CHEMWATCH

Bulletin Board

Contents

JUN. 07, 2024

(click on page numbers for links)

CONTACT US

subscribers@chemwatch.net
tel +61 3 9572 4700
fax +61 3 9572 4777

1227 Glen Huntly Rd
Glen Huntly
Victoria 3163 Australia

CHEMWATCH

Bulletin Board

Contents

JUN. 07, 2024

CHEMWATCH

Bulletin Board

Contents

JUN. 07, 2024

ASIA PACIFIC

Preparing for the engineered stone ban

2024-05-28

Safe Work Australia has finalised amendments to the model WHS Regulations to give effect to the engineered stone ban from 1 July 2024.

On 22 March 2024, WHS ministers agreed to progress amendments to the model WHS Regulations to give effect to a ban on engineered stone benchtops, panels and slabs. WHS ministers also endorsed a stronger regulatory framework to manage risks of exposure to respirable crystalline silica (RCS) from any material or product that contain at least 1% crystalline silica. The amendments are designed to protect thousands of workers from the health and safety risks from exposure to RCS.

The amendments prohibit a PCBU from carrying out, or directing or allowing a worker to carry out, work involving the manufacture, supply, processing or installation of engineered stone benchtops, panels and slabs.

This ban will not apply to the removal, repair or minor modification of engineered stone benchtops, panels or slabs installed prior to the 1 July 2024. Other limited exceptions to the prohibition are provided in relation to disposal of engineered stone benchtops, panels or slabs and in relation to research and sampling.

The amendments additionally provide a notification framework for PCBUs working with previously installed engineered stone, and a national framework for WHS regulators to grant exemptions from the prohibition.

For the amendments to the model WHS Regulations to apply, each jurisdiction will need to implement them separately through amendments to their own WHS laws.

Safe Work Australia is developing guidance to support PCBUs and workers understand how amendments to the model WHS Regulations will affect them and to help them prepare for the changes.

Visit our website for the latest information on the engineered stone ban, and contact your WHS regulator for information about transitional arrangements and the implementation of the ban in your jurisdiction.

CHEMWATCH
Bulletin Board
Regulatory Update
JUN. 07, 2024

Read More

SWA, 28-05-24

https://www.safeworkaustralia.gov.au

China Notice on the public solicitation of opinions on the national ecological environment standard "Technical Guidelines for Environmental Impact Assessment - Format and Content of Environmental Impact Report for Near-Surface Disposal of Radioactive Solid Waste (Draft for Comments)"

2024-05-15

In order to implement the Environmental Protection Law of the People's Republic of China, the Nuclear Safety Law of the People's Republic of China, the Environmental Impact Assessment Law of the People's Republic of China, and the Radioactive Pollution Prevention and Control Law of the People's Republic of China, standardize the environmental impact assessment of radioactive solid waste near-surface disposal construction projects, our Ministry organized the preparation of the "Technical Guidelines for Environmental Impact Assessment - Format and Content of Environmental Impact Report for Near-Surface Disposal of Radioactive Solid Waste (Draft for Comments)", which is now open for public comment. The draft for comments and the preparation instructions can be searched in the "Comments Collection" column of our ministry's website (http://www.mee.gov.cn).

All agencies, groups, enterprises, institutions and individuals can put forward opinions and suggestions. Please provide feedback to our department in writing if you have any comments. Please send the electronic version of the materials to the contact person's email address at the same time. The deadline for soliciting comments is May 31, 2024.

Read More

Ministry of Ecology and Environment of China, 15-05-24

https://www-mee-gov-cn.translate.goog/xxgk2018/xxgk/xxgk06/202405/t20240508_1072636.html?_x_tr_sl=auto&_x_tr_tl=en&_x_tr_hl=en&_x_tr_pto=wapp

China MEE Adds 41 Substances to IECSC (Updated on May 20, 2024)

2024-05-24

These 41 substances are regulated as existing chemical substances in China.

Updates:

China MEE recently issued two notices to announce the addition of 41 chemical substances to the IECSC.

- **Notice I**

The proposal of adding 7 substances to the IECSC made in January 2024 has been adopted. Details of the 7 substances can be accessed here.

- **Notice II**

34 substances, which were previously registered under the Measures on Environmental Management of New Chemical Substances (MEP Order No. 7 of 2010), are now qualified for listing in the IECSC as existing chemical substances in China. They are now regulated as existing chemical substances in China, and thus free from new chemical registration or notification requirements under the MEE Order No.12. However, if the substance is used for industrial applications other than the permitted uses, new usage registration will be required. Details of the 34 substances are available here.

Read More

Chemlinked, 24-05-24

https://chemical.chemlinked.com/news/chemical-news/china-mee-consults-on-adding-7-chemicals-to-iecsc

Protecting workers from airborne contaminants

2024-05-28

Following extensive consultation and an expert review, WHS ministers have approved new workplace exposure limits for airborne contaminants, which will come into effect on 1 December 2026 following a harmonised transitional period.

Work processes can release dusts, gases, fumes, vapours or mists into the air – known as airborne contaminants. These may be invisible or odourless, and breathing them in can increase the risk of adverse health effects,

CHEMWATCH
Bulletin Board
Regulatory Update
JUN. 07, 2024

including occupational lung diseases. Under the model WHS Regulations, persons conducting a business or undertaking (PCBUs) must ensure that workers are not exposed to a level of airborne contaminant that exceeds the WES.

From WES to WEL: what's changing

The workplace exposure standards will be known as workplace exposure limits, or WEL, when the WEL is implemented on 1 December 2026. The change from standards to limits aligns with terms used internationally and makes it clear that these are limits that should not be exceeded. There are no changes to the concept or units of measurement.

"Based on contemporary health data, the updated workplace exposure limits for airborne contaminants will help better protect workers and make workplaces safer."

Fiona Leves, Director, Chemicals Policy

While most exposure limits remained unchanged, the WES Review did result in some reductions and increases in limits and the removal or introduction of new limits. These include:

- reductions in 160 exposure limits
- increases in 11 exposure limits
- amendments to 79 exposure limits, including:
- introduction or removal of 8-hour time weighted average, short term exposure limit or peak limitation for a particular airborne contaminant
- merging multiple pre-existing exposure standards into a singular WEL
- splitting pre-existing exposure standards into 2 WELs to account for differences in the inhalation and respirable fraction
- introduction of 30 exposure limits
- removal of 6 exposure limits.

Compliance with the WEL list will only become mandatory following 1 December 2026 and once adopted into the WHS laws of each jurisdiction. Until then, PCBUs must ensure they still adhere to the current WES and fulfil their existing duty to eliminate or minimise risks to workers from hazardous chemicals so far as is reasonably practicable.

"Breathing in dusts, gases, fumes, vapours or mists at work may cause lung damage. Eliminating or reducing exposure to airborne contaminants can lower the risk of developing occupational lung disease later in life."

Maryanne Shoobridge, Director, Occupational Diseases and Hygiene Policy

What's next?

We will be doing further impact analysis for the following chemicals and substances to inform changes to their workplace exposure limit in the WEL:

- respirable crystalline silica
- formaldehyde
- benzene
- chlorine
- copper (fumes, dusts and mists)
- hydrogen cyanide
- hydrogen sulphide
- nitrogen dioxide, and
- titanium dioxide.

Find out more about the WEL, the changes from the WES, and the transitional period, on our website.

Read More

SWA, 28-05-24

https://www.safeworkaustralia.gov.au

AMERICA

Protecting children and families from lead and cadmium

2024-05-21

To protect children and families from short- and long-term health impacts that can come from exposure to lead and cadmium, Minnesota passed a law in 2023 that restricts a broader array of consumer products, including toys and school supplies, from containing those toxic chemicals. The MPCA has developed additional guidance on the law.

Investigation leads to action

While Minnesota had already regulated lead and cadmium content in children's jewellery, an interagency team including representatives from the MPCA, Department of Health, and Department of Commerce

CHEMWATCH
Bulletin Board
Regulatory Update
JUN. 07, 2024

found that some inexpensive toys and jewellery contained lead and cadmium levels well above regulatory limits. Those findings spurred recommendations for tighter restrictions on lead and cadmium content in toys, jewellery, and other consumer items that children can likely encounter in the home.

Getting toxic metals out of products

Under the new law (Minn. Stat. § 325E.3892), which went into effect July 1, 2023, a person or business cannot import, manufacture, sell, hold for sale, distribute, or offer products in certain categories containing lead at more than 0.009 percent by total weight (90 parts per million) or cadmium at more than 0.0075 percent by total weight (75 parts per million). That list of categories includes:

- jewelry
- toys
- cosmetics and personal care products
- puzzles, board games, card games, and similar games
- play sets and play structures
- outdoor games
- school supplies
- pots and pans
- cups, bowls, and other food containers
- craft supplies and jewelry-making supplies
- chalk, crayons, paints, and other art supplies
- fidget spinners
- costumes, costume accessories, and children's and seasonal party supplies
- keys, key chains, and key rings
- clothing, footwear, headwear, and accessories

Read More

US Minnesota Pollution Control Agency, 21-05-24

https://www.pca.state.mn.us/air-water-land-climate/protecting-children-and-families-from-lead-and-cadmium#guidance

Publication after assessment of 16 substances in the Gas Oils and Kerosenes with Uses in Products Available to Consumers Group specified on the Domestic Substances List (section 77 of the Canadian Environmental Protection Act, 1999)

2024-05-21

Whereas a summary of the draft assessment conducted on the Gas Oils and Kerosenes with Uses in Products Available to Consumers Group pursuant to paragraphs 68(b) or (c) of the Act is annexed hereby;

And whereas it is proposed to conclude that the substances meet one or more of the criteria set out in section 64 of the Act;

Notice therefore is hereby given that the Minister of the Environment and the Minister of Health (the ministers) propose to recommend to Her Excellency the Governor in Council that these substances be added to Part 2 of Schedule 1 to the Act.

Notice is furthermore given that the ministers have released a risk management scope document for these substances to initiate discussions with stakeholders on the development of risk management options.

Public comment period

Any person may, within 60 days after publication of this notice, file with the Minister of the Environment written comments on the measure the ministers propose to take and on the scientific considerations on the basis of which the measure is proposed. More information regarding the scientific considerations may be obtained from the Canada.ca (Chemical substances) website. All comments must cite the Canada Gazette, Part I, and the date of publication of this notice and be addressed to the Executive Director, Substance Prioritization, Assessment and Coordination Division, Department of the Environment, Gatineau, Quebec K1A 0H3, by email to substances@ec.gc.ca or by using the online reporting system available through Environment and Climate Change Canada's Single Window.

In accordance with section 313 of the Canadian Environmental Protection Act, 1999, any person who provides information in response to this notice may submit with the information a request that it be treated as confidential.

CHEMWATCH
Bulletin Board
Regulatory Update
JUN. 07, 2024

Read More

Canada Gazette, 21-05-24

https://gazette.gc.ca/rp-pr/p1/2024/2024-05-04/html/notice-avis-eng.html#na3

Bill that would restrict PFAS in consumer products heads to governor

2024-05-07

The Vermont Legislature gave its final approval Tuesday to a bill that restricts toxic so-called "forever chemicals" in a suite of commercial goods.

The bill bans PFAS in clothing, makeup, menstrual products, diapers and nonstick frying pans starting in 2026. It also bans them in turf starting in 2028.

The tiny chemicals don't break down on their own and are increasingly ubiquitous in drinking water and the natural environment.

The Environmental Protection Agency has said virtually no level of exposure to them is safe, and the agency added the chemicals to its "Superfund" list this spring.

Paul Burns of the Vermont Public Interest Research Group said the bill will go a long way to protect Vermont consumers from chemical toxins.

"This legislation, I think, will stand as perhaps the most comprehensive legislation thus far passed in the country dealing with PFAS pollution," he said.

Read More

Vermont Public, 07-05-24

https://www.vermontpublic.org/local-news/2024-05-07/bill-that-would-restrict-pfas-in-consumer-products-heads-to-governor

EUROPE

Denmark wants to ban PFAS in clothing and shoes

2024-05-29

As part of a new action plan on the use of per- and polyfluoroalkyl substances (PFAS), the Danish government has proposed to introduce a

national ban on PFAS in clothing, footwear and sealants, as these are one of the largest sources of PFAS in the local environment. Notably, PFAS in workwear and safety clothing should not be affected by the ban.

"We must take the lead in working to limit PFAS at the source. A national ban will benefit our health and the environment in Denmark," commented Environment Minister Magnus Heunicke in a statement.

PFAS belong to the so-called "eternal chemicals", as they are difficult to break down and therefore spread everywhere in the environment. There they are absorbed by plants and animals, which become food and are eaten by humans. In the long term, PFAS can weaken the immune system, cause hormonal disorders and are suspected of increasing the risk of cancer.

"A national ban on the import and sale of clothing, footwear and waterproofing products containing PFAS is an important step towards limiting emissions and will have a real impact on the environment in Denmark. It also sends a strong signal to the rest of the world that we need to phase out these substances wherever possible," added Heunicke.

Read More

Fashion United, 29-05-24

https://fashionunited.com/news/business/denmark-wants-to-ban-pfas-in-clothing-and-shoes/2024050259699

Sweden, France and Denmark calls for new global rules on exporting textile waste to developing countries

2024-03-24

Opinion piece by Romina Pourmokhtari, Minister for Climate and the Environment in Sweden, Christophe Béchu, Minister for Ecological Transition and Cohesion of the Territories in France and Magnus Heunicke, Minister for the Environment in Denmark, published in Dagens industri, March 25 2024.

We must put an end to exporting our textile waste problems to developing countries. That is why Sweden, France and Denmark today are proposing new global rules for exporting textile waste under the Basel Convention.

There have never been so many clothes sold in the world, with over 100 billion new pieces of clothing sold every year. This impressive growth

CHEMWATCH
Bulletin Board
Regulatory Update
JUN. 07, 2024

comes with environmental challenges, as the production of textiles requires large amounts of energy, water and use of chemicals. The lifecycle of textiles is another source of pollution, including the release of increasing quantities of microplastics in the environment. The textile sector is also a significant contributor to climate change, as it accounts for 10% of global greenhouse gas emissions, more than air or maritime transport.

Over the past 20 years, the EU's exports of used textiles have tripled. In 2019 alone 1.7 million tons of textiles were exported outside the EU, mainly to countries in Africa and Asia who do not have the capacity to ensure proper waste management. Mismanaged textile waste frequently ends up in landfills or in nature, where it causes harm to both humans, animals and the environment.

Read More

The Government of Sweden, 25-03-24

https://www.government.se/opinion-pieces/2024/03/sweden-france-and-denmark-calls-for-new-global-rules-on-exporting-textile-waste-to-developing-countries

INTERNATIONAL

Construction machinery manufacturers seek exemptions on forever chemicals

2024-05-23

Construction machinery manufacturers have joined a worldwide industrial lobbying movement to support the continued use of toxic chemicals.

The European Union has been tightening the rules concerning per- and polyfluoroalkyl substances (PFAS) in recent years and is heading in the direction of a total ban.

PFAS are also known as forever chemicals because they rarely break down and cannot be cleaned.

Various global authorities are looking at clamping down further on these chemicals, or even an outright ban.

Construction machinery manufacturers are worried. Manufacturers' organisations from Europe, the USA, Japan, Korea, India and Australia

have come together to formulate a joint response to what they regard as a threat – a threat to machine safety, a threat to durability and a threat to their businesses.

"Regarding our internationally intertwined supply chains, we believe a coordinated approach to regulating PFAS across regions is needed. It has become apparent that any general restriction on PFAS will have severe repercussions over both import and export of equipment, thereby threatening the quality of the trade relationships between our regions."

They say: "We stand for a substance-specific approach to regulating diverse PFAS as it contributes to making proportionate decisions while ensuring a level-playing field across industries. Referring to the Montreal Protocol, multiple authorities around the world are considering extending application of essential use criteria to PFAS restriction and authorization procedures. Considering our need for legal certainty, our numerous PFAS industrial applications, to which few credible alternatives can be proposed today, should remain regulated in accordance with the principle of proportionality.

"Our construction equipment manufacturers design products to effectively operate for decades mostly in harsh and demanding environments whilst satisfying safety, environmental, regulatory, durability, quality, and customer requirements. Construction equipment manufacturers use state-of-the-art and innovative technologies to meet the challenging variety of requirements, with PFAS performing a variety of essential use functions to help achieve these goals. It is crucial to understand that without the functionality provided by certain PFAS chemicals, the future construction equipment products able to meet air quality, climate, safety, durability, waste, sustainability, and alternative power goals is imperilled."

Read More

The Construction Index, 23-05-24

https://www.theconstructionindex.co.uk/news/view/construction-machinery-manufacturers-seek-exemptions-on-forever-chemicals

Six language webinars on mercury-added products

2024-05-28

The Minamata Convention Secretariat, in collaboration with its partners, is organizing a series of webinars on the Minamata Convention and mercury-added products. Funded by the European Union, this series will be available in all six UN languages. With the European Union's financial

CHEMWATCH
Bulletin Board
Regulatory Update
JUN. 07, 2024

support, the Secretariat is also developing a capacity-building material in six languages to help control mercury-added products. This material, along with updates on the latest amendments to the Convention and decisions from COP-5, will be presented during the webinars. The series will run from June 6 to July 3. Check the dedicated page for more information.

ABOUT THE UNEP GLOBAL MERCURY PARTNERSHIP

The Global Mercury Partnershipaims to protect human health and the environment from the releases of mercury to air, water and land. With over 250 partners to date, from governments, IGOs, NGOs, industry and academia, the Partnership focuses on supporting timely and effective implementation of the Minamata Convention, providing state of the art knowledge and science and raising awareness towards global action on mercury.

Read More

UNEP, 28-05-24

https://minamataconvention.org/en/events/six-language-webinars-mercury-added-products

Consultations on potential candidates for substitution and on derogations conditions

2024-05-29

If an active substance meets any of the criteria for substitution listed in Article 10(1) of the Biocidal Products Regulation (BPR), then the evaluating competent authority may identify the substance as a potential candidate for substitution (CfS).

If this is the case, normally before submitting its opinion on the approval or renewal of the renewal of the active substance to the Commission, ECHA will launch a consultation to collect information on potential alternatives to this substance (Article 10(3) if the BPR).

In addition to be a candidate for substitution, an active substance might meet the exclusion criteria listed in Article 5(1) of the BPR:

- carcinogens, mutagens and reprotoxic substances categories 1A or 1B according to the CLP Regulation
- endocrine disruptors
- persistent, bioaccumulative and toxic (PBT) substances
- very persistent and very bioaccumulative (vPvB) substances

Active substances meeting these exclusion criteria should normally not be approved. However, derogations may be possible as laid down in Article 5(2) of the BPR, when it is shown that:

1. the risk to humans, animals or the environment from exposure to the active substance in a biocidal product, under realistic worst-case conditions of use, is negligible, in particular where the product is used in closed systems or under other conditions which aim to exclude contact with humans and release into the environment;
2. there is evidence that the active substance is essential to prevent or control a serious danger to human health, animal health or the environment; or
3. not approving the active substance would have a disproportionate negative impact on society when compared with the risk to human health, animal health or the environment arising from the use of the substance.

Moreover, Article 5(2) of the BPR specifies that the availability of suitable and sufficient alternative substances or technologies shall be a key consideration when deciding on the approval of substances meeting the exclusion criteria.

CHEMWATCH
Bulletin Board
REACH Update
JUN. 07, 2024

If at least one of the derogation conditions is met, approval of an active substance may be granted for a maximum period of five years, and for restricted uses. In addition, Member States may only authorise biocidal products where they consider that conditions are met on their territory.

ECHA collects additional information whether these substances meet at least one of the derogation conditions through third-party consultations.

This page lists the ongoing third-party consultations on the availability of alternatives for substances which are potential candidate for substitution and, in addition, for substances meeting the exclusion criteria, on argumentation for meeting at least one of the derogation conditions.

Read More

ECHA, 29-05-24

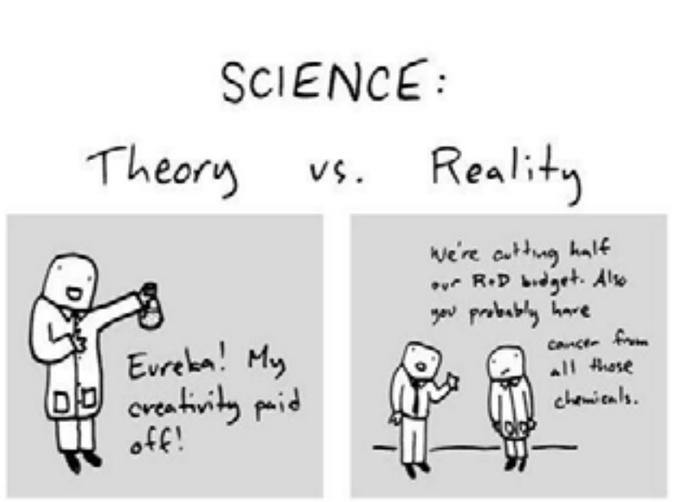
https://echa.europa.eu/current-candidates-for-substitution-and-derogations-conditions

Janet's Corner

JUN. 07, 2024

Theory vs Reality

2024-06-07



https://www.toothpastefordinner.com/

CHEMWATCH
Bulletin Board

Hazard Alert

JUN. 07, 2024

Acetophenone

2024-06-07

USES [2,3]

Acetophenone is used in perfumery as a fragrance ingredient in soaps, detergents, creams, lotions, and perfumes; as a flavouring agent in foods, non-alcoholic beverages, and tobacco; as a specialty solvent for plastics and resins; as a catalyst for the polymerisation of olefins; and in organic syntheses as a photosensitiser.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Exposure Sources

- Occupational exposure to acetophenone may occur during its manufacture and use.
- Acetophenone has been detected in ambient air and drinking water; exposure of the general public may occur through the inhalation of contaminated air or the consumption of contaminated water.

Routes of Exposure

Acetophenone can be absorbed into the body by inhalation, through the skin and by ingestion. A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20°C; on spraying or dispersing, however, much faster and may pose a risk via inhalation.

HEALTH EFFECTS [4]

Acute Health Effects

- Acute exposure of humans to acetophenone vapour may produce skin irritation and transient corneal injury. One study noted a decrease in light sensitivity in exposed humans.
- Acute oral exposure has been observed to cause hypnotic or sedative effects, haematological effects, and a weakened pulse in humans.
- Congestion of the lungs, kidneys, and liver were reported in rats acutely exposed to high levels of acetophenone via inhalation.
- Tests involving acute exposure of rats, mice, and rabbits have demonstrated acetophenone to have moderate acute toxicity from oral or dermal exposure.

Acetophenone is the organic compound with the formula C6H5C(O)CH3. It is the simplest aromatic ketone. Is a colour-less or yellow-tinted liquid with a sweet, strong odour. [1,2]

Carcinogenicity

- No information is available on the carcinogenic effects of acetophenone in humans or animals.
- EPA has classified acetophenone as a Group D, not classifiable as to human carcinogenicity.

Other Effects

- Phenanthrene may cause a skin allergy. If allergy develops, very low future exposure can cause itching and a skin rash.

SAFETY

First Aid Measures [5]

- No information is available on the chronic effects of acetophenone in humans.
- Degeneration of olfactory bulb cells was reported in rats chronically exposed via inhalation. In another study, chronic inhalation exposure of rats produced haematological effects and, at high doses, congestion of cardiac vessels and pronounced dystrophy of the liver.
- In two studies, no effects were observed in rats chronically exposed to acetophenone in their diet.
- EPA has not established a Reference Concentration (RfC) for acetophenone.
- The Reference Dose (RfD) for acetophenone is 0.1 milligram per kilogram body weight per day (mg/kg/d) based on general toxicity in rats.

Workplace Controls & Practices [4]

Engineering controls include:
Exhaust ventilation or other engineering controls should be provided to keep the airborne concentrations of acetophenone vapours below their respective threshold limit value.

- Ensure that eyewash stations and safety showers are proximal to the workstation location.

Personal Protective Equipment [5]

The following personal protective equipment should be used when handling acetophenone:

CHEMWATCH
Bulletin Board
Hazard Alert
JUN. 07, 2024

- Splash goggles;
- Lab coat;
- Gloves

Personal Protection in Case of a Large Spill:

- Splash goggles;
- Full suit;
- Boots;
- Gloves;
- Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product

REGULATION

United States

ACGIH: The American Conference of Governmental Industrial Hygienists has set a Threshold Limit Value (TLV) for acetophenone of 10 ppm, 49 mg/m3 Time Weighted Average

REFERENCES

1. http://en.wikipedia.org/wiki/Acetophenone
2. http://nj.gov/health/eoh/rtkweb/documents/fs/2961.pdf
3. http://www.epa.gov/ttn/atw/hlthef/acetophe.html
4. http://www.cdc.gov/niosh/ipcsneng/neng1156.html
5. http://www.sciencelab.com/msds.php?msdsId=9922778
6. https://www.osha.gov/dts/chemicalsampling/data/CH_216750.html

100% of cancer patients cured long-term in 'remarkable' human trial

2024-06-05

In what researchers have called an "unprecedented" response, a new drug that treats locally advanced rectal cancer has shown to have completely eradicated tumors in all 42 patients who took part in the Phase II trial.

The drug, Jemperli (dostarlimab-gxly), had earlier shown great potential for eliminating mismatch repair deficient (dMMR) cancers, which make up 5-10% of colorectal cancers. Following the Phase II trial, the first 24 patients assessed showed a "sustained complete clinical response" – no cancer evident – after an average of 26.3 months.

"These findings demonstrate the potential of dostarlimab-gxly as a novel approach to treating locally advanced dMMR rectal cancer that leads to durable complete tumor regression without the need for life-altering treatment," said Dr Andrea Cercek, researcher and oncologist at the Memorial Sloan Kettering Cancer Center (MSK). "As a clinician, I've seen firsthand the debilitating impact of standard treatment of dMMR rectal cancer and am thrilled about the potential of dostarlimab-gxly in these patients."

The drug is a hugely promising first-line treatment option, bypassing the need for chemotherapy and radiation. Right now, while traditional treatment is effective, it's incredibly invasive and impacts long-term quality of life. And ultimately, a third of patients will see their cancer metastasize and become terminal.

Those who do undergo surgery often experience life-long life-changing impacts, including bowel, urinary and sexual dysfunction, as well as secondary cancers and infertility.

"We wanted to see if we could make a tumor with the MMR(d) mutation recede and eventually disappear using only immunotherapy to spare patients these life-altering consequences of standard treatment," Dr Luis Diaz Jr said last year, after preliminary trial research showed how effective this drug was at targeting the cancer.

Unlike chemotherapy, dostarlimab-gxly is a programmed death receptor-1 (PD-1)-blocking monoclonal antibody, which enters the body and binds to the protein PD-1 T cells, encouraging these immune cells to attack cancer cells. While still in its early stages before clinical use, it's already been hyped up as a 'wonder drug' for successful, non-invasive cancer treatment.

CHEMWATCH
Bulletin Board
Gossip
JUN. 07, 2024

Last year, the drug was approved by the FDA as a complementary treatment alongside chemotherapy for endometrial cancer. The pharmaceutical company behind Jemperli, GSK, will now undertake studies on other types of colorectal cancers, hoping for similar impactful results.

"The data showing no evidence of disease in 42 patients is remarkable," said Hesham Abdullah, GSK Senior Vice President. "These results bring us one step closer to understanding the potential of dostarlimab-gxly in this curative-intent setting for patients with dMMR locally advanced rectal cancer. We look forward to evaluating dostarlimab-gxly in certain colorectal cancers in our ongoing AZUR-1 and AZUR-2 registrational studies."

In a statement, GSK said patients didn't experience side-effects above grade three, with most experiencing mild or moderate adverse reactions. The company noted that the drug's safety and tolerance is "consistent with the known safety profile of the agent."

The results of the long-term follow-up examinations were presented at the 2024 American Society of Clinical Oncology (ASCO) annual meeting in Chicago this week.

New Atlas, 5 June 2024

https://newatlas.com

Turning Up the Heat on Next-Generation Semiconductors

2024-05-24

The scorching surface of Venus, where temperatures can climb to 480 degrees Celsius (hot enough to melt lead), is an inhospitable place for humans and machines alike. One reason scientists have not yet been able to send a rover to the planet's surface is because silicon-based electronics can't operate in such extreme temperatures for an extended period of time.

For high-temperature applications like Venus exploration, researchers have recently turned to gallium nitride, a unique material that can withstand temperatures of 500 degrees or more.

The material is already used in some terrestrial electronics, like phone chargers and cell phone towers, but scientists don't have a good grasp of

how gallium nitride devices would behave at temperatures beyond 300 degrees, which is the operational limit of conventional silicon electronics.

In a new paper published in Applied Physics Letters, which is part of a multiyear research effort, a team of scientists from MIT and elsewhere sought to answer key questions about the material's properties and performance at extremely high temperatures.

They studied the impact of temperature on the ohmic contacts in a gallium nitride device. Ohmic contacts are key components that connect a semiconductor device with the outside world.

The researchers found that extreme temperatures didn't cause significant degradation to the gallium nitride material or contacts. They were surprised to see that the contacts remained structurally intact even when held at 500 degrees Celsius for 48 hours.

Understanding how contacts perform at extreme temperatures is an important step toward the group's next goal of developing high-performance transistors that could operate on the surface of Venus. Such transistors could also be used on Earth in electronics for applications like extracting geothermal energy or monitoring the inside of jet engines.

"Transistors are the heart of most modern electronics, but we didn't want to jump straight to making a gallium nitride transistor because so much could go wrong. We first wanted to make sure the material and contacts could survive, and figure out how much they change as you increase the temperature. We'll design our transistor from these basic material building blocks," says John Niroula, an electrical engineering and computer science (EECS) graduate student and lead author of the paper.

Turning up the heat

While gallium nitride has recently attracted much attention, the material is still decades behind silicon when it comes to scientists' understanding of how its properties change under different conditions. One such property is resistance, the flow of electrical current through a material.

A device's overall resistance is inversely proportional to its size. But devices like semiconductors have contacts that connect them to other electronics. Contact resistance, which is caused by these electrical connections, remains fixed no matter the size of the device. Too much contact resistance can lead to higher power dissipation and slower operating frequencies for electronic circuits.

CHEMWATCH
Bulletin Board
Gossip
JUN. 07, 2024

"Especially when you go to smaller dimensions, a device's performance often ends up being limited by contact resistance. People have a relatively good understanding of contact resistance at room temperature, but no one has really studied what happens when you go all the way up to 500 degrees," Niroula says.

For their study, the researchers used facilities at MIT.nano to build gallium nitride devices known as transfer length method structures, which are composed of a series of resistors. These devices enable them to measure the resistance of both the material and the contacts.

They added ohmic contacts to these devices using the two most common methods. The first involves depositing metal onto gallium nitride and heating it to 825 degrees Celsius for about 30 seconds, a process called annealing.

The second method involves removing chunks of gallium nitride and using a high-temperature technology to regrow highly doped gallium nitride in its place, a process led by Rajan and his team at Ohio State. The highly doped material contains extra electrons that can contribute to current conduction.

"The regrowth method typically leads to lower contact resistance at room temperature, but we wanted to see if these methods still work well at high temperatures," Niroula says.

A comprehensive approach

They tested devices in two ways. Their collaborators at Rice University, led by Zhao, conducted short-term tests by placing devices on a hot chuck that reached 500 degrees Celsius and taking immediate resistance measurements.

At MIT, they conducted longer-term experiments by placing devices into a specialized furnace the group previously developed. They left devices inside for up to 72 hours to measure how resistance changes as a function of temperature and time.

Microscopy experts at MIT.nano (Aubrey N. Penn) and the Technology Innovation Institute (Nitul S. Rajput) used state-of-the-art transmission electron microscopes to see how such high temperatures affect gallium nitride and the ohmic contacts at the atomic level.

"We went in thinking the contacts or the gallium nitride material itself would degrade significantly, but we found the opposite. Contacts made with both methods seemed to be remarkably stable," says Niroula.

While it is difficult to measure resistance at such high temperatures, their results indicate that contact resistance seems to remain constant even at temperatures of 500 degrees, for around 48 hours. And just like at room temperature, the regrowth process led to better performance.

The material did start to degrade after being in the furnace for 48 hours, but the researchers are already working to boost long-term performance. One strategy involves adding protective insulators to keep the material from being directly exposed to the high-temperature environment.

Moving forward, the researchers plan to use what they learned in these experiments to develop high-temperature gallium nitride transistors.

"In our group, we focus on innovative, device-level research to advance the frontiers of microelectronics, while adopting a systematic approach across the hierarchy, from the material level to the circuit level. Here, we have gone all the way down to the material level to understand things in depth. In other words, we have translated device-level advancements to circuit-level impact for high-temperature electronics, through design, modeling and complex fabrication. We are also immensely fortunate to have forged close partnerships with our longtime collaborators in this journey," Xie says.

Technology Networks, 24 May 2024

https://technologynetworks.com

Researchers successfully fabricate magneto-optical ceramics

2024-06-05

A team of material scientists led by Jiang Li from Shanghai Institute of Ceramics, Chinese Academy of Sciences, in Shanghai, China recently reported (Tb1-xYx)3Al5O12 magneto-optical ceramics with high optical quality. The optical transmittance, microstructure, Verdet constant, and thermal conductivity of (Tb1-xYx)3Al5O12 with different Y content were investigated in detail.

It was found that Y2O3 can suppress the secondary phase and improve the optical quality of TAG ceramics. As optical quality occupies one of the most

CHEMWATCH
Bulletin Board
Gossip
JUN. 07, 2024

important parts of the practical performance of magneto-optical ceramics, Y2O3 is considered to be a promising and effective additive.

The team published their research article in Journal of Advanced Ceramics on April 30, 2024.

In high-performance laser devices, Faraday isolators are one of the important components that can prevent the front-end system from disturbance and damage caused by a back-reflected beam. Magneto-optical materials are thus widely studied as they are key elements of Faraday isolators.

Among magneto-optical materials applied in the visible to near-infrared wavelength band, TAG ceramics have been considered to be one of the most promising materials thanks to their high Verdet constant and good thermo-optic properties. However, the manufacturing process of TAG ceramics should be further optimized to reduce the optical loss and make them applicable for practical use.

Optical scattering from the secondary phases is one of the most important problems for TAG ceramics, originating from the narrow solid-solution range. Based on the existing problems and difficulties of TAG ceramics, the research team proposed their own solutions.

"As Y3+ has a smaller ionic radius compared with Tb3+, anti-site defect can more easily form after Y substitution in TAG, which implies a possibility of increasing the solid-solution range, suppressing the secondary phases, and improving the optical quality of TAG ceramics," said Jiang Li, senior author of the research paper, vice director of the Transparent Ceramics Research Center, Shanghai Institute of Ceramics, Chinese Academy of Sciences. Dr. Li is also a professor in Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences.

"In this work, Y2O3 was added in various amounts as an additive to investigate the mechanisms leading to improvement of the optical quality of TAG ceramics. (Tb1-xYx)3Al5O12 (x=0, 0.05, 0.1, 0.2, 0.3) ceramics were fabricated by solid-state reaction sintering. Vacuum sintering combined with hot isostatic pressing (HIP) post-treatment was conducted. The crystal structure, microstructure, optical transmittance, Verdet constant, and thermal properties for obtained ceramics were investigated in details," Jiang Li said.

The result is that Y2O3 improves the optical transmittance of the ceramics by suppressing the secondary phase, probably due to the increase of solubility.

"The (Tb0.8Y0.2)3Al5O12 ceramics possess the highest in-line transmittance value in this work, which is 82.9% at 1064 nm and 82.2% at 633 nm. The optical loss of the (Tb0.8Y0.2)3Al5O12 ceramics is nearly one order of magnitude lower than that of the obtained TAG ceramics in this work and in our previous works, showing that adding Y2O3 is a suitable method for improving the optical quality of TAG ceramics," said Jiang Li.

Phys Org, 5 June 2024

https://phys.org

Pregnancy Workouts Alter Brain Chemistry to Fight Offspring Obesity

2024-06-04

A study reveals that maternal obesity in mice increases microRNA levels in the hypothalamus in offspring, leading to overeating.

Maternal obesity impacts the eating behaviors of offspring via long-term overexpression of the microRNA miR-505-5p. This is according to a study published today (June 4th) in the open-access journal PLOS Biology by Laura Dearden and Susan Ozanne from the MRC Metabolic Diseases Unit, Institute of Metabolic Science, University of Cambridge, UK, and colleagues.

Link Between Maternal Obesity and Offspring Health Risks

Previous studies in both humans and animal models have shown that the offspring of obese mothers have a higher risk of obesity and type 2 diabetes. While this relationship is likely the result of a complex relationship between genetics and environment, emerging evidence has implicated that maternal obesity can disrupt the hypothalamus—the region of the brain responsible for nutrition sensing and energy homeostasis.

In animal models, offspring exposed to overnutrition during key periods of development eat more, but little is known about the molecular mechanisms that lead to these changes in eating behavior.

Study Findings on MicroRNA and Eating Behaviors

CHEMWATCH
Bulletin Board
Gossip
JUN. 07, 2024

In this study, researchers found that mice born from obese mothers had higher levels of the microRNA miR-505-5p in their hypothalamus—from as early as the fetal stage into adulthood. The researchers found that the mice ate more and showed a preference for high-fat foods.

Interestingly, the effect of maternal obesity on miR-505-5p and eating behaviors was mitigated if the mothers exercised during pregnancy.

Molecular Mechanisms and Preventative Measures

Cell culture experiments showed that miR-505-5p expression could be induced by exposing hypothalamic neurons to long-chain fatty acids and insulin, which are both high in pregnancies complicated by obesity. The researchers identified miR-505-5p as a novel regulator of pathways involved in fatty acid uptake and metabolism, therefore high levels of the miRNA make the offspring brain unable to sense when eating high-fat foods.

Several of the genes that miR-505-5p regulates have been associated with high body mass index in human genetic studies. The study is one of the first to demonstrate the molecular mechanism linking nutritional exposure in utero to eating behavior.

Sci Tech Daily, 4 June 2024

https://scitechdaily.com

Marine fungus takes a bite out of plastic waste

2024-06-05

That we have a huge plastic waste problem is clear, but there are numerous efforts to stem the tide while also cleaning up the mess. Nature is also joining the battle, and scientists have now identified a marine fungus at the plastic-devouring front line.

The fungus, named Parengyodontium album, was found living with other marine organisms on samples of plastic trash drawn from the North Pacific Garbage Patch in December 2019 during the Ocean Cleanup's North Pacific Mission 3.

It was subsequently identified and isolated by marine biologists from the Royal Netherlands Institute for Sea Research, in cooperation with Utrecht University and institutes in Paris, Copenhagen and Switzerland. The fungus was then grown in the lab and found to break down polyethylene, one of

the most commonly used plastics and found in such things as packaging film, grocery bags, bottles, toys and housewares.

Though previous research has revealed bacteria and enzymes capable of chomping through plastic waste, plastic-eating marine fungi are something of a rarity, with P.album now becoming the fourth member of this elite club. But what makes this latest discovery so compelling is that the scientists have managed to quantify the rate of degradation.

Laboratory experiments suggest that polyethylene (PE) marine waste exposed to ultraviolet light would be broken down and used as an energy source by the fungus at a rate of 0.044% per day.

"In the lab, P. album only breaks down PE that has been exposed to UV-light at least for a short period of time. That means that in the ocean, the fungus can only degrade plastic that has been floating near the surface initially," said study lead author, Annika Vaksmaa. "It was already known that UV-light breaks down plastic by itself mechanically, but our results show that it also facilitates the biological plastic breakdown by marine fungi."

A potential negative here is that the fungus doesn't seem to devour much of the carbon in the polyethylene during the process, instead converting most of it as carbon dioxide and excreting the greenhouse gas. But the small amount produced – reported to be "the same as the low amount humans release while breathing" – is not viewed by the researchers as causing a whole new environmental problem.

Vaksmaa suggests that there are likely other – as yet unidentified – fungi that are breaking down plastics on the surface and below as well.

"Marine fungi can break down complex materials made of carbon," she said. "There are numerous amounts of marine fungi, so it is likely that in addition to the four species identified so far, other species also contribute to plastic degradation."

A paper detailing the research has been published in the journal Science of The Total Environment.

Meanwhile, the Ocean Cleanup reported in April that it has so far removed 10 million kilograms (22 million lb) of marine trash from the Great Pacific

CHEMWATCH
Bulletin Board
Gossip
JUN. 07, 2024

Garbage Patch and from key polluting rivers around the world since making its first haul in 2019.

New Atlas, 5 June 2024

https://newatlas.com

Uptake of tire wear additives by vegetables grown for human consumption

2024-06-05

Car tires contain hundreds of chemical additives that can leach out of them. This is how they end up in crops and subsequently in the food chain. Researchers at the Center for Microbiology and Environmental Systems Science at the University of Vienna and the Hebrew University of Jerusalem have now detected these chemical residues in leafy vegetables for the first time. Although the concentrations were low, the evidence was clear, a finding that is also known for drug residues in plant-based foods. The study was published in the journal Frontiers in Environmental Science.

The presence of drug residues in commercially sold fruit and vegetables has already been scientifically investigated many times. However, chemical substances from tire wear, so-called additives, also find their way into the food chain. This has now been shown in a new study by an international research team led by Thilo Hofmann at the Center for Microbiology and Environmental Systems Science at the University of Vienna (CeMESS) in collaboration with a team the Hebrew University of Jerusalem led by Benny Chefetz. Vegetables from Switzerland and Israel were examined. Some of these substances and their transformation products can potentially pose ecological and toxicological risks.

Car tires consist of a complex mixture of materials that improve their performance and durability. These include 5-15% chemical additives, which comprise hundreds of substances, for example antioxidants, antiozonants, vulcanizing agents, anti-aging agents and many more, to enable the hig-tech performance of a modern tire. "The toxicity of tire and road wear particles is related to their organic additives and associated transformation products," explains Anya Sherman, PhD student at CeMESS and first author of the recently published study.

The compounds extracted from car tires find their way into agriculture through atmospheric deposition, irrigation with treated wastewater and the use of sewage sludge as fertilizer. "There they can be taken-up by

plants and thus also reach humans," adds Thilo Hofmann, head of the research group.

Residues of tire wear in leafy vegetables from the supermarket and field

Finally, the researchers extrapolated the measured values from the vegetables to the intake of these substances in the diet. "We calculated the intake per day based on what people in Switzerland and Israel eat," says Sherman. The concentrations of the tire additives in leafy vegetables are low overall and are, for example, 238 nanograms ng/kg for benzothiazole (BTZ), or 0.4 ng/kg for 6PPD, a substance whose transformation product 6PPD quinone is known to be highly toxic for aquatic species like coho salmon. Depending on the diet, this leads to a daily intake per person of 12 to 1,296 ng for BTZ, or 0.06 to 2.6 ng for 6PPD. This is comparable in magnitude to drug residues, which also enter the food chain. According to Thilo Hofmann, the study shows clear results: "While the concentrations and daily intake are fortunately relatively low, additives from car tires are still found in food. That's not where they belong." According to Hofmann, the next steps should now be to investigate the environmental and human health aspects.

From the street, to the plant, into the body

As early as 2023, the scientists were able to show that additives from car tires can in principle be absorbed by plants. "However, the question was whether this only happens in our mechanistic laboratory study or also in the field," explains first author Anya Sherman. In the current study, the Viennese and Israeli environmental scientists therefore analyzed whether lettuce plants absorb the chemicals released by car tires under natural growing conditions. "We examined real samples from supermarkets in Switzerland and field vegetables from Israel," says Thilo Hofmann, explaining the background to the study published last week.

The international team of researchers used high-resolution mass spectrometry to analyze the samples for a total of sixteen tire-associated compounds. The countries of origin of the leafy vegetables in the Swiss samples from the supermarket were Italy, Spain, and Switzerland. In the Israeli samples, field vegetables from Israel directly after harvest.

Science Daily, 5 June 2024

https://sciencedaily.com

CHEMWATCH
Bulletin Board
Gossip
JUN. 07, 2024

Researchers Find a Way To Scale Up Carbon Dioxide Capturing "Wonder Material"

2024-05-03

Researchers at the University of Virginia School of Engineering and Applied Science have figured out how to take a miracle material, one capable of extracting value from captured carbon dioxide, and do what no one else has: make it practical to fabricate for large-scale application.

The breakthrough from chemical engineering assistant professor Gaurav "Gino" Giri's lab group has implications for the cleanup of the greenhouse gas, a major contributor to the climate change dilemma. It could also help solve the world's energy needs.

The substance, called MOF-525, is in a class of materials called metal-organic frameworks.

"If you can make these MOFs cover large areas, then new applications become possible, like making a membrane for carbon capture and electrocatalytic conversion all in one system," Giri said.

Electrocatalytic conversion creates a bridge from renewable energy sources to direct chemical synthesis, taking the burning of carbon-dioxide producing fossil fuels out of the equation.

What gives MOFs superpowers is their ultra-porous, crystalline structures — 3D networks of minute nanoscale cavities that create vast internal surface area and act like a sponge — that can be designed to trap all sorts of chemical compounds.

A Cutting-Edge Solution

Giri's group reasoned that starting with an inherently scalable synthesis technique — solution shearing — would better their odds. They had already had success shearing simpler MOFs.

In Giri's process, the MOF's components are mixed in a solution, then spread across a substrate with the shearing blade. As the solution evaporates, chemical linkages form the MOF as a thin film on the substrate. Applying MOF-525 in this way produces an all-in-one membrane for carbon trapping and conversion.

"The bigger the membrane, the more surface area you have for the reaction, and the more product you could get," said Prince Verma, a

December 2023 Ph.D. graduate from Giri's lab. "With this process, you can increase the shearing blade width to whatever size you need."

The team targeted CO2 conversion to demonstrate their solution shearing approach because carbon capture is widely used to reduce industrial emissions or to remove it from the atmosphere — but at a cost to operators with minimal return on the investment: Carbon dioxide has little commercial value and most often winds up stored indefinitely underground.

However, with minimal energy input, using electricity to catalyze a reaction, MOF-525 can take away an oxygen atom to make carbon monoxide — a chemical that is valuable for manufacturing fuels, pharmaceuticals and other products.

UVA's Grand Challenges

The process of accelerating reactions through catalysis, especially electrocatalysis, which consumes less energy than reactions driven by heat or pressure, is essential to a green-energy future — so much so that UVA invested $60 million in catalysis study as part of UVA's Grand Challenges Investments.

For that expertise, Giri collaborated with UVA associate professor of chemistry Charles W. Machan.

"The materials from Gino's lab help us understand how to enable new, scalable technologies for capture and conversion, which we're going to need to address the environmental challenges posed by current carbon dioxide concentrations in the atmosphere and rate of emissions," Machan said.

Technology Networks, 3 June 2024

https://technologynetworks.com

Atomizer of history: How perfume research has shaped a century of scientific innovation

2024-06-05

Is the quest for the perfect top notes responsible for some of the world's most influential scientific discoveries? A new article in the journal Isis argues that fragrance research has stimulated scientific endeavor for over a century, but that its contributions have been overlooked due to perfume's stigma as a frivolous, feminine luxury.

CHEMWATCH
Bulletin Board
Gossip
JUN. 07, 2024

In "Musk and the Making of Macromolecules: Perfumes and Polymers in the History of Organic Chemistry," author Galina Shyndriayeva demonstrates how tracing the history of perfume production clarifies and enriches the history of chemical innovation and industrial development.

Leopold Ružička, a recipient of the 1939 Nobel Prize in chemistry, was granted this honor in part due to a discovery he made while working for a Geneva-based perfume supplier: the synthesis of muscone, or artificial musk. Musk, a vital ingredient in the production of perfume, was expensive and time-consuming to source in its natural form, as it involved the hunting of male deer in Russia and the Himalayas region, and the musk pouches of up to fifty bucks were required to generate a single kilogram.

Ružička reproduced the substance chemically by identifying a molecular structure involving large rings, defying the prevailing theories of the time regarding atomic composition. The breakthrough was not only of great value to M. Naef, his employer, and the perfume industry at large, but also opened up avenues of other scientific research, "including study of previously unseen arrangements of atoms in space, new ring closure techniques, and identification of other biologically important molecules with a large ring structure, such as oxytocin."

Ružička's muscone work and his study of large rings additionally paved the way for further inquiry by American scientist Wallace H. Carothers, a research chemist at the industrial behemoth DuPont. During the First World War, DuPont and other American industries had greatly expanded, and by the late 1920s and early 1930s the company was leveraging this prosperity to diversify its holdings and develop new products.

While Carothers was not directly engaged in work with perfume, he and organic chemist Julian W. Hill used Ružička's large ring findings to inform a new method of polymer synthesis that would ultimately lead to the invention of nylon and polyester.

"The codevelopment of knowledge about perfume and polymers," writes Shyndriayeva, "points to what was driving Ružička's and Carothers's research: investigation of some of the most pertinent theoretical questions about chemical structure at the time."

The unappreciated significance of perfume research reflects, Shyndriayeva notes, a more general disdain for scholarship regarding the "aesthetic-industrial complex." Some historians—and female historians, in particular—have attempted to correct this imbalance, turning their

analysis to "the importance of looks and attractiveness as attributes mobilized for national and political agendas, as essential components for understanding race, class, and gender."

The article argues that the story of perfume is hardly just a frivolous footnote in the history of science—instead intersecting with the legacies of war, molecular structure, and global networks of commerce and development. The study of fragrance and other trivialized subjects could yield a richer, more diverse study of history, and offer up "new paths for reflection."

Phys Org, 5 June 2024

https://phys.org

New metal-free MOFs show early promise for nuclear chemistry

2024-06-03

Metal-free organic frameworks, featuring inexpensive and abundant non-metallic elements, have been designed and then made with the help of computational crystal-structure prediction software.

It is hoped the new materials will have a range of applications such as catalysis, water capture and hydrogen storage and offer an alternative to their metal-based equivalents.

The researchers, who are based at the Universities of Liverpool, Southampton and Nottingham, used computational design methods in combination with synthetic know-how to develop non-metal organic porous framework (N-MOF) materials using non-metallic ions such as chloride.

'We guided the discovery of these materials using a computational method called crystal structure prediction,' said Graeme Day, an expert in chemical modelling at the University of Southampton. 'This allows us to predict which non-metal salts will form stable porous frameworks, which salts will not and to anticipate the precise crystal structure in advance of experimental work. We don't have to assume a specific geometry for the joints in the framework, which is a fundamental principle in MOF chemistry.'

The researchers said the new frameworks could be thought of as 'inverted' MOFs, in which the halide anions are analogous to the metal cations

CHEMWATCH
Bulletin Board
Gossip
JUN. 07, 2024

and that, like MOFs, they could be structurally diversified by using other counter-ions such as nitrates, sulfates and phosphates.

The synthesis of these materials is also scalable, as it involves simple acid–base neutralisation, the researchers pointed out. They added that the first examples of these materials already showed 'practical promise', outperforming most MOFs for iodine capture, which is important for the nuclear industry.

Other applications could take advantage of the highly charged pore channels in the frameworks for proton conduction, catalysis, water capture or hydrogen storage.

Chemistry World, 3 June 2024

https://chemistryworld.com

Shining a light on molecules: L-shaped metamaterials can control light direction

2024-06-04

Polarized light waves spin clockwise or counterclockwise as they travel, with one direction behaving differently than the other as it interacts with molecules. This directionality, called chirality or handedness, could provide a way to identify and sort specific molecules for use in biomedicine applications, but researchers have had limited control over the direction of the waves -- until now.

Using metamaterials, a team of electrical engineering researchers from Penn State and the University of Nebraska-Lincoln (UNL) created an ultrathin optical element that can control the direction of polarized electromagnetic light waves. This new control allows researchers to not only direct the light's chirality, but also to identify the chirality of molecules by determining how polarized light interacts with them.

Identifying the chirality of molecules can reveal critical information about how they will interact with other systems, such as whether specific drugs will help heal diseased or damaged tissue without harming healthy cells. The researchers published their findings in Nature Communications.

Chirality refers to mirror images, like left and right hands joining in a handshake, explained Christos Argyropoulos, associate professor of electrical engineering at Penn State and co-corresponding author on the paper. In physics, among other responsibilities, chirality influences the direction that light waves spin.

Argyropoulos and his colleagues fabricated an optical element, akin to a glass slide, that uses a forest of tiny, antenna-like nanorods that together create a metamaterial -- or material engineered to have specific properties not typically found in nature -- able to control the spin of light. The metamaterial nanorods appear to be shaped like the letter "L" when seen at the nanoscale.

"When the light-matter interaction is mediated by the metamaterials, you can image a molecule and identify its chirality by inspecting how chiral light interacts with it," Argyropoulos said.

Researchers at UNL used an emerging fabrication approach called glancing angle deposition to fabricate the optical element out of silicon.

"Silicon does not substantially dissipate the incident light that was problematic with metal, which we used in previous attempts to create the element," said Ufuk Kilic, a research professor at UNL and co-corresponding author on the paper. "And silicon allowed us to adjust the shape and length of the nanopillars on the platform, which in turn allows us to change how we control the light."

Identifying the chirality of molecules can have wide-ranging impacts in biomedicine, particularly in pharmaceutical drugs, which sometimes have right- or left-handed chirality, Argyropoulos explained. While a right-handed molecular structure can be effective at treating disease, the same molecule with a left-handed structure can be toxic to healthy cells.

Argyropoulos mentioned the classic example of thalidomide, a drug with a chiral structure that was prescribed to women to treat morning sickness between 1957 and 1962. The right-handed molecule could appease nausea but was highly toxic to developing fetuses and caused birth defects for thousands of babies around the world. The optical element, Argyropoulos said, can quickly image the molecular structure of pharmaceuticals, allowing scientists to better understand the nuances of drug behavior.

Additionally, the optical element can be used to create right- or left-handed electromagnetic waves, Argyropoulos said, which are necessary for the development and maintenance of classical and quantum communications systems, like encrypted Wi-Fi and cell phone service.

CHEMWATCH
Bulletin Board
Gossip
JUN. 07, 2024

"Previously, for optical communication systems, you needed big, bulky devices that only operated at one frequency," Argyropoulos said. "This new optical element is lightweight and easily tunable to multiple frequencies."

Science Daily, 4 June 2024

https://sciencedaily.com

A cracking discovery: Eggshell waste can recover rare earth elements needed for green energy

2024-06-05

A collaborative team of researchers has made a cracking discovery with the potential to make a significant impact in the sustainable recovery of rare earth elements (REEs), which are in increasing demand for use in green energy technologies. The team found that humble eggshell waste could recover REES from water, offering a new, environmentally friendly method for their extraction.

The researchers, from Trinity College Dublin's School of Natural Sciences, and iCRAG, the Ireland Research Centre in Applied Geosciences, have just published their findings in the journal ACS Omega.

REEs, which are essential for the technologies used in electric cars and wind turbines, for example, are in increasing demand but in relatively short supply. As a result, scientists must find new ways of extracting them from the environment—and in sustainable ways, with current methods often harmful.

Here, the researchers discovered that calcium carbonate (calcite) in eggshells can effectively absorb and separate these valuable REEs from water.

The researchers placed eggshells in solutions containing REEs at various temperatures from a pleasant 25°C to a scorching 205°C, and for different time periods of up to three months. They found that the elements could enter the eggshells via diffusion along the calcite boundaries and the organic matrix, and, at higher temperatures, that the rare earth built new minerals on the eggshell surface.

At 90°C, the eggshell surface helped recover formations of a rare earth compound called kozoite. As things got hotter, the eggshells underwent a complete transformation with the calcite shells dissolving and being replaced by polycrystalline kozoite. And at the highest temperature of 205°C, this mineral gradually transitioned into bastnasite, the stable rare earth carbonate mineral that is used by industry to extract REEs for technology applications.

This innovative method suggests that waste eggshells could be repurposed as a low-cost, eco-friendly material to help meet the growing demand for REES, as the eggshells trap distinct rare earths within their structure over time.

CHEMWATCH
Bulletin Board
Curiosities
JUN. 07, 2024

Lead author Dr. Remi Rateau says, "This study presents a potential innovative use of waste material that not only offers a sustainable solution to the problem of rare earth element recovery but also aligns with the principles of circular economy and waste valorization."

Principal Investigator, Prof. Juan Diego Rodriguez-Blanco, emphasized the broader implications of the findings, adding, "By transforming eggshell waste into a valuable resource for rare earth recovery, we address critical environmental concerns associated with traditional extraction methods and contribute to the development of greener technologies."

Phys Org, 5 June 2024

https://phys.org

Towards next-gen functional materials: direct observation of electron transfer in solids

2024-06-04

Electron transfer (ET) is a process in which an electron is transferred from one atom or molecule to another. ET is fundamental to electrochemical reactions with applications in many fields. Nanoscale ET, which involves the transfer of electrons in the range of 1-100 nanometers in solids is fundamental to the design of multifunctional materials. However, this process is not yet clearly understood.

Nanotubes, nanomaterials with unique cylindrical nanostructures, offer a variety of ET properties that can be realized through electron and hole (vacant spaces left by electrons) injections into the nanotubes, making them a suitable candidate for studying nanoscale ET. Although carbon-based nanotubes have fascinating ET properties, they are particularly difficult to control in terms of their shape and size due to extreme conditions, such as high temperatures, required for their synthesis.
A viable approach for fabricating well-defined tunable nanotubes is bottom-up fabrication of non-covalent nanotubes, which sometimes result in crystalline-form nanotubes. Non-covalent nanotubes are formed through the inherent attractive interactions or non-covalent interactions between atoms, instead of the strong covalent interactions seen in carbon nanotubes. However, they are not strong enough to endure electron and hole injections, which can break their non-covalent interactions and destroy their crystalline structure.

In a recent study, a team of researchers from the Department of Applied Chemistry at Tokyo University of Science, led by Professor Junpei Yuasa

and including Dr. Daiji Ogata, Mr. Shota Koide, and Mr. Hiroyuki Kishi, used a novel approach to directly observe solid-state ET. Prof. Yuasa explains, "We have developed crystalline nanotubes with a special double-walled structure. By incorporating electron donor molecules into the pores of these crystalline nanotubes through a solid-state oxidation reaction, we succeeded in directly observing the electron transfer reaction in the solid using X-ray crystal structure analysis." Their findings were published in the journal Nature Communications on May 23, 2024.

The researchers used a novel supramolecular crystallization method, which involves oxidation-based crystallization, to fabricate zinc-based double-walled crystalline nanotubes. This double-walled structure with large windows in the nano-tube walls makes the crystal robust and flexible enough to maintain its crystalline state when subjected to ET oxidation processes. Moreover, this structure allows the crystal to absorb electron donor molecules. The researchers used ferrocene and tetrathiafulvalene as electron donor molecules, which were absorbed through the windows of the nanotube crystals. This allows electrons to be removed from the absorbed electron donors through solid-state ET oxidation reactions, resulting in the accumulation of holes in the donors inside the nanotube. Due to the robustness of the crystals, the researchers were able to observe this ET oxidation process using X-ray crystal structure analysis directly, uncovering key insights.

This novel approach is highly valuable for direct observation of ET in solid nanomaterials. Highlighting the potential applications of this study, Prof. Yuasa says, "Understanding ET can lead to the development of novel functional materials, which in turn can lead to the design of more efficient semiconductors, transistors, and other electronic devices. Optoelectronic devices, such as solar cells, rely heavily on ET. Hence, direct observation of ET can help improve these devices' performance. Additionally, this approach can lead to advancements in energy storage, nanotechnology, and materials science research."

Overall, this study is a striking example of direct observation of solid-state ET, which can be expanded to observe ET and related phenomena in other nanomaterials.

Science Daily, 4 June 2024

https://sciencedaily.com

CHEMWATCH
Bulletin Board
Curiosities
JUN. 07, 2024

Hazards in Your Chocolate? New Study Reveals Potential Risks

2024-06-01

A study reveals that while chocolate contains potentially harmful chemicals at safe levels, these compounds appear in much higher, possibly unsafe concentrations in some baked desserts.

What makes chocolate taste and smell so delicious? Chemistry, of course! A variety of molecules work together to create that unmistakable aroma, but those same molecules might carry some unwanted health effects if there are too many around.

According to research published in ACS' Journal of Agricultural and Food Chemistry, while many of the compounds appeared in chocolate in low enough concentrations to be safe, higher amounts were found in some baked sweet treats.

When making chocolate, cocoa beans are roasted to help their chocolatey flavors shine. During this process, new molecules like α,β-unsaturated carbonyls are formed when they react with other ingredients under high temperatures. This class of carbonyls is highly reactive and potentially genotoxic, or able to cause damage to DNA when consumed. Though naturally found in many foods, these carbonyls are also used as flavoring additives, and some have been banned in the European Union, including the buttery-tasting furan-2(5H)-one.

Research on Carbonyls in Chocolates and Desserts

To better understand how these molecules form naturally in foods, and whether or not they are present in levels that could pose a health concern, Alexandre Dusart and colleagues tested chocolates and other sweet treats for 10 different α,β-unsaturated carbonyls — some of which have been confirmed as safe by the European Food Safety Authority, while others are still under evaluation.

The team created its own chocolates and found that α,β-unsaturated carbonyls formed during roasting and after the addition of cocoa butter; however, their concentrations remained too low to pose any health concerns from consuming the chocolates. Next, researchers screened 22 commercially available desserts, including crepes, waffles, cakes, and biscuits, either with or without chocolate. In these packaged treats, they found even lower concentrations of nine of the 10 carbonyls compared to the chocolates.

Potential Health Risks in Packaged Desserts

The remaining carbonyl — genotoxic furan-2(5H)-one — appeared in much higher concentrations in the crepe and cake samples, reaching up to 4.3 milligrams per kilogram. Considering that the recommended threshold for genotoxic substances is only 0.15 micrograms per person per day, consuming these desserts could exceed that limit, though additional studies are needed to accurately assess the potential health risk.

Researchers concluded that the furan-2(5H)-one molecule likely formed during the baking process and did not seem to correlate with the amount of chocolate present in the packaged desserts. The team says that this work helps to better understand where these carbonyls come from in chocolate and highlights the importance of monitoring flavorings in food to keep consumers informed and safe.

Sci Tech Daily, 1 June 2024

https://scitechdaily.com

Cool paint made sustainable using recycled plastics

2024-06-05

An NTU research team has successfully developed new methods to create a type of "cool paint" using recycled plastics—namely acrylic, old PVC pipes and polystyrene foam—and barium sulfate, offering a sustainable and efficient alternative to new plastics.

The NTU methods not only help in cooling temperatures in tropical environments, but also contribute to effective plastic waste management.

In the first method (sol-gel), the research team used recycled plastics and mixed them with barium sulfate ($BaSO_4$), to create their cool paint.

A 24-hour test on the roof-top of a building in Singapore showed that the newly created coating can reach 1.2° C below the surrounding air temperature when exposed to direct sunlight. At night, the coating could reach 3° C below the ambient temperature. The coating can reflect about 97.7% of sunlight and emits 95% of its heat in the infra-red band.

In a second method (phase inversion), the team also used recycled plastics and barium sulfate to make the cool paint but focused on making the recycled plastics porous by creating tiny air-filled holes in them during the production process. This is because air pores help to scatter sunlight across its spectrum.

CHEMWATCH
Bulletin Board
Curiosities
JUN. 07, 2024

Results showed that the surfaces coated with this version of the paint could almost match the surrounding air temperature at noon and achieve night temperature of 2.5° C below the ambient temperature.

The cool paint developed using both methods outperforms commercially available cool paints which typically are unable to bring surface temperatures below ambient.

Further investigations using a mix of unsorted plastic waste (mix of acrylic, PVC pipes and polystyrene foam) also showed that results were comparable to those from cool paints developed using only a single type of plastic waste. This suggests that the NTU team's approaches reduce the need for sorting different types of plastic.

Phys Org, 5 June 2024

https://phys.org

Scientists develop 'x-ray vision' technique to see inside crystals

2024-06-03

A team of New York University researchers has created a new way to visualize crystals by peering inside their structures, akin to having X-ray vision. Their new technique -- which they aptly named "Crystal Clear" -- combines the use of transparent particles and microscopes with lasers that allow scientists to see each unit that makes up the crystal and to create dynamic three-dimensional models.

"This is a powerful platform for studying crystals," says Stefano Sacanna, professor of chemistry at NYU and the principal investigator for the study, published in the journal Nature Materials. "Previously, if you looked at a colloidal crystal through a microscope, you could only get a sense of its shape and structure of the surface. But we can now see inside and know the position of every unit in the structure."

Atomic crystals are solid materials whose building blocks are positioned in a repeating, orderly fashion. Every now and then, an atom is missing or out of place, resulting in a defect. The arrangement of atoms and defects is what creates different crystalline materials -- from table salt to diamonds -- and gives them their properties.

To study crystals, many scientists, including Sacanna, look to crystals composed of miniscule spheres called colloidal particles rather than atoms. Colloidal particles are tiny -- often around a micrometer in

diameter, or dozens of times smaller than a human hair -- but are much larger than atoms and therefore easier to see under a microscope.

A see-through structure

In their ongoing work to understand how colloidal crystals form, the researchers recognized the need to see inside these structures. Led by Shihao Zang, a PhD student in Sacanna's lab and the study's first author, the team set out to create a method to visualize the building blocks inside a crystal. They first developed colloidal particles that were transparent and added dye molecules to label them, making each particle possible to distinguish under a microscope using their fluorescence.

A microscope alone wouldn't allow the researchers to see inside a crystal, so they turned to an imaging technique called confocal microscopy, which uses a laser beam that scans through material to produce targeted fluorescence from the dye molecules. This reveals each two-dimensional plane of a crystal, which can be stacked on top of each other to build a three-dimensional digital model and identify the location of each particle. The models can be rotated, sliced, and taken apart to look inside the crystals and see any defects.

In one set of experiments, the researchers used this imaging method on crystals that form when two of the same type of crystals grow together -- a phenomenon known as "twinning." When they looked inside models of crystals having structures equivalent to table salt or an alloy of copper and gold, they could see the shared plane of the adjoined crystals, a defect that gives rise to these particular shapes. This shared plane revealed the molecular origin of twinning.

Crystals in motion

In addition to looking at static crystals, this new technique allows scientists to visualize crystals as they change. For example, what happens when crystals melt -- do particles rearrange, and do defects move? In an experiment in which the researchers melted a crystal with the structure of the mineral salt cesium chloride, they were surprised to find that the defects were stable and did not move around as expected.

In order to validate their experiments on static and dynamic crystals, the team also used computer simulations to create crystals with the same characteristics, confirming that their "Crystal Clear" method accurately captured what is inside crystals.

CHEMWATCH
Bulletin Board
Curiosities
JUN. 07, 2024

"In a sense, we're trying to put our own simulations out of business with this experiment -- if you can see inside the crystal, you may not need simulations anymore," jokes Glen Hocky, assistant professor of chemistry at NYU, a faculty member in the Simons Center for Computational Physical Chemistry at NYU, and the study's co-corresponding author.

Now that scientists have a method for visualizing the inside of crystals, they can more easily study their chemical history and how they form, which could pave the way for building better crystals and developing photonic materials that interact with light.

"Being able to see inside crystals gives us greater insight into how the crystallization process works and can perhaps help us to optimize the process of growing crystals by design," adds Sacanna.

Additional study authors include Adam Hauser and Sanjib Paul of NYU. The research was supported by the US Army Research Office (award number W911NF-21-1-0011), with additional support from the National Institute of Health (R35GM138312), and used NYU IT High Performance Computing resources, including those supported by the Simons Center for Computational Physical Chemistry at NYU (grant number 839534).

Science Daily, 3 June 2024

https://sciencedaily.com

Some metals actually grow more resilient when hot

2024-5-23

Heating metals can sometimes make them stronger, despite the common conception that higher temperatures just make them pliable. This surprising phenomenon could lead to a better understanding of important industrial processes and make for tougher aircraft.

"It was just so unexpected or backwards of what you might conventionally see," says Ian Dowding at the Massachusetts Institute of Technology. Together with Christopher Schuh at Northwestern University in Illinois, he uncovered the odd effect by bombarding metals with tiny projectiles.

The researchers used a laser to launch microscopic aluminium oxide particles towards heated samples of the metals copper, gold and titanium at velocities of thousands of kilometres per hour.

A high-speed camera recorded the impact and rebound of these tiny projectiles as they hit each metal sample, a process illuminated by another

laser. Based on the particles' trajectories and the size of the craters they left on the metals, Dowding and Schuh calculated the strength of each metal and determined how it changed at rising temperatures.

The copper grew roughly 30 per cent stronger after the team increased its temperature by 157°C. Most strikingly, at 177°C (350°F) this typically soft material proved as sturdy as some types of steel.

Usually, heat softens metals because it loosens some of the bonds between metal atoms, Schuh says. So when you put pressure on the metal, some atoms "sloppily" slide around and reconnect elsewhere within it, deforming the material and making it pliable.

After diving into other researchers' calculations on metals' properties under extreme conditions, Schuh says he and Dowding learned that the microparticles hit the metals too quickly for this sloppy sliding to occur. And at higher temperatures, more waves of heat or sound passed through the metal and made it harder for bond-breaking to spread across the metal.

Although this outcome had been predicted before, "this research now provides experimental evidence for the concept", says Mostafa Hassani at Cornell University in New York.

While the "hotter is stronger" phenomenon occurred under carefully controlled laboratory conditions, Schuh says it may happen undetected in a range of real-world industrial processes. For instance, cutting and smoothing processes, which involve blasting materials with fast particles of sand or jets of water, may be inadvertently changing the materials' strength. The effect could also come into play in some types of 3D printing where "ink" particles move very quickly.

Still, some of the physics behind this finding remain unclear. Researchers know that turning up the heat will eventually warm the metal to its melting point, but future experiments must pinpoint the highest possible temperatures for this strengthening effect to occur, says Schuh.

New Scientist, 23 May 2024

https://newscientist.com

CHEMWATCH
Bulletin Board
Curiosities
JUN. 07, 2024

"Monstrous" Discovery: Scientists Identify Key to Stopping Cancer Recurrence

2024-06-05

Researchers at MUSC Hollings Cancer Center have made a breakthrough that may reveal why cancer sometimes returns in patients who have received chemotherapy or radiotherapy.

Both forms of therapy aim to stress cancer cells into self-destruction. However, these treatments often lack long-term effectiveness because cancer cells can adapt to the stress, escape, and enable the tumor to rebound after a a short time.

Recently, scientists have begun to look at the role of polyploid giant cancer cells, or PGCCs, in cancer recurrence. Although these cells have been known to scientists since the invention of the microscope and have been observed by pathologists in cancerous tissues, their exact function in cancer recurrence remained unknown.

In a recent article in the Journal of Biological Chemistry, a MUSC Hollings Cancer Center research team led by Christina Voelkel-Johnson, Ph.D., reports that it has identified select genes that prostate cancer cells manipulate to become PGCCs, thereby protecting themselves from therapy stress. The Hollings team also found that PGCCs later regain their capacity for cell division, setting the stage for cancer recurrence.

Unexpected Discoveries in Lab Experiments

Voelkel-Johnson and her lab made this discovery while studying an inhibitor, or a drug designed to block a biological mechanism, which was associated with durable cures after radiotherapy. "We initially thought that combination of radiation with the inhibitor killed cancer cells better," said Voelkel-Johnson. "It was only when the inhibitor failed to make a difference in short-term experiments that the time frame was extended, which allowed for an unusual observation."

Lab members had observed giant abnormal-looking cells during the short-term experiments but had considered them to be "doomed." When the time frame was extended, they were surprised to observe that these cells generated small offspring.

"They looked really funky," said Voelkel-Johnson. "When we didn't use the inhibitor, those giant cancer cells generated daughter cells, creating the appearance of a colony with smaller cells surrounding the large one."

These funky-looking PGCCs were visually different from other cancer cells. They were able to make copies of their genetic information, increasing the number of nuclei. However, the cytoplasm was not dividing, and so the cells grew monstrously, containing multiple nuclei instead of only one.

The surprise findings that the monster cells were not "doomed" led Voelkel-Johnson and her team to suspect that their inhibitor stopped cancer recurrence in a different way than they had hypothesized.

"The inhibitor did not kill cancer cells better," said Voelkel-Johnson. "Instead, it prevented the generation of offspring from the polyploid giant cancer cells."

The team also observed that the daughter cells of the PGCCs continued to divide, mimicking tumor recurrence that some patients experience after undergoing therapy. It became clear that this inhibitor was creating durable cures not by causing cell death but by stopping PGCCs from transitioning back into single-nucleus cancer cells with the capacity for division.

To understand what made PGCCs and their daughter cells different from their parent cancer cells, Voelkel-Johnson, with the help of other collaborators, set out to investigate the changes in gene expression among the different cells that appeared during their experiments. This information would help to explain how cancer cells can transition into and out of PGCC states after being exposed to therapy stress.

Genetic Insights and Therapeutic Implications

Voelkel-Johnson and her team were able to identify cell-signaling pathways that cancer cells manipulate to become PGCCs in response to therapy stress and then later to transition back to cells capable of producing daughter cells.

One protein that specifically piqued their interest was p21, which is induced by a protein called p53 when normal cells are stressed. In normal cells, p21 prevents duplication of damaged DNA, enabling DNA damage to be repaired. Cells in which damage cannot be repaired commit suicide.

The Hollings research team showed that stress in cancer cells lacking p53 also increased p21, but the protein did not stop the duplication of damaged DNA, as it did in normal cells. As a result, p21 helped to set the stage for the generation of the PGCCs.

CHEMWATCH
Bulletin Board
Curiosities
JUN. 07, 2024

When increases in p21 were blocked, the stressed cancer cells did not transform into these monstrous cells. Interfering with p21 in cells that were already monstrous prevented them from generating daughter cells that could be responsible for tumor relapse.

The team's findings provide insights into novel mechanisms that could be targeted to improve patient outcomes after cancer therapy. Although it may not be feasible to block p21 as a therapy, both the breast cancer drug tamoxifen and cholesterol-lowering statins have been shown to interfere with the pathways identified by the team. Further research is needed to assess whether they can reduce recurrence rates by blocking PGCCs from regaining the ability to generate daughter cells.

The findings also provide new insight into the optimal timing for the administration of these drugs.

"One of the questions we had was, 'At what point of the therapy do you treat?'" said Voelkel-Johnson. "Our findings suggest that treatment should occur at the same time as chemotherapy or radiotherapy. It is important to administer one of these drugs in conjunction with therapy stress to prevent PGCCs from generating the daughter cell. Once they are generated, it is too late."

Voelkel-Johnson plans to continue to investigate ways to prevent the generation of daughter cells from PGCCs to increase therapy efficacy. She is also interested in assessing how various combination treatment regimens delivered at the time of cancer therapy affect recurrence rates in a wide range of cancers.

Sci Tech Daily, 5 June 2024

https://scitechdaily.com

An AI tool for predicting protein shapes could be transformative for medicine, but it challenges science's need for proof

2024-05-31

An advanced algorithm that has been developed by Google DeepMind has gone some way to cracking one of the biggest unsolved mysteries in biology. AlphaFold aims to predict the 3D structures of proteins from the "instruction code" in their building blocks. The latest upgrade has recently been released. The latest upgrade has recently been released.

Proteins are essential parts of living organisms and take part in virtually every process in cells. But their shapes are often complex, and they are difficult to visualise. So being able to predict their 3D structures offers windows into the processes inside living things, including humans.

This provides new opportunities for creating drugs to treat disease. This in turn opens up new possibilities in what is called molecular medicine. This is where scientists strive to identify the causes of disease at the molecular scale and also develop treatments to correct them at the molecular level.

The first version of DeepMind's AI tool was unveiled in 2018. The latest iteration, released this year, is AlphaFold3. A worldwide competition to evaluate new ways of predicting the structures of proteins, the Critical Assessment of Structure Prediction (Casp) has been held biannually since 1994 In 2020, the Casp competition got to test AlphaFold2 and was very impressed. Since then, researchers eagerly anticipate each new incarnation of the algorithm.

However, as a masters student I was once reprimanded for using AlphaFold2 in some of my coursework. This was because it was deemed only a predictive tool. In other words, how could anyone know whether what was predicted matched the real-life protein without experimental verification?

This is a legitimate point. The area of experimental molecular biology has undergone its own revolution in the past decade with strong advances in a microscope technique called cryo-electron microscopy (cryo-EM), which uses frozen samples and gentle electron beams to capture the structures of biomolecules in high resolution.

The advantage of AI tools such as AlphaFold is that it can elucidate protein structures much faster (in a matter of minutes) at almost no cost. Results are more readily available and accessible globally online. They can also predict the structure of proteins that are notoriously difficult to experimentally verify, such as membrane proteins.

However, AlphaFold2 was not designed to address something called the quaternary structure of proteins, where multiple protein subunits form a larger protein. This involves a dynamic visualisation of how different units of the protein molecule are folded. And some researchers reported that it sometimes appeared to have difficulty predicting structural elements of proteins known as coils.

CHEMWATCH
Bulletin Board
Curiosities
JUN. 07, 2024

When my professor contacted me in May to relay the news that AlphaFold3 had been released, my first question was about its ability to predict quaternary structures. Had it succeeded? Were we now able to take the massive leap towards predicting a complete structure? Early reports suggest the answers to those questions are positive.

Experimental methods are slower. And when they are able to capture the 3D structure of molecules, it is more akin to looking at a statue –- a snapshot of the protein – rather than seeing how it moves and interacts to carry out actions in the body. In other words, we want a movie, rather than a photo.

Experimental methods have also traditionally struggled with membrane proteins – key molecules that are attached to or are associated with the membranes of cells. These are often crucial in understanding and treating many of the worst diseases.

Here is where AlphaFold3 could truly change the landscape. If it is successful at predicting quaternary structures at a level equal to or greater than experimental methods such as crystallography, cryo-EM and others, and it can visualise membrane proteins better than the competition, then we will indeed have a gigantic leap forwards in our race towards true molecular medicine.

AlphaFold3 can only be accessed from a DeepMind server, but it is easy to use. Researchers can get their results in minutes simply from the sequence. The other promise of AlphaFold3 is further disruption. DeepMind is not alone in its ambitions to master the problem of protein folding. As the next Casp competition approaches there are others looking to win the race. For example, Liam McGuffin and his team at the University of Reading are making gains in quality assessment and predicting the stoichiometry of protein complexes. Stoichiometry refers to the proportions in which elements or chemical compounds react with one another.

Not all scientists in this area are chasing the goal in the same way. Others are trying to solve similar challenges in terms of the quality of the 3D models or specific barriers such as those presented by membrane proteins. The competition has been marvellous for progress in this field.

However, experimental methods are not going away anytime soon, and nor should they. The progress of cryo-EM is laudable, and X-ray crystallography still gives us the finest resolution on biomolecules. The European XFEL laser in Germany could be the next breakthrough. These technologies will only continue to improve.

My biggest question as we survey this new field is whether our human instinct to relent until we have absolute proof will fold with AlphaFold. If this new technology is able to give results comparable to, or greater than, experimental verification, will we be prepared to accept it? If we can, its speed and accuracy could have a major effect on areas such as drug development.

For the first time, with AlphaFold3, we may have cleared the most significant hurdle in the protein prediction revolution. What will we make of this new world? And what medicine can we make with it?

The Conversation, 31 May 2024

https://theconversation.com

Scientists develop 'X-ray vision' technique to see inside crystals

2024-06-03

A team of New York University researchers has created a new way to visualize crystals by peering inside their structures, akin to having X-ray vision. Their new technique—which they aptly named "Crystal Clear"—combines the use of transparent particles and microscopes with lasers that allow scientists to see each unit that makes up the crystal and to create dynamic three-dimensional models.

"This is a powerful platform for studying crystals," says Stefano Sacanna, professor of chemistry at NYU and the principal investigator for the study, published in the journal Nature Materials.

"Previously, if you looked at a colloidal crystal through a microscope, you could only get a sense of its shape and structure of the surface. But we can now see inside and know the position of every unit in the structure."

Atomic crystals are solid materials whose building blocks are positioned in a repeating, orderly fashion. Every now and then, an atom is missing or out of place, resulting in a defect. The arrangement of atoms and defects is what creates different crystalline materials—from table salt to diamonds—and gives them their properties.

To study crystals, many scientists, including Sacanna, look to crystals composed of miniscule spheres called colloidal particles rather than atoms. Colloidal particles are tiny—often around a micrometer in diameter, or dozens of times smaller than a human hair—but are much larger than atoms and therefore easier to see under a microscope.

CHEMWATCH
Bulletin Board
Curiosities
JUN. 07, 2024

A see-through structure

In their ongoing work to understand how colloidal crystals form, the researchers recognized the need to see inside these structures. Led by Shihao Zang, a Ph.D. student in Sacanna's lab and the study's first author, the team set out to create a method to visualize the building blocks inside a crystal.

They first developed colloidal particles that were transparent and added dye molecules to label them, making each particle possible to distinguish under a microscope using their fluorescence.

A microscope alone wouldn't allow the researchers to see inside a crystal, so they turned to an imaging technique called confocal microscopy, which uses a laser beam that scans through material to produce targeted fluorescence from the dye molecules.

This reveals each two-dimensional plane of a crystal, which can be stacked on top of each other to build a three-dimensional digital model and identify the location of each particle. The models can be rotated, sliced, and taken apart to look inside the crystals and see any defects.

In one set of experiments, the researchers used this imaging method on crystals that form when two of the same type of crystals grow together—a phenomenon known as "twinning."

When they looked inside models of crystals having structures equivalent to table salt or an alloy of copper and gold, they could see the shared plane of the adjoined crystals, a defect that gives rise to these particular shapes. This shared plane revealed the molecular origin of twinning.

Phys Org, 3 June 2024

https://phys.org

Ultra-Processed Foods May Increase Insomnia Risk

2024-06-03

Ultra-processed food (UPF) could be behind the insomnia experienced by one third of adults, according to a new study.

After analyzing health and sleep surveys filled out by 38,570 participants, the researchers from Sorbonne Paris Nord University found that those who reported chronic insomnia, on average, consumed a higher proportion of UPFs.

This effect could be due to the lack of healthy, sleep-promoting chemicals in UPFs, the researchers posit.

The results were published in the Journal of the Academy of Nutrition and Dietetics.

Losing sleep over food

UPFs are a now staple part of Western diets. From ice cream to white bread, instant soup to soda, these products are thought to account for 57.9% of the diets of US citizens. They're often rich in saturated fat, salt and sugar, and poor in fiber and essential nutrients like calcium.

For these reasons, the foods have been blamed for increasing rates of obesity, heart disease and cancer rates in Western countries.

To find out if the foods have any effect on sleep quality, the Sorbonne Paris Nord University researchers first accessed data from an ongoing online health study in France, the NutriNet-Santé cohort. All 38,570 selected participants (76.6% female, average age 50) had provided reports of their sleep quality and diet.

On average, participants consumed around 16% of their energy from UPFs. Close to 20% reported chronic insomnia.

These individuals who reported insomnia, on average, consumed more UPFs. This association between insomnia and UPF intake was seen in both males and females, but the risk was slightly higher in males.

Although concerned by their findings, the researchers weren't necessarily surprised.

"Our research team had previously reported associations of healthy dietary patterns, like the Mediterranean diet, with a reduced risk of insomnia and poor sleep quality (both cross-sectionally and longitudinally), and high carbohydrate diets with an elevated risk of insomnia," said Marie-Pierre St-Onge, an associate professor of Nutritional Medicine at Columbia University and co-author of the study.

"The consumption of UPF is on the rise worldwide, and it has been linked to numerous health conditions such as diabetes, obesity, and cancer," she added.

While St-Onge and her colleagues admit that their findings were observational – and no biochemical causation between UPFs and insomnia could be proven – they nonetheless conclude that regular

CHEMWATCH
Bulletin Board
Curiosities
JUN. 07, 2024

consumption of such manufactured treats and meals may be a risk factor for chronic sleeplessness.

After all, they say, the sleep–wake cycle is promoted by melatonin, which is synthesized exclusively from tryptophan present in the diet. This amino acid can be typically found in dairy, fish, fruit and vegetables, but is scarcer in processed foods.

The team say epidemiological and clinical research will be needed to uncover any such causational mechanism by which UPFs induce insomnia.

Technology Networks, 3 June 2024

https://technologynetworks.com

CHEMWATCH

Bulletin Board

Technical Notes

JUN. 07, 2024

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

CHEMICAL EFFECTS

Insight into the mechanisms of combined toxicity of cadmium and flotation agents in luminescent bacteria: Role of micro/nano particles

Indigo dyes: Toxicity, teratogenicity, and genotoxicity studies in zebrafish embryos

Occurrence and dissipation mechanisms of organic contaminants during sewage sludge anaerobic digestion: A critical review

ENVIRONMENTAL RESEARCH

Emerging contaminants in water environments: progress, evolution, and prospects

Ultrafine CuO/graphene oxide cellulose nanocomposites with complementary framework for polycyclic aromatic hydrocarbon pollutants removal

Sixty years of research on bracken fern (Pteridium spp.) toxins: environmental exposure, health risks and recommendations for bracken fern control

PHARMACEUTICAL/TOXICOLOGY

Hazard identification of endocrine-disrupting carcinogens (EDCs) in relation to cancers in humans

Children's exposure to halogenated flame retardants and organophosphate esters through dermal absorption and hand-to-mouth ingestion in Swedish preschools

OCCUPATIONAL

Letter re: Regulatory toxicology approaches in workplaces of Iran

Reduced protein levels in latex gloves may play an alternative approach to lowering latex sensitization risks among health workers; a cross-sectional analytical study