvesting, imaging, and various other domains. Acoustic lenses are fundamental in all these applications as they are instrumental in accurately focusing sound waves.

Professor Junsuk Rho's team, known for their work on metalens, is attracting acclaim for their advancements in optical metalens for light wave manipulation as well as acoustic metalens for sound control. Metalens, comprised of artificial structures usually smaller than the wavelength of the waves, enables unrestricted manipulation of waves while significantly reducing lens thickness. This research extends the concept of a "wide field-of-view," currently trending in next-generation AR and VR devices and displays, into the realm of acoustics, opening avenues for novel applications of "wide field-of-hearing" technology.

Wide field-of-hearing measures the breadth of angles through which a lens can display a sound image. Traditional acoustic metalenses suffer from undesired sound distortion (aberration) when waves approach at non-perpendicular angles. The team devised a method to meticulously control the phase of the metalens, ensuring precise focusing of sound waves regardless of their angle of incidence. This marks the first successful achievement and demonstration of a wide field-of-hearing using ultra-thin metalenses, achieving up to 140 degrees of field-of-hearing without sound distortion.

Professor Junsuk Rho of POSTECH stated, "By first demonstrating the significance and necessity of field-of-hearing, we've established a new paradigm in the realm of acoustic metalenses." He added, "We will continue our work to further explore its applications in acoustic imaging and high-sensitivity sensing along with explorations in energy harvesting and submarine monitoring within underwater environments."

Science Daily, 14 May 2024

https://sciencedaily.com

Is hyaluronic acid as effective at hydration and moisturising as skincare brands claim?

2024-03-23

Hyaluronic acid has become a huge buzzword in the beauty industry, with everything from creams and cleansers to shampoos containing it.

Often, these products are marketed to consumers with the promise that hyaluronic acid will boost hydration — important for keeping the skin looking its best.

Hyaluronic acid is ubiquitous in our organs and tissues, playing a crucial role in the function of our cells and tissues. It has been in clinical use for decades, for example, as an injectable between joints to help lubricate cartilage.

But at the turn of the century, cosmetic companies began using it as a moisturising ingredient in cosmetic products.

Topically, it's thought that hyaluronic acid works by holding and retaining water molecules in order to hydrate the skin and restore elasticity, preventing wrinkles.

When combined with sunscreen, hyaluronic acid may be capable of protecting the skin against ultraviolet radiation as it has antioxidant properties (meaning it prevents damage caused by oxidising agents, such as ultraviolet radiation).

Is it just hyaluronic hype?

One of the most frequent marketing claims used to sell hyaluronic acid is the long-held belief that hyaluronic acid holds 1,000 times its weight in water.

This means it can maintain moisture and reduce moisture loss.

But this claim has been called into question recently, with numerous publications recently discussing the findings of a pre-print paper which suggests this claim is not true.

The authors of the pre-print, researchers from the University of California, looked into the molecule-binding properties of hyaluronic acid and water to test the claim that it can hold 1,000 times its weight in water.

CHEMWATCH
Bulletin Board
Curiosities
MAY. 17, 2024

To do this, the researchers created a solution containing 1g of hyaluronic acid and 1,000g of water (0.1 per cent of hyaluronic acid), which was compared with just water.

They then applied heat to both solutions, measuring the thermal changes that occurred.

They found that there was not much difference in the changes that occurred in the 0.1 per cent hyaluronic acid solution compared with the pure water. They therefore concluded that the long-held claim is not true.

These findings may have consumers wondering how well their hyaluronic acid products actually work if it doesn't hydrate the skin as much as previously claimed.

How hyaluronic acid works

While there's no disputing the experimental results obtained, the conclusion on hyaluronic acid's water-holding capacity is not applicable to all forms of hyaluronic acids.

Hyaluronic acid comes in different molecular sizes. This pre-print only looked at one medium-sized hyaluronic acid molecule in their experiments. This means the results may only be true for products containing medium and smaller hyaluronic acid molecules.

When hylauronic acid interacts with water, its water-loving and water-hating parts lead to electrostatic repulsion. This enables large numbers of hyaluronic acid molecules to form networks, which look a bit like honeycombs, and expand.

The larger the hyaluronic acid's molecule size, the more capable it is of forming these honeycomb structures — and also the more able it is to retain water relative to its own weight.

Hyaluronic acid with larger molecular sizes will form these networks at a concentration of 0.1 per cent, meaning it can hold 1,000 times its own weight in water. Some very large molecules will even form these networks at a concentration as low as 0.05 per cent. This means it can hold 2,000 times its weight in water.

It's also worth noting that hyaluronic acid doesn't just hold moisture and hydrate the skin. Because of its hydrating and antioxidant effects, it also promotes cell regeneration and stimulates collagen production. So hyaluronic acid's benefits go beyond its ability to retain water.

Although this paper may have partially debunked one popular claim about hyaluronic acid's moisturising abilities, that doesn't mean you should stop using it.

The research still shows there's no doubt about hyaluronic acid's moisturising abilities, which can leave skin softer, smoother and with fewer wrinkles. Plus, hyaluronic acid's antioxidant effects promote the growth of new skin cells and collagen.

But if you want to make sure you're getting the most effective product possible, look for one containing multiple weights of hyaluronic acid molecules (sometimes labelled as "triple weight", "multiweight" or "multi-molecular weight").

Also look for a product containing a minimum hyaluronic acid concentration of 0.1 per cent.

This is because research suggests products containing a formulation of multiple sizes of hyaluronic acid molecules could be more beneficial for skin than formulations containing only one molecule size. This is partly due to smaller molecules permeating skin better, while the larger ones hold more water.

ABC News, 23 March 2024

https://abc.net.au

Bionanomachine Breakthrough: A Master Key for Sustainable Chemistry

2024-04-14

Enzymes are powerful biomolecules that can be used to produce many substances at ambient conditions. They enable "green" chemistry, which reduces environmental pollution resulting from processes used in synthetic chemistry. One such tool from nature has now been characterized in detail by PSI researchers: the enzyme styrene oxide isomerase. It is the biological version of the Meinwald reaction, an important chemical reaction in organic chemistry.

"The enzyme, discovered decades ago, is made by bacteria," says Richard Kammerer of PSI's Biomolecular Research Laboratory. His colleague Xiaodan Li adds: "But because the way it functions was not known, its practical application has been limited up to now." The two researchers and their team have elucidated the structure of the enzyme as well as the way it works.

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Curiosities
MAY. 17, 2024

Simple Mechanism for a Complicated Reaction

Microorganisms possess specific enzymes with which they can, for example, break down harmful substances and use them as nutrients. Styrene oxide isomerase is one of these. Together with two other enzymes, it enables certain environmental bacteria to grow on the hydrocarbon styrene.

The styrene oxide isomerase catalyzes a very specific step in the reaction: it splits a three-membered ring in the styrene oxide consisting of one oxygen and two carbon atoms, a so-called epoxide. Thereby the enzyme is highly specific and creates only one product. It is also capable of converting a number of additional substances, producing important precursors for medical applications.

One particular advantage has to do with the fact that in many chemical reactions, both an image and a mirror image of a chemical compound are formed, which may have completely different biological effects. But this enzyme specifically creates only one of the two products. In chemistry this property is called stereospecificity – it is particularly important for the generation of precursor molecules for drugs. "The enzyme is an impressive example of how nature makes chemical reactions possible in a simple and ingenious way," Xiaodan Li says.

Extremely Useful in Chemical and Pharmaceutical Industries

In the course of their investigations, which they conducted in part at the Swiss Light Source SLS, the PSI researchers discovered the enzyme's secret: an iron-containing group in its interior, similar to the iron-containing pigment in our red blood cells. This haem group binds the epoxide ring, and that's how it makes the reaction so simple and efficient. Other parts of the investigations were carried out by the group of Volodymyr Korkhov, also from the PSI Laboratory for Biomolecular Research and Associate Professor in the Department of Biology at ETH Zurich, using cryo-electron microscopy.

Xiaodan Li and Richard Kammerer feel certain that the enzyme will prove extremely useful in the chemical and pharmaceutical industries. "It is so far the only bacterial enzyme known to catalyze the Meinwald reaction," Richard Kammerer emphasizes. With the enzyme's help, industry could produce precursors for drugs and important chemicals under energy-saving and environmentally friendly conditions.

Xiaodan Li adds: "The enzyme could potentially be altered so that it can produce a great many new substances." In addition, the enzyme is very stable and thus is suitable for large-scale industrial applications. "It will certainly become a new, important tool for the circular economy and green chemistry," the PSI researchers are convinced.

Sci Tech Daily, 14 May 2024

https://scitechdaily.com

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PHARMACEUTICAL/TOXICOLOGY

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OCCUPATIONAL

Carbon Monoxide Poisoning: From Occupational Health to Emergency Medicine

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