CHEMWATCH

Bulletin Board

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ASIA PACIFIC

Veterinary chemical products and approved labels

2024-11-12

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

Table 6: Veterinary products based on existing active constituents

Application no.	144699
Product name	Quad Multi-Combination Sheep Drench
Active constituents	37.5 g/L closantel, 34 g/L levamisole (as levamisole hydrochloride), 25 g/L albendazole, 1 g/L abamectin
Applicant name	Four Seasons Agribusiness Pty Ltd
Applicant ACN	115 133 189
Date of registration	24 October 2024
Product registration no.	95108
Label approval no.	95108/144699
Description of the application and its purpose, including the intended use of the chemical product	Registration of a 37.5 g/L closantel, 34 g/L levamisole (as levamisole hydrochloride), 25 g/L albendazole, 1 g/L abamectin oral suspension product for the treatment and control of worms in sheep

Read More

APVMA, 12-11-24

https://www.apvma.gov.au/news-and-publications/publications/gazette/gazette-23-12-november-24

Approved active constituents

2024-11-12

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

Table 8: Approved active constituents

Application no.	142052
Active constituent	Ametryn
Applicant name	Syngenta Australia Pty Ltd
Applicant ACN	002 933 717
Date of approval	18 October 2024
Approval no.	94312
Description of the application and its purpose, including the intended use of the active constituent	Approval of the active constituent ametryn for use in agricultural chemical products

Read More

APVMA, 12-11-24

https://www.apvma.gov.au/news-and-publications/publications/gazette/gazette-23-12-november-24

Licensing of veterinary chemical manufacturers

2024-11-12

Pursuant to Part 8 of the Agricultural and Veterinary Chemicals Code (Agvet Code), scheduled to the Agricultural and Veterinary Chemicals Code Act 1994, the APVMA hereby gives notice that it has taken action with respect to the licensing of the following veterinary chemical manufacturers with effect from the dates shown.

For a comprehensive listing of all licensed manufacturers please see the APVMA website.

New licenses

The APVMA has issued the following licenses under subsection 123(1) of the Agvet Code:

Table 10: New licenses issued by the APVMA under subsection 123(1) of the Agvet Code

	Licence number		Address	Product types	Steps of	Date issued
Alltech Lienert Australia Pty LTD	2274	008 293 007	7 Durham Street Forbes NSW 2871	Category 2: Pellets Category 4: Premixes	Quality	17 October 2024
Alltech Lienert Australia Pty LTD	2274	008 293 007	7 Durham Street Forbes NSW 2871	Category 2: Pellets Category 4: Premixes	Quality	17 October 2024
Inline	2198	120 276 995	28 Horizon Drive	Category 2: creams	Quality	30 October 2024
Scientest Analytical Services Pty Ltd	6250	116 585 936	64 Blanck Street Ormeau QLD 4208	Category 6: all dosage forms	Analysis and testing (physical	31 October 2024

Read More

APVMA, 12-11-24

https://www.apvma.gov.au/news-and-publications/publications/gazette/gazette-23-12-november-24

Proposed revisions to the Categorisation Guidelines in 2025

2024-11-22

We propose to revise the Industrial Chemicals Categorisation Guidelines (the Guidelines) in September 2025.

The revisions mainly affect the list of chemicals with high hazards for categorisation (the list), which is a downloadable resource that some importers and manufacturers must use when working out their introduction category. We invite your comments on the proposed revisions.

Have your say by 5 December 2024:

Updating the Guidelines

The Guidelines (which include the list) were originally published in July 2020. They were updated on 24 April 2024 and 24 September 2024. We intend to update the Guidelines and list annually from here on, unless an urgent change is required.

- The updates would come into effect in September each year, to coincide with the start of the registration year.
- We propose to consult publicly on the changes in September/October of the preceding year.
- We would publish the final changes 6 months before they come into effect for changes that may have a regulatory impact.

This consultation and publication schedule provides stakeholders with certainty about the timing of public consultations and time to prepare for upcoming changes that may affect them.

Read More

AICIS, 22-11-24

https://www.industrialchemicals.gov.au/consultations/proposed-revisions-categorisation-guidelines-2025

AMERICA

FDA Update on Phthalates in Food Packaging and Food Contact Applications

2024-10-29

The U.S. Food and Drug Administration (FDA) responded to objections on the agency's final rule that removed the authorized food contact uses of most phthalates because industry abandoned these uses. The FDA evaluated the objections and concluded that they did not provide a basis for modifying the final rule. However, the FDA is working on an updated safety assessment of the remaining authorized uses, including considering information we have received through our request for information, and phthalates are included on the list of select chemicals under FDA review.

The FDA issued the final rule in 2022 which granted a petition demonstrating that industry has abandoned the food contact use of most

phthalates that were previously authorized for food contact uses. An objection from several public interest groups followed. Today's response to this objection explains that the FDA's action on the final rule was reasonable.

The FDA also received objections to the agency's denial of a separate food additive petition requesting that the agency revoke authorized food contact uses of 28 phthalates due to alleged safety concerns. We have concluded that the objectors have not established a basis for modifying or revoking the denial order as requested in the objections.

Today's response to these objections explains that we denied the food additive petition because it did not establish, through data and information, sufficient support to take the requested action of grouping the 28 phthalates as a class and revoking the authorizations for the 28 phthalates on the basis that they were unsafe as a class. Fundamental to the petition was the claim that all 28 phthalates could be reviewed together as a class, applying data from one chemical to the entire set of 28. The FDA assessment found that available information does not support grouping all 28 phthalate chemicals into a single class assessment.

For the 28 phthalates that were the subject of the safety-based petition, we note that the authorization of 23 of the 28 phthalates were no longer in use and have been revoked in the final rule issued at the same time as the denial of the safety-based petition.

We will continue to keep the food industry and the public informed of updates related to our activities on phthalates in food contact applications. Up to date information is available on the FDA's phthalates page.

Read More

US FDA, 29-10-24

https://www.fda.gov/food/hfp-constituent-updates/fda-update-phthalates-food-packaging-and-food-contact-applications

Pesticide Registration Review; Proposed Decisions for Several Pesticides; Notice of Availability

2024-11-05

EPA is conducting its registration review of the chemicals listed in the table 1 of unit I pursuant to the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) section 3(g) (7 U.S.C. 136a(g)) and the Procedural

Regulations for Registration Review at 40 CFR part 155, subpart C. FIFRA Section 3(g) provides, among other things, that pesticide registrations are to be reviewed every 15 years. Consistent with 40 CFR 155.57, in its final registration review decision, EPA will ultimately determine whether a pesticide continues to meet the registration standard in FIFRA section 3(c)(5) (7 U.S.C. 136a(c)(5)). As part of the registration review process, the Agency has completed a proposed interim or proposed decision for each of the pesticides listed in table 1 of unit I.

The registration review docket for a pesticide includes documents related to the registration review case. Among other things, these documents describe EPA's rationales for conducting additional risk assessments for the registration review of the pesticides included in table 1 of unit I, as well as the Agency's subsequent risk findings and consideration of possible risk mitigation measures. The proposed interim and proposed registration review decisions are supported by the rationales included in those documents.

Read More

US Federal Register, 05-11-24

https://www.federalregister.gov/documents/2024/11/05/2024-25618/pesticide-registration-review-proposed-decisions-for-several-pesticides-notice-of-availability

Consumer demands drive sustainable trends in packaging design

2024-11-08

Shifting consumer attitudes and the increased demand for eco-friendly solutions continue to shape changes to the way goods are packaged and distributed across industries. Key trends in the shifting packaging landscape include the rise of biodegradable and compostable materials, such as PLA and mycelium, which decompose naturally and reduce environmental impact compared to traditional plastics. Minimalist packaging design is also gaining popularity, focusing on reducing waste, cutting costs, and using recyclable materials like cardboard and paper. Additionally, reusable and refillable packaging solutions are becoming more common, particularly in sectors like cosmetics and food, as part of the zero-waste movement. Companies adopting these sustainable packaging strategies can reduce waste, lower costs, and build stronger

relationships with eco-conscious consumers, ultimately contributing to a more sustainable future.

Read More

RPRA, 08-11-24

https://rpra.ca/the-hub/consumer-demands-drive-sustainable-trends-in-packaging-design/

Toronto relaunches ChemTRAC program to track hazardous substances

2024-11-21

With the relaunch of a program which implements Toronto's community right to know bylaw, advocates hope reductions in harmful chemical exposures will follow.

While environmental and workplace exposures are known and significant contributors to the burden of cancer and other diseases, cancer prevention efforts mostly continue to focus on individual modifiable risk factors such as smoking, diet and lack of exercise. Thus, the onus for cancer prevention is shifted to individual workers and residents.

In Ontario occupational cancers claim more worker lives than traumatic injuries by far. Conservative estimates conclude that occupational exposures are responsible for an estimated 2 to 10 per cent of newly diagnosed cancers, but some believe it may be as high as 20 per cent. Similarly, environmental carcinogens are associated with two to as much as 19 per cent of all new cancer cases in Ontario each year.

With the substantial contribution of environmental and occupational carcinogens bold policy initiatives with the potential for population level impacts are much needed and long overdue.

Read More

HSC Workers Health & Safety, 21-11-24

https://www.whsc.on.ca/What-s-new/News-Archive/Toronto-relaunches-ChemTRAC-program-to-track-hazardous-substances

EUROPE

Czechia, Italy push to postpone fines for missing emission targets

2024-11-04

Czech Transport Minister Martin Kupka (ODS, ECR) revealed the plan on CNN Prime News on Sunday, expressing concern that the recent drop in demand for electric vehicles across the EU will make it increasingly difficult for carmakers to meet the required 15% reduction in emissions by 2025.

"They can't meet the target because interest in electric cars has fallen across the European Union," Kupka explained.

To meet these targets, European carmakers need to increase the proportion of electric vehicles in their fleets, driven by EU regulations that aim for a 100% reduction in emissions by 2035. However, recent market trends show declining electric vehicle sales, causing concern among manufacturers and policymakers.

Kupka also pointed out that Czechia formally proposed the delay two weeks ago, with Italy joining shortly afterwards. Germany has also indicated its support, with German Economy Minister Robert Habeck (Greens) - a strong supporter of e-mobility - agreeing that a temporary suspension of the fines would benefit the industry.

Kupka stressed that forcing manufacturers to pay penalties for not meeting quotas would reduce the funds available for further investment in electric vehicle technology, which could hinder the sector's progress in the long term.

Read More

Euractiv, 04-11-24

https://www.euractiv.com/section/politics/news/czechia-italy-push-to-postpone-fines-for-missing-emission-targets/

Climate report shows the largest annual drop in EU greenhouse gas emissions for decades

2024-11-05

EU greenhouse gas emissions fell by 8.3% in 2023, compared to 2022, reveals the latest climate action progress report by the European Commission. The report states that net greenhouse gas emissions are now

37% below 1990 levels. Over the same period, EU Gross Domestic Product (GDP) grew by 68%. This points to the fact that reducing emissions and economic growth are compatible. It also confirms that the EU remains on track to reach its goal of reducing emissions by at least 55% by 2030.

Among the report's findings are:

- a record 16.5% decrease in 2023 emissions from power and industrial installations that are listed under the EU Emissions Trading System.
- a 24% decrease in emissions from electricity production and heating, under the EU Emissions Trading System, driven by the growth of renewable energy sources, in particular wind and solar energy.
- the EU Emissions Trading System generated revenues of €43.6 billion in 2023 for climate action investments.
- around a 2% decrease in 2023 of overall buildings, agriculture, domestic transport, small industry and waste emissions.
- an 8.5% increase in 2023 in the EU's natural carbon absorption, reversing the recent declining trend in the land use and forestry sector.

Read More

European Commission, 05-11-24

https://commission.europa.eu/news/climate-report-shows-largest-annual-drop-eu-greenhouse-gas-emissions-decades-2024-11-05_en

New IUCLID Service Release (v8.13.2)

2024-11-11

The latest service release of IUCLID is now available, bringing a host of fixes and improvements to enhance user experience and functionality.

This release does not introduce any format changes but focuses on resolving existing issues and implementing valuable enhancements.

Among the key fixes, the document comparison functionality has been restored, text wrapping for long strings has been improved, and the .csv file upload mapping for phrases in picklists has been corrected.

Key improvements include enhanced data entry with full-screen mode for rich text fields and an improved date-picker control. The automatic selection of legal entity in dossier headers upon creation has been added, along with the ability to re-order records in multi-reference fields.

This release also contains specific user group enhancements such as improved validation rules and report templates. For EU CLP (Poison Centres), the labelling calculator has been extended to include non-GHS hazard statements, and the PCN report now displays new hazard classes. Improvements for EU PPP include better filtering of mixture components, a new report for analytical methods, and enhanced quality rules. For EU BPR, a new set of quality rules is introduced for active substance applications.

Read More

IUCLID News, 11-11-24

https://iuclid6.echa.europa.eu/view-article/-/journal_content/title/new-iuclid-service-release-v8.13.2

New substance evaluation conclusions published

2024-11-15

- Bis(isopropyl)naphthalene (EC 254-052-6, CAS 38640-62-9), evaluated by Sweden.
- Imidazolium compounds, 2-C17-unsatd.-alkyl-1-(2-C18-unsatd. amidoethyl)-4,5-dihydro-N-methyl, Me sulfates (EC 931-745-8), evaluated by Sweden.

Read More

ECHA, 15-11-24

https://echa.europa.eu/information-on-chemicals/evaluation/community-rolling-action-plan/corap-table

Assessment of regulatory needs report published

2024-11-15

Report for the following substance group is now available on our website:

- Fluoride salts with counterions of low hazard

If you have questions or feedback related to the assessment work, you can send them to us using this webform.

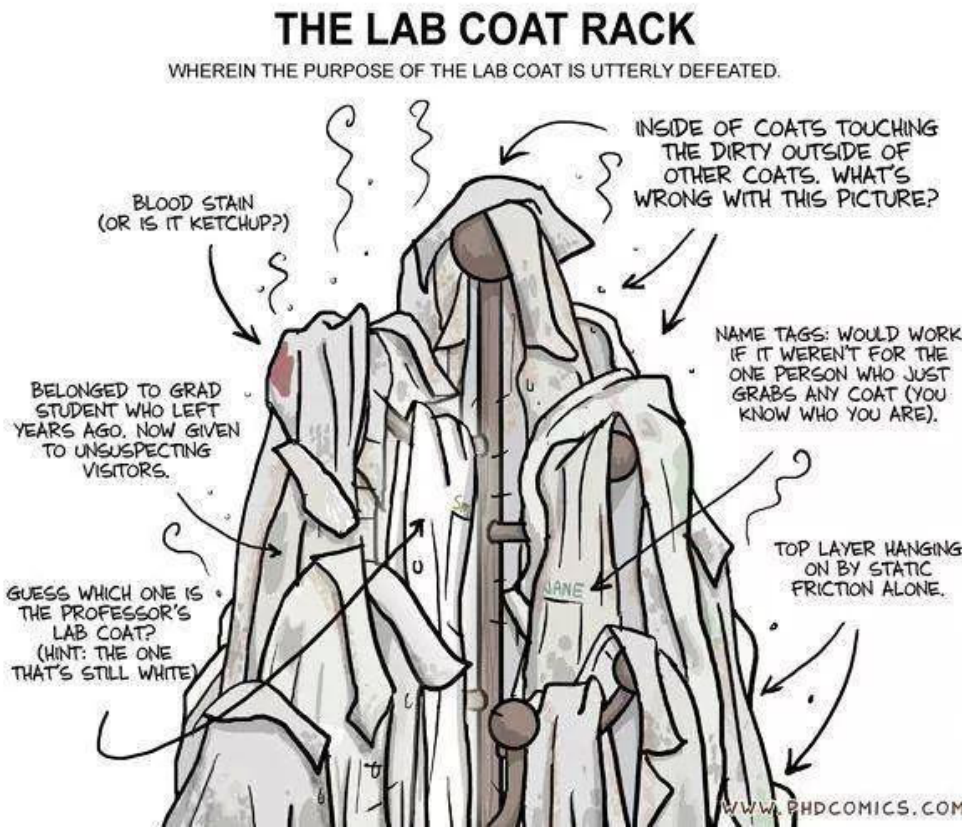
Read More

ECHA, 15-11-24

https://echa.europa.eu/assessment-regulatory-needs

The Lab Coat Rack

2024-12-13



Science Jokes Daily

http://sciencejokesdaily.com/

Dichlorvos

2024-12-13

Dichlorvos is an insecticide that is a dense colourless liquid. It has a sweetish smell and readily mixes with water. Dichlorvos used in pest control is diluted with other chemicals and used as a spray. It can also be incorporated into plastic that slowly releases the chemical. [1,2]

USES [2,3]

houses, and barns, and control of insects on livestock. It is not generally used on outdoor crops. Dichlorvos is sometimes used for insect control in workplaces and in the home. [2] It is effective against mushroom flies, aphids, spider mites, caterpillars, thrips, and white flies in greenhouse, outdoor fruit, and vegetable crops. Dichlorvos is used to treat a variety of parasitic worm infections in dogs, livestock, and humans. Dichlorvos can be fed to livestock to control botfly larvae in the manure. It acts against insects as both a contact and a stomach poison. It is used as a fumigant and has been used to make pet collars and pest strips. It is available as an aerosol and soluble concentrate. Veterinarians use it to control parasites on pets.

Dichlorvos or 2,2-dichlorovinyl dimethyl phosphate is a organophosphate with the molecular formula C4H7Cl2O4P.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Exposure Sources

- The general population is not likely to be exposed to dichlorvos.
- It has been found on some fruits, vegetables, and grain, but washing and processing destroys the dichlorvos.
- Breathing contaminated air or touching contaminated soil could expose people who live near a hazardous waste site containing dichlorvos.
- Workers who manufacture the chemical or use it are likely to be exposed.
- Breathing contaminated air or touching surfaces where dichlorvos was applied could expose people whose homes have been sprayed with dichlorvos.

Routes of Exposure

The routes of exposure to dichlorvos are:

- Inhalation;

- Skin absorption;
- Ingestion; and
- Skin and/or eye contact

Dichlorvos is highly toxic by inhalation, dermal absorption, and ingestion. Because it is volatile, inhalation is the most common route of exposure. As with all organophosphates, dichlorvos is readily absorbed through the skin.

HEALTH EFFECTS [4]

Acute Health Effects

- Dichlorvos exerts its toxic effects in humans and animals by inhibiting the enzyme, acetylcholinesterase. Effects from acute exposure include perspiration, nausea, vomiting, diarrhoea, drowsiness, fatigue, headache, and at very high concentrations, convulsions, and coma.
- Tests involving acute exposure of rats, mice, and rabbits have demonstrated dichlorvos to have high to extreme acute toxicity from oral or dermal exposure and extreme acute toxicity from inhalation.

Carcinogenicity

- No information is available on the carcinogenic effects of dichlorvos in humans.
- In a gavage study by the NTP, there was an increased incidence of tumours of the pancreas and leukaemia in male rats, tumours of the pancreas and mammary gland in female rats, and tumours of the forestomach in both sexes of mice.
- Dichlorvos was not found to be carcinogenic in an animal study by the National Cancer Institute (NCI) in which the compound was administered in the diet.
- EPA has classified dichlorvos as a Group B2, probable human carcinogen.

Other Effects

- Acetylcholinesterase inhibition may also occur in humans from chronic exposure to dichlorvos.
- Symptoms in animals orally exposed to dichlorvos include ataxia, salivation, dyspnea, tremors, and diarrhoea.

- The Reference Concentration (RfC) for dichlorvos is 0.0005 milligrams per cubic metre (mg/m3) based on decreased brain cholinesterase activity in rats.
- The Reference Dose (RfD) for dichlorvos is 0.0005 milligrams per kilogram body weight per day (mg/kg/d) based on plasma and red blood cell cholinesterase inhibition in male and female dogs and brain cholinesterase inhibition in male dogs.

SAFETY

First Aid Measures [5]

- If inhaled: If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
- In case of skin contact: Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.
- In case of eye contact: Flush eyes with water as a precaution.
- If swallowed: Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Workplace Controls & Practices [4]

Control measures include:

- Avoid contact with skin, eyes and clothing.
- Wash hands before breaks and immediately after handling the product.

Personal Protective Equipment [5]

The following personal protective equipment is recommended when handling dichlorvos:

- **Eye/face protection:** Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
  Skin protection: Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.
  Body Protection: Complete suit protecting against chemicals, the

type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

- **Respiratory Protection:** Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

REGULATION

United States

OSHA: The Occupational Safety & health Administration has established the following Permissible Exposure Limit (PEL) for dichlorvos:

General Industry: 29 CFR 1910.1000 Z-1 Table -- 1 mg/m3 TWA; Skin

Construction Industry: 29 CFR 1926.55 Appendix A -- 1 mg/m3 TWA; Skin

Maritime: 29 CFR 1915.1000 Table Z-Shipyards -- 1 mg/m3 TWA; Skin

ACGIH: The American Conference of Governmental Industrial Hygienists has set a Threshold Limit Value (TLV) for dichlorvos of 0.1 mg/m3 TWA (Inhalable Fraction) (Vapour and Aerosol); Skin; SEN; Appendix A4 - Not Classifiable as a Human Carcinogen; BEI

NIOSH: The National Institute for Occupational Safety and Health has set a Recommended Exposure Limit (REL) for dichlorvos of 1 mg/m3 TWA; Skin.

REFERENCES

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7. https://www.osha.gov/dts/chemicalsampling/data/CH_234230.html
8. http://www.safeworkaustralia.gov.au/sites/SWA/about/Publications/Documents/772/Workplace-exposure-standards-airborne-contaminants.pdf

Beyond Silicon: How DNA Is Powering Next-Gen Computers

2024-12-11

Researchers have developed a new, fast, and rewritable method for DNA computing that promises smaller, more powerful computers.

This method mimics the sequential and simultaneous gene expression in living organisms and incorporates programmable DNA circuits with logic gates. The improved process places DNA on a solid glass surface, enhancing efficiency and reducing the need for manual transfers, culminating in a 90-minute reaction time in a single tube.

Advancements in DNA-Based Computation

DNA carries the instructions for life, guiding everything from physical traits like hair color to disease susceptibility. Its ability to store vast amounts of information and perform complex biological processes has inspired scientists to explore DNA-based computers. These futuristic devices could be faster and more compact than today's silicon-based computers. In a new study published today (December 11) in ACS Central Science, researchers unveiled a new DNA computing method that is both fast and rewritable — much like modern digital computers.

"DNA computing as a liquid computing paradigm has unique application scenarios and offers the potential for massive data storage and processing of digital files stored in DNA," explains Fei Wang, one of the study's co-authors.

Developing Programmable DNA Devices

In living organisms, DNA expression follows a precise sequence: Genes are transcribed into RNA, which is then translated into proteins. This process happens simultaneously across numerous genes and is continuously repeated. If scientists can replicate this intricate biological process within DNA-based computers, they could create machines far more powerful than current silicon-based systems. While sequential DNA computing has been demonstrated for specific, narrowly focused tasks, developing flexible and programmable DNA devices that can be reused across multiple applications has remained a challenge — until now.

Innovations in DNA Circuit Design

In previous research, Chunhai Fan, Wang, and colleagues developed a programmable DNA integrated circuit with many logic gates that act as instructions for the circuit's operations. Here's how it worked:

- Data, 0 or 1, was represented by a short piece of single-stranded DNA, called an oligonucleotide, that contained a series of bases: adenine, thymine, guanine and cytosine. (In nature, the sequence of bases codes for a gene.)
- For example, two inputs of 1 (DNA strands 1 and 2) would interact with an OR logic gate DNA molecule.
- Then in a fluid-filled tube, the input oligonucleotide interacted with a logic gate DNA molecule and generated an output oligonucleotide.
- The output oligonucleotide bound to a different single-stranded DNA that was folded into an origami-like structure, called a register in computer lingo.
- The oligonucleotide was "read" by reviewing its base sequence, released and used in a vial containing the next gate, and so on.

Enhancing DNA Computing Efficiency

This process took hours, and someone had to manually transfer the oligonucleotide from one gate to another vial for the next computing operation. So the team, along with Hui Lv and Sisi Jia, wanted to speed things up.

To make the reaction processes more efficient and compact, the team first placed the DNA origami register onto a solid glass 2D surface. The output oligonucleotide floating in liquid from a specific logic gate then attached to the glass-mounted register. After the output oligonucleotide was read and the logic gate instructions determined, it detached, which reset the register so it could be rewritten, thereby avoiding the need to move or replace registers. The researchers also designed an amplifier that boosted the output signal so all the pieces — the gates, oligonucleotides and registers — could find one another more easily. In a proof-of-concept experiment, all the DNA computing reactions took place in a single tube within 90 minutes.

Future Perspectives

"This research paves the way for developing large-scale DNA computing circuits with high speed and lays the foundation for visual debugging and automated execution of DNA molecular algorithms," says Wang.

Sci Tech Daily, 11 December 2024

https://scitechdaily.com

'Superman' bacteria offer a sustainable boost to chemical production

2024-12-11

Trillions of bacteria work in the chemical and pharmaceutical industries, helping produce everything from beer and facial creams to biodiesel and fertilizer. The pharmaceutical industry, in particular, relies heavily on bacteria for producing substances like insulin and penicillin.

Harnessing bacteria's industrial contributions have revolutionized global health, but their work comes at a high energy cost.

Additionally, solvents and continuous production of new bacteria are often necessary, as they don't last long in their jobs.

Changzhu Wu, a chemist and associate professor at the Department of Physics, Chemistry, and Pharmacy, University of Southern Denmark, is focused on making industrial bacteria more robust and useful.

His goal is to reduce the energy, time, and unwanted chemicals required to maintain bacteria, while also making them reusable so they can work longer before needing to be replaced.

His latest innovation introduces a type of "super-powered" bacterium and is now published in Nature Catalysis.

"We took a common industrial bacterium, E. coli, and essentially gave it a 'Superman cape' to enhance its catalysis capabilities. This reduces energy use and makes the production process more sustainable," Changzhu Wu explains.

While E. coli is often associated with foodborne illness, it is widely used in the pharmaceutical industry to produce essential medicines like insulin and growth hormone through various chemical reactions.

The industry uses vast quantities of E. coli, and replacing them takes a toll on the environment, energy, and time due to factors like high temperatures, extreme pH levels, UV radiation, and exposure to solvents.

In developing his "Superman cape," Changzhu Wu sought a material that could envelop the bacteria while still allowing them to interact with their environment to carry out the desired complex chemical reactions.

The solution: a polymer coating that integrates with the bacterial cell membrane.

Polymers are large molecules made up of billions of identical units called monomers.

"We essentially grafted an E. coli bacterium's cell membrane with polymers, achieving two important outcomes: First, the bacteria became stronger and more efficient, and could carry out complex chemical reactions more quickly. Second, the bacteria became more protected, allowing for multiple uses. So, it's a kind of 'Superman bacterium' that is more sustainable," explains Changzhu Wu.

Science Daily, 11 December 2024

https://sciencedaily.com

Small RNAs Hold the Key to Butterfly Wing Color Diversity

2024-11-09

Lepidopterans (butterflies and moths) exhibit a splendid diversity of wing colour patterns, and many species display black and white, or dark and bright, wing colour pattern variants associated with the presence and absence of melanin. Many of these wing colour pattern variants are textbook examples of natural selection and evolution. Iconic examples include the rapid increase in frequency of the melanic form of the British peppered moth Biston betularia, driven by the sootier and darker environment caused by carbon burning and industrialisation in the late 1800s in the United Kingdom, and the mimetic radiation of Heliconius butterflies, among others.

Despite the often well-understood ecological drivers that favour the presence or absence of melanin in the wings of these lepidopterans, the genetic and developmental basis of changes in colouration has remained unclear.

How do butterflies and moths paint their wings either black or white?

Over the past two decades, scientists discovered that the majority of melanic wing colour variants are controlled by a single genomic region surrounding the protein-coding gene "cortex". It was assumed, then, that cortex was the melanic colour switch. A team of international researchers from Singapore, Japan, and the United States of America, led by Professor Antónia MONTEIRO and Dr Shen TIAN from the Department of Biological Sciences at the National University of Singapore (NUS), discovered that

cortex does not affect melanic colouration. Instead, a previously ignored microRNA (miRNA), is the actual colour switch.

The findings were published in the journal Science.

Dr Tian, the lead author of this work said, "Piles of evidence from previous studies cast doubt on whether cortex was really the melanic colour switch, which inspired me to test the function of some other genomic features within this genomic region – miRNAs." He conducted this research work as a PhD/postdoctoral researcher in Professor Monteiro's laboratory at NUS, and is now a postdoctoral researcher at Duke University, USA.

"MiRNAs are small RNA molecules that do not encode proteins like most genes do, yet they play essential roles in gene regulation by repressing the expression of target genes," added Dr Tian.

In this study, Dr Tian and colleagues found a miRNA located next to cortex, mir-193. The team disrupted mir-193 using a gene editing tool CRISPR-Cas9 in three deeply diverged lineages of butterflies. The complete disruption of mir-193 eliminated black and dark wing colours in the African squinting bush brown butterfly, Bicyclus anynana, the Indian cabbage white butterfly, Pieris canidia, and the common mornon butterfly, Papilio polytes. In contrast, disrupting cortex and three other protein-coding genes from the same genomic region in B. anynana had no effect on wing colours. This indicated that mir-193, not cortex or any other nearby gene, is the key melanic colour regulator across these Lepidoptera.

The team further confirmed that mir-193 is processed from a long non-protein-coding RNA, ivory, and it functions by directly repressing multiple pigmentation genes. Since the sequence of mir-193 is deeply conserved not only in Lepidoptera but across the animal kingdom, the team also tested the role of mir-193 in Drosophila flies. Surprisingly, mir-193 was also found to control melanic colouration in these flies, suggesting a deeply conserved role for mir-193 beyond Lepidoptera.

Prof Monteiro said, "While previous studies exclusively focused on the role of cortex in generating melanic colour variations, this work brings a twist to this long-standing hypothesis and demonstrates that a small, non-protein coding RNA is the switch that, by being expressed or not expressed, brings about the diverse melanic wing colour variations in nature."

"This study shows that poorly annotated non-protein-coding RNAs, such as miRNAs, should never be ignored in genotype-phenotype association

studies, which would otherwise lead to misleading conclusions," added Prof Monteiro.

Dr Tian said, "The role of non-coding RNAs in phenotypic diversification is largely understudied. This study prompts further investigations on how non-coding RNAs such as miRNAs can contribute to phenotypic diversifications in organisms."

Technology Networks, 9 December 2024

https://technologynetworks.com

Supercharged E. coli: The Future of Eco-Friendly Chemical Production

2024-12-11

Scientists have innovated a polymer-coated bacterium that enhances its catalytic efficiency and sustainability in industrial applications.

This new "super-powered" bacterium, designed to be more robust and reusable, aims to minimize the environmental and resource burdens associated with bacterial production in industries like pharmaceuticals.

Bacteria's Role in Industry

Bacteria play a crucial role in the chemical and pharmaceutical industries, helping create products as diverse as beer, facial creams, biodiesel, and fertilizer. In the pharmaceutical sector, bacteria are essential for producing life-saving substances like insulin and penicillin.

While bacteria-driven production has revolutionized medicine and industry, it comes with significant challenges. The process requires substantial energy and often involves harsh solvents. Additionally, bacteria used in production have limited lifespans and must be frequently replaced, increasing costs and environmental impact.

Enhancing Bacterial Durability and Efficiency

Changzhu Wu, a chemist and associate professor at the Department of Physics, Chemistry, and Pharmacy at the University of Southern Denmark, aims to make industrial bacteria tougher and more efficient. His research focuses on reducing the energy, time, and chemicals needed to sustain bacteria while making them reusable, allowing them to work longer before replacement is necessary.

His latest innovation introduces a type of "super-powered" bacterium and is published today (December 11) in Nature Catalysis.

"We took a common industrial bacterium, E. coli, and essentially gave it a 'Superman cape' to enhance its catalysis capabilities. This reduces energy use and makes the production process more sustainable," Changzhu Wu explains.

E. coli in Industrial Applications

While E. coli is often associated with foodborne illness, it is widely used in the pharmaceutical industry to produce essential medicines like insulin and growth hormone through various chemical reactions.

The industry uses vast quantities of E. coli, and replacing them takes a toll on the environment, energy, and time due to factors like high temperatures, extreme pH levels, UV radiation, and exposure to solvents.

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The Polymer Solution

The solution: a polymer coating that integrates with the bacterial cell membrane. Polymers are large molecules made up of billions of identical units called monomers.

"We essentially grafted an E. coli bacterium's cell membrane with polymers, achieving two important outcomes: First, the bacteria became stronger and more efficient, and could carry out complex chemical reactions more quickly. Second, the bacteria became more protected, allowing for multiple uses. So, it's a kind of 'Superman bacterium' that is more sustainable," explains Changzhu Wu.

Sci Tech Daily, 11 December 2024

https://scitechdaily.com

Scientists develop material with almost perfect water repellency

2024-12-08

Scientists from Karlsruhe Institute of Technology (KIT) and the Indian Institute of Technology Guwahati (IITG) have developed a surface material that repels water droplets almost completely. Using an entirely innovative

process, they changed metal-organic frameworks (MOFs)—artificially designed materials with novel properties—by grafting hydrocarbon chains.

The resulting superhydrophobic (extremely water-repellent) properties are interesting for use as self-cleaning surfaces that need to be robust against environmental influences, such as on automobiles or in architecture. The study was published in the journal Materials Horizons.

MOFs (metal-organic frameworks) are composed of metals and organic linkers that form a network with empty pores resembling a sponge. Their volumetric properties—unfolding two grams of this material would yield the area of a football pitch—make them an interesting material in applications such as gas storage, carbon dioxide separation, or novel medical technologies.

The outer surfaces exposed by these crystalline materials also offer unique characteristics, which the research team took advantage of by grafting hydrocarbon chains onto thin MOF films. They observed a water contact angle of more than 160 degrees—the larger the angle formed by the surface of a water drop with the substrate, the better the hydrophobic properties of the material.

"With our method, we are able to achieve superhydrophobic surfaces with contact angles that are significantly higher than those of other smooth surfaces and coatings," states Professor Christof Wöll from KIT's Institute of Functional Interfaces. "Although the wetting properties of MOF powder particles have been explored before, the use of monolithic MOF thin films for this purpose is a groundbreaking concept."

Next-generation 'superhydrophobic' materials

The team attributes these results to the brush-like arrangement (polymer brushes) of the hydrocarbon chains on the MOFs. After being grafted to the MOF materials, they tend to form "coils"—a state of disorder that scientists call "high-entropy state," which is essential for its hydrophobic properties. The scientists asserted that this state of the grafted hydrocarbon chains could not be observed on other materials.

It is remarkable that the water contact angle did not increase even when they used perfluorinated hydrocarbon chains for grafting, i.e., substituting hydrogen atoms with fluorine. In materials such as Teflon, perfluorination brings about superhydrophobic properties. In the newly developed

material, however, it decreased the water contact angle significantly, as the team found out.

Further analyses in computer simulations confirmed that the perfluorinated molecules—in contrast to hydrocarbon chains—could not assume the energetically favorable high-entropy state.

In addition, the scientists varied the surface roughness of their SAM@ SURMOF systems in the nanometer range, thereby further reducing the water adhesion strength. Even with extremely small inclination angles, water droplets started rolling off, and their hydrophobic and self-cleaning properties were significantly improved.

"Our work also includes a detailed theoretical analysis, which links the unexpected behavior shown in experiments to the high-entropy state of the molecules grafted to the MOF films," says Professor Uttam Manna from IITG's Chemistry department. "This study will change the design and production of next-generation materials with optimum hydrophobic properties."

Phys Org, 9 December 2024

https://phys.org

A greener, cleaner way to extract cobalt from 'junk' materials

2024-11-10

Penn researchers led a collaborative effort pioneering safer, more sustainable technique to extract elements critical to battery-powered technologies. Findings pave the way for getting value from materials that would otherwise be considered waste.

Siddarth Kara's bestseller, "Cobalt Red: How the Blood of Congo Powers Our Lives," focuses on problems surrounding the sourcing of cobalt, a critical component of lithium-ion batteries that power many technologies central to modern life, from mobile phones and pacemakers to electric vehicles.

"Perhaps many of us have read how lithium-ion batteries are vital for energy storage technologies," says Eric Schelter, the Hirschmann-Makineni Professor of Chemistry at the University of Pennsylvania. "But how material that make up such batteries are sourced can be concerning and problematic, both ethically and environmentally."

Schelter says that cobalt mining in the Democratic Republic of Congo, which supplies about 70% of the world's cobalt, raises concerns due to environmental degradation and unsafe working conditions, and that large-scale mining disrupts ecosystems, can contaminate water supplies, leaving lasting environmental damage. In addition, he notes that a looming cobalt shortage threatens to strain global supply chains as demand for battery technologies continues to grow.

To that end, an area of research his lab has been focusing on is the separation of battery-critical metals like nickel and cobalt. In a new paper, published in the journal Chem, Schelter's team and collaborators at Northwestern University presented an "easier, more sustainable, and cheaper way to separate both from materials that would otherwise be considered waste."

"Our chemistry is attractive because it's simple, works well, and efficiently separates nickel and cobalt -- one of the more challenging separation problems in the field," Schelter says. "This approach offers two key benefits: increasing the capacity to produce purified cobalt from mining operations with potentially minimal environmental harm, addressing the harshness of traditional purification chemicals, and creating value for discarded batteries by providing an efficient way to separate nickel and cobalt."

The right ingredients for selective separation

Typically, the researchers say, cobalt is often produced as a byproduct of nickel mining by way of hydrometallurgical methods such as acid leaching and solvent extraction, which separates cobalt and nickel from ores. It's an energy-intensive method that generates significant hazardous waste.

The process Schelter and the team developed to circumvent this is based on a chemical-separation technique that leverages the charge density and bonding differences between two molecular complexes: the cobalt (III) hexammine complex and the nickel (II) hexammine complex.

"A lot of separations chemistry is about manifesting differences between the things you want to separate," Schelter says, "and in this case we found conditions where ammonia, which is relatively simple and inexpensive, binds differently to the nickel and cobalt hexammine complexes."

By introducing a specific negatively charged molecule, or anion, like carbonate into the system, they created a molecular solid structure that causes the cobalt complex to precipitate out of the solution while leaving the nickel one dissolved. Their work showed that the carbonate anion

selectively interacts with the cobalt complex by forming strong "hydrogen bonds" that create a stable precipitate. After precipitation, the cobalt-enriched solid is separated through filtration, washed with ammonia, and dried. The remaining solution contains nickel, which can then be processed separately.

"This process not only achieves high purities for both metals -- 99.4% for cobalt and more than 99% for nickel -- but it also avoids the use of organic solvents and harsh acids commonly used in traditional separation methods," says first author Boyang (Bobby) Zhang, a graduate student in Penn's School of Arts & Sciences and a Vagelos Institute for Energy Science and Technology Graduate Fellow. "It's an inherently simple and scalable approach that offers environmental and economic advantages."

Techno-economic and life cycle analyses

In evaluating the real-world applicability of their new method, the team, led by Marta Guron, conducted both techno-economic analysis and life-cycle assessment, with the former revealing an estimated production cost of $1.05 per gram of purified cobalt, substantially lower than the $2.73 per gram associated with a reported separations process.

"We focused on minimizing chemical costs while also using readily available reagents, which makes our method potentially competitive with existing technologies," Schelter says.

The life-cycle analysis found that eliminating volatile organic chemicals and hazardous solvents allows the process to significantly reduce environmental and health risks, which was supported by metrics like Smog Formation Potential and Human Toxicity by Inhalation Potential, where the process scored at least an order of magnitude better than traditional methods.

"This means fewer greenhouse gas emissions and less hazardous waste, which is a seriously big win for both the environment and public health," says Zhang.

Cleaner path forward

Owing to how the team accomplished their separation, Schelter says, there's an exciting fundamental science aspect of this work that he thinks they can take in many different directions, even for other metal separation problems.

"Based on the unique set of molecular recognition principles we identified through the course of this work, I think we can extend this work in many different directions," he says. "We could apply it to other metal separation problems, ultimately driving broader innovation in sustainable chemistry and materials recovery."

Eric Schelter is the Hirschmann-Makineni Professor of Chemistry in the Department of Chemistry at the School of Arts & Sciences at the University of Pennsylvania.

Boyang (Bobby) Zhang is a Vagelos Institute for Energy Science and Technology Graduate Fellow in the Schelter Group at Penn Arts & Sciences.

Marta Guron is an adjunct lecturer in the Department of Chemistry and project manager in the Office of Environmental and Radiation Safety.

Other authors are Andrew J. Ahn, Michael R. Gau, and Alexander B. Weberg from Penn and Leighton O. Jones and George C. Schatz of Northwestern University.

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Sciene Daily, 10 December 2024

https://sciencedaily.com

Revolutionizing Carbon Capture: Scientists Double MOF Efficiency

2024-12-06

OSU scientists enhanced a MOF's carbon capture capacity by over 100% using ammonia gas, creating a stable, energy-efficient alternative to traditional sorbents. This development showcases MOFs' potential in reducing industrial CO2 emissions and other applications.

Scientists at Oregon State University have developed a method to more than double the uptake ability of a chemical structure that can be used for scrubbing carbon dioxide from factory flues.

The study involving metal-organic frameworks, or MOFs, is important because industrial activities, among them burning fossil fuels for energy, account for a significant percentage of the greenhouse gas in the Earth's atmosphere. In the United States, 16% of total carbon dioxide emissions are from industry, according to the Environmental Protection Agency.

OSU researchers led by Kyriakos Stylianou of the College of Science worked with a copper-based MOF and found that its effectiveness at adsorbing carbon dioxide more than doubled when first exposed to ammonia gas.

"The capture of CO2 is critical for meeting net-zero emission targets," said Stylianou, associate professor of chemistry. "MOFs have shown a lot of promise because of their porosity and their structural versatility."

Understanding MOFs: Structure and Applications

MOFs are crystalline materials made up of positively charged metal ions surrounded by organic "linker" molecules known as ligands. The metal ions make nodes that bind the linkers' arms to form a repeating structure that looks something like a cage; the structure has nanosized pores that adsorb gases, similar to a sponge.

MOFs can be designed with a variety of components, which determine the MOF's properties, and there are millions of possible MOFs, Stylianou said. More than 100,000 of them have been synthesized by chemistry researchers, and the properties of hundreds of thousands of others have been predicted.

In addition to the capture of carbon dioxide and other types of gases, MOFs can be used as catalysts and for energy storage, drug delivery and water purification.

When exposed to ammonia gas, the MOF in this study, mCBMOF-1, showed a carbon uptake capacity comparable to or greater than that of the traditional amine-based sorbents that are widely used for carbon dioxide capture in industrial applications. And compared to amine-based sorbents, MOFs are more stable and can be regenerated using less energy – in this case, by immersion in water.

"The MOF is activated by removing water molecules to expose four closely positioned open copper sites," Stylianou said. "Then we introduce the ammonia gas, which causes one of the sites to be occupied by an ammonia molecule. The remaining sites attract CO2, promoting interaction with ammonia to form carbamate species."

The carbamates – compounds with a range of uses in industry, agriculture, and medicine – are released during the water immersion that regenerates the MOF's pristine structure, making it reusable for ongoing carbon capture.

Implications for Future Research and Applications

The findings emphasize that MOF structures can be tailored with functional groups to enhance their interactions with specific target molecules, such as carbon dioxide, Stylianou said; similar strategies could be applied to other MOFs and gases.

"Our study's use of sequential pore functionalization to enhance CO2 uptake without significantly increasing regeneration energy is a terrific development," he said. "The formation of a copper-carbamic acid complex within the pores suggests strong and selective interactions with CO2, which is crucial for ensuring that CO2 is preferentially adsorbed over other gases in flue emissions."

Sci Tech Daily, 6 December 2024

https://scitechdaily.com

Enzymes evolved mix-and-match characteristics to shape nitrogen metabolism diversity across the planet

2024-12-12

To boost crops more efficiently in the future, the evolutionary past may hold key insights. The way that plants process nutrients has a rich back story—they rely on enzymes that have been evolving for billions of years. However, these enzymes are often loosely understood, leaving potential targets for crop engineering untouched.

Research recently published in the Proceedings of the National Academy of Sciences bridges this gap, by tracing the evolution of a specific enzyme family called aminotransferases (ATs). These enzymes play a crucial role in how an organism processes both carbon and nitrogen.

This research team combined computational and experimental approaches to look at how this enzyme family evolved across 90 species. "One unique thing about this work was our focus on all the kingdoms, including animals, plants, bacteria, archaea and fungi. We thought this kind of analysis would provide a framework for the evolution of this enzyme family," said Sang-Woo Han, one of the co-first authors of this work.

Han is an Assistant Professor at Konkuk University in South Korea as well as a faculty affiliate in the Environmental Genomics and Systems Biology Division of Lawrence Berkeley National Laboratory (Berkeley Lab). He completed this work with collaborators at the University of Wisconsin-Madison as well as the U.S. Department of Energy (DOE) Joint Genome Institute (JGI), a DOE Office of Science User Facility located at Berkeley Lab.

In addition to providing metagenome mining for computational analysis of the AT enzyme family, the JGI provided DNA synthesis capabilities to enable functional testing of these enzymes.

Yasuo Yoshikuni, head of the JGI's DNA Synthesis Science program, underscored the value of taking a look at the AT family. "Essentially, the aminotransferases that we studied are involved in transfer of the amine group, or the N group, to a variety of different molecules. So they're involved anytime you make an amine-based molecule—a very critical role," he said. These enzymes are crucial for creating nucleic acids and proteins, as well as recycling nitrogen.

Now, with insight into a specific enzyme class that's important to the way many organisms function, they have a sense of why nitrogen metabolisms can be so varied.

As evolution has progressed, organisms have developed metabolisms that function with a toolkit of enzymes. It's useful to differentiate these enzyme tools into two groups: core metabolism and specialized metabolism.

For enzymes involved in core metabolism, organisms tend to have enzymes evolved to high performance, with specificity—a bit like including hex keys in many different sizes in a toolkit. This makes it possible to process more molecules efficiently, with just the right tool for the job.

For enzymes in specialized metabolism, organisms tend to evolve multiple copies of enzymes, similar to including half a dozen slightly different screwdrivers in a toolkit. This way, these important tools are always around, regardless of malfunction or misplacement.

In studying this family of ATs, researchers found that these enzymes have evolved distinctly from both core and specialized enzymes. Even during specializing or multiplying, ATs have maintained functional versatility with fewer enzyme copies. In this way, this family is more like including a Swiss Army knife within a toolkit—a tool with some redundancy, that is both functionally versatile as well as compact. Because these ATs can facilitate

reactions with multiple types of molecules, they're versatile in ways other enzymes are not.

"It turns out that all of life created the minimum set of ATs that act together to create the robust network to supply amino acids fast enough for life to grow," Yoshikuni said.

To gain this insight into the evolution of ATs, this team traced the evolution of these enzymes across 90 species. They queried the genomes of 15 species from each of six kingdoms: eubacteria, archaea, protist, plant, fungi and animal. This analysis led them to identify 2,938 putative AT genes.

Within the AT genes identified across different species, each organism has a relatively small set of around 20 ATs. These ATs have maintained a small and relatively constant number across different kingdoms, with archaea having around 15, eubacteria around 25, and eukaryotes having slightly larger numbers due to their expanded metabolisms. These ATs can operate in a relatively small set because of their unique functional redundancy.

To understand how founder AT enzymes became integral to core nitrogen metabolism, this team built a phylogenetic tree using bioinformatic software called FastTree and identified 62 distinct AT groups. However, no single AT group was conserved across all species—a surprise for an enzyme that plays a central role in metabolism.

This lack of conservation is likely due to the fact that AT enzymes have undergone non-orthologous gene displacements, where they replaced other ATs in different species, seemingly driven by the functional versatility of ATs. This replacement has allowed AT enzymes to evolve in complex ways.

Finally, to take a closer look at the functional redundancy of ATs, this team leveraged the JGI's DNA synthesis capabilities to express, purify and characterize recombinant enzymes to determine substrate specificity. They found that even enzymes that evolved separately for billions of years have some common signatures of muli-substrate specificity. However, different organisms use different active residues to achieve this, a bit like having slightly different Swiss Army knives—explaining a bit more about why and how nitrogen metabolism is so robust and varied.

Phys Org, 12 December 2024

https://phys.org

New Catalyst Turns Methane Into Useful Polymers

2024-11-05

Although it is less abundant than carbon dioxide, methane gas contributes disproportionately to global warming because it traps more heat in the atmosphere than carbon dioxide, due to its molecular structure.

MIT chemical engineers have now designed a new catalyst that can convert methane into useful polymers, which could help reduce greenhouse gas emissions.

"What to do with methane has been a longstanding problem," says Michael Strano, the Carbon P. Dubbs Professor of Chemical Engineering at MIT and the senior author of the study. "It's a source of carbon, and we want to keep it out of the atmosphere but also turn it into something useful."

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The new catalyst works at room temperature and atmospheric pressure, which could make it easier and more economical to deploy at sites of methane production, such as power plants and cattle barns.

Daniel Lundberg PhD '24 and MIT postdoc Jimin Kim are the lead authors of the study, which appears today in Nature Catalysis. Former postdoc Yu-Ming Tu and postdoc Cody Ritt also authors of the paper.

Capturing methane

Methane is produced by bacteria known as methanogens, which are often highly concentrated in landfills, swamps, and other sites of decaying biomass.

Agriculture is a major source of methane, and methane gas is also generated as a byproduct of transporting, storing, and burning natural gas. Overall, it is believed to account for about 15 percent of global temperature increases.

At the molecular level, methane is made of a single carbon atom bound to four hydrogen atoms. In theory, this molecule should be a good building block for making useful products such as polymers. However, converting methane to other compounds has proven difficult because getting it to react with other molecules usually requires high temperature and high pressures.

To achieve methane conversion without that input of energy, the MIT team designed a hybrid catalyst with two components: a zeolite and a naturally occurring enzyme. Zeolites are abundant, inexpensive clay-like minerals, and previous work has found that they can be used to catalyze the conversion of methane to carbon dioxide.

In this study, the researchers used a zeolite called iron-modified aluminum silicate, paired with an enzyme called alcohol oxidase. Bacteria, fungi, and plants use this enzyme to oxidize alcohols.

This hybrid catalyst performs a two-step reaction in which zeolite converts methane to methanol, and then the enzyme converts methanol to formaldehyde. That reaction also generates hydrogen peroxide, which is fed back into the zeolite to provide a source of oxygen for the conversion of methane to methanol.

This series of reactions can occur at room temperature and doesn't require high pressure. The catalyst particles are suspended in water, which can absorb methane from the surrounding air. For future applications, the researchers envision that it could be painted onto surfaces.

"Other systems operate at high temperature and high pressure, and they use hydrogen peroxide, which is an expensive chemical, to drive the methane oxidation. But our enzyme produces hydrogen peroxide from oxygen, so I think our system could be very cost-effective and scalable," Kim says.

Creating a system that incorporates both enzymes and artificial catalysts is a "smart strategy," says Damien Debecker, a professor at the Institute of Condensed Matter and Nanosciences at the University of Louvain, Belgium.

"Combining these two families of catalysts is challenging, as they tend to operate in rather distinct operation conditions. By unlocking this constraint and mastering the art of chemo-enzymatic cooperation, hybrid catalysis becomes key-enabling: It opens new perspectives to run complex reaction systems in an intensified way," says Debecker, who was not involved in the research.

Building polymers

Once formaldehyde is produced, the researchers showed they could use that molecule to generate polymers by adding urea, a nitrogen-containing molecule found in urine. This resin-like polymer, known as urea-formaldehyde, is now used in particle board, textiles and other products.

The researchers envision that this catalyst could be incorporated into pipes used to transport natural gas. Within those pipes, the catalyst could generate a polymer that could act as a sealant to heal cracks in the pipes, which are a common source of methane leakage. The catalyst could also be applied as a film to coat surfaces that are exposed to methane gas, producing polymers that could be collected for use in manufacturing, the researchers say.

Strano's lab is now working on catalysts that could be used to remove carbon dioxide from the atmosphere and combine it with nitrate to produce urea. That urea could then be mixed with the formaldehyde produced by the zeolite-enzyme catalyst to produce urea-formaldehyde.

Technology Networks, 5 December 2024

https://technologynetworks.com

Scientists examine how roasting affects the perfect brew

2024-12-11

A new study in published in Scientific Reports suggests that the perfect cup of coffee is influenced by a complex blend of variables such as bean processing method, brewing time, and grind size, not just the roast level.

Caffeine content and extraction yield are two of the most vital variables for coffee enthusiasts, especially those who approach it with precision.

Extraction yield is a measure of the amount of soluble material from the coffee grounds that gets dissolved in the brewed coffee. It essentially

reflects the efficiency of the brewing process in extracting compounds from the coffee grounds.

Led by Dr. Zachary R. Lindsey, Assistant Professor of Physics at Berry College, U.S., the study focuses on how the degree of roast affects these two variables. Phys.org spoke to Dr. Lindsey, a self-proclaimed coffee nerd about the study.

"Over 20 years ago, I heard a barista claim that dark roasts have more caffeine, but a decade later, I was exposed to the contrasting idea that light roasts were the king of caffeine. Yet, I couldn't find any convincing data."

"It wasn't until I picked up coffee roasting as a hobby in 2022 that I started to see the missing pieces of the puzzle. Luckily, two passionate undergraduate students on my research team were also intrigued by this mystery, and we got to work," said Dr. Lindsey.

Choice of coffee, roast, and brew method

The researchers chose Ethiopian coffee to conduct their study. Ethiopia has a long tradition of producing coffee dating back centuries as it is the country where Coffee arabica, aka the coffee plant, originates.

In this, they are investigating natural and washed processed coffee.

In the natural method, the coffee cherries are dried with the seeds still inside. The seeds are separated after drying, resulting in fruity and complex flavors in the coffee beans. On the other hand, in the washed method, the seeds are separated from the coffee cherries and then dried, leading to a cleaner and brighter flavor profile.

The researchers then used five different degrees of roasts for the green coffee beans, choosing a brewing time of one, two, and ten minutes.

The researchers chose the AeroPress brewing method with a 15:1 water-to-coffee ratio. The AeroPress is a pressure-based brewing method, similar to an espresso machine, but on a smaller scale. The AeroPress steeps the coffee and uses pressure to extract the brew through a paper filter.

Dr. Lindsey explained the choice behind the AeroPress, saying, "When selecting a brew method, the main goal was to implement a procedure that could consistently produce brews within a wide range of extraction yields by only varying the brew time."

"The AeroPress stood out as a means to achieve these desired outcomes with minimal variation across all roast batches."

Overall, the researchers had 30 unique combinations of brewed coffee to study.

Analyzing the coffee

The researchers used three analysis techniques to analyze caffeine content and extraction yield.

To measure compounds like caffeine, chlorogenic acids, and other soluble compounds in the brewed coffee, they used high-performance liquid chromatography (HPLC).

This method separates different compounds in the coffee based on their interactions with a standard material, quantifying individual concentrations.

Next, they used refractometry. This method measures the bending of light through the brewed coffee, indicating the extraction yield, i.e., how much soluble material is dissolved from the coffee grounds.

Finally, they used scanning electron microscopy (SEM) to observe the surface of the coffee beans and grounds. This helped them to examine the grain size and porosity. SEM provides information about the impact of roasting on the physical features of the coffee beans.

"SEM allows for a straightforward characterization approach that provides two-dimensional information about the structure of the roasted coffee. The evolving porosity of the roasting coffee plays a pivotal role in compound mobility during roasting and brewing," explained Dr. Lindsey.

Porosity, caffeine, and extraction

The researchers found that caffeine content in the brewed coffee depended on the roasting process and the extraction yield.

"During roasting, the volume and porosity of the coffee seeds increase as the roast progresses, which makes it easier for compounds to move in or out of the system," explained Dr. Lindsey.

A greater porosity implies more of the inner surface area of the coffee grounds is exposed, making it easier for water to penetrate and dissolve compounds like caffeine and flavors. This has an impact on the entire extraction process that occurs during brewing.

For the caffeine content, the researchers found that when using identical brewing setups, light and medium roasts had a higher caffeine content than darker roasts. This is due to the caffeine loss during roasting, resulting in typically lower extraction yields for darker roasts.

Conversely, they found that the darker roast's caffeine content was higher when the extraction yield was kept consistent for all the roasts.

"However, darker roasts consistently exhibited lower extraction yields than light and medium roasts, so it was not always possible to achieve a common extraction yield for all degrees of roast," added Dr. Lindsey.

New insights

The competing mechanisms of increased porosity improving extraction efficiency and darker roasts losing extractable compounds revealed a unique insight contradicting previous assumptions.

Caffeine sublimation—the process of caffeine transitioning directly from a solid to a gas—occurs at higher temperatures than previously thought.

"Although the interplay between roast degree and caffeine content has been addressed over 20 times in the literature, the prevailing theory is that caffeine remains stable during the roasting process."

"However, we establish a clear relationship between roast degree, caffeine content, and extraction yield," said Dr. Lindsey.

The researchers plan to extend this work to study the relationship between roast degree and extraction yield for decaffeinated coffees. They also aim to test it with percolation-based brewing methods to see if they yield similar results.

The bottom line is, if you want a cup of coffee with the maximum caffeine content choose a medium roast, says Dr. Lindsey.

Phys Org, 11 December 2024

https://phys.org

Application of Tantalum and Molybdenum in Mobile Phones

2024-11-27

Metal elements have many applications in mobile phones. And today we tend to mention two important ones–molybdenum and titanium. The main use of tantalum materials in electronic products comes in the creation of the tantalum capacitor; and the main use of molybdenum in mobile phones mainly related to the liquid crystal display coating: using magnetron sputtering to sputter metal molybdenum from the molybdenum target onto the surface of a liquid crystal display.

Tantalum

Tantalum could be a vital component within the industry. And it's widely used in every kind of electronic devices, such as phones and computers. Tantalum plays its role in the electronic industry mainly by the creation of the tantalum capacitor. Tantalum capacitors have their distinctive advantages over other capacitors. They do not use electrolytes like normal electrolytic capacitors, enabling them ideal for operation at high temperatures. Solid tantalum capacitors have wonderful electronic properties, wide operating temperature range, varied forms, and excellent volumetrical potency.

In addition to capacitors, tantalum is also used as wave filters in mobile phones to realize high audio property, since electronic signal wave dampening can provide clearer and crisper audio and video output.

A mobile phone has average forty milligrams of titanium inside. Well, compared with the overall weight of a phone, it's not an enormous variety. However, this forty milligrams tantalum is irreplaceable. Thanks to the massive demand for mobile phones, the demand for tantalum has conjointly multiplied. Believe it or not, 50% of tantalum is consumed every year in the electronics industry.

Molybdenum

Molybdenum has a high melting point, high electrical physical phenomenon, low specific resistance, smart corrosion resistance, and smart environmental protection. Therefore, it's wide employed in the electronics industry, mainly for flat panel displays, electrodes of skinny film star cells, and barrier materials for semiconductors. Coating the phone screen with molybdenum sputtering target will greatly improve the brightness, contrast, color, and lifetime of the screen.

In the process of film coating, the quality of the sputtering target has a great influence on the quality of the produced film. Stanford Advanced Materials (SAM) specializes in producing high purity molybdenum sputtering targets with the highest possible density and smallest possible average grain sizes for use in the PVD, CVD, APS and VPS coating processes. We have both of planar molybdenum target and rotatory molybdenum target. Please visit for https://www.sputtertargets.net/ more information.

Stanford Advanced Materials, 27 November 2024

https://sputtertargets.net

Engineered Immune Cells Act As "Referees" To Soothe Inflammation

2024-12-06

When the immune system overreacts and starts attacking the body, the only option may be to shut the entire system down and risk developing infections or cancer.

But now, scientists at UC San Francisco may have found a more precise way to dial the immune system down.

The technology uses engineered T cells that act as immune "referees" to soothe overreacting immune responses. They also can mop up inflammatory molecules.

The new approach could be used to stop the body from rejecting transplanted organs and tissues, such as pancreatic islet cells, which are sometimes used to treat type 1 diabetes. That way, recipients would not need to take harsh immunosuppressant drugs.

"This technology can put the immune system back into balance," said Wendell Lim, PhD, UCSF professor of cellular and molecular pharmacology and co-senior author of the paper, which appears Dec. 5 in Science. "We see it as a potential platform for tackling all kinds of immune dysfunction."

Lim and his colleagues were inspired by "suppressor" cells, which are the immune system's natural brakes. They wanted to take advantage of these suppressor cells' power to temper immune responses, such as inflammation.

Unfortunately, suppressor cells can't always stop a dangerous immune response. In type 1 diabetes, for example, the immune system destroys pancreatic islet cells, while these suppressor cells just stand by.

The team adapted the suppressor cells' anti-inflammatory abilities to work in CD4 immune cells. These are the same cells that are used to make cancer-killing CAR T cells. They also gave these cells a molecular sensor to guide them to their target tissue in the body.

Proof of principle in type 1 diabetes

The scientists tailored a batch of immune referees to search for human pancreatic islet cells and then produce TGF-Beta and CD25, molecules that can muzzle killer T cells.

They introduced the engineered referee cells into mice that had received a transplant of human islet cells, modeling the treatment for type 1 diabetes.

The referee cells found the vulnerable islet cells and stopped the killer T cells from attacking, and the islet cells survived.

"It would be life changing for people with type 1 diabetes if they could get new islet cells without needing to take immunosuppressants, and stop having to take insulin every day," said Audrey Parent, PhD, associate professor in the UCSF Diabetes Center and a co-senior author of the paper.

Lim envisions a future in which organ transplant patients, or those with autoimmune diseases, receive therapies that only treat the specific regions of the body where the immune system is misbehaving.

This could prevent the significant side effects from general immunosuppressants as well as the infections and cancers that arise when the immune system is disabled completely.

The new technology also could be used to finetune CAR T cell therapies for cancer, so these CAR T cells only attack tumors, and not healthy tissue.

"This puts so many more options on the table for dealing with some of the biggest challenges in medicine," said Lim, who directs the UCSF Cell Design Institute. "We hope this can benefit patients in the not-so-distant future."

Technology Networks, 6 December 2024

https://technologynetworks.com

'Breakthrough' dementia drug looks to stop disease in its tracks

2024-12-04

Filamon Limited, an Australian biotech company focused on developing next-gen anti-inflammatory drugs, has announced its breakthrough dementia treatment. ALPHA-003 is designed to preserve the integrity of vital brain cell structures and protect them against destruction caused by brain inflammation.

In healthy neurons, the tau protein stabilizes microtubules, crucial tube-like structures that, together with neurofilaments, maintain the neurons' shape and provide mechanical support. However, when it's modified, tau can form toxic aggregates – tangles that degrade these key structures. This is seen in a group of diseases called tauopathies, such as dementia, including Alzheimer's disease, and chronic traumatic encephalopathy (CTE).

Existing dementia treatments focus on reducing the consequences of this structural damage but have enjoyed only moderate success. Now, an Australian biotech company, Filamon Limited, has announced its breakthrough treatment, ALPHA-003, which is aimed at halting the progression of dementia by preventing microtubular destruction.

"The underlying problem with most forms of dementia is the destruction of a key structural component of brain cells known as microtubules," said Associate Professor Kieran Scott, Professor of Oncology at Western Sydney University, and co-founder of Filamon. "These long, hollow tubes are vital to healthy brain function. In dementia, these microtubules degrade, resulting in the death of brain cells.

"To date, no one has found a way of preventing microtubular destruction," Scott said. "We believe ALPHA-003 has the potential to be that first drug by stabilizing the two main brain cell components whose job is to protect microtubules from damage – tau and neurofilaments."

ALPHA-003 is designed to prevent damaging brain inflammation by binding to tau and neurofilaments, providing the microtubular protection that Scott is referring to. The result of deep-learning, computational drug design technology developed in Australia, ALPHA-003 started life as a more general anti-inflammatory drug, countering the effects of human group IIA secretory phospholipase A2 (hGIIA), a significant player in inflammatory conditions, before its developers realized its potential for treating neuroinflammation, specifically.

"ALPHA-003 was under development as a new form of anti-inflammatory drug that worked by blocking the activating effects of the key inflammatory ligand, hGIIA, on a range of cell structural proteins," Professor Graham Kelly, Filamon's co-founder, CEO, and Managing Director said in an interview with New Atlas. "Activation of those proteins underlies most chronic inflammatory changes. Recent published data has shown that tau is another structural protein that responds to hGIIA, so we simply asked the question whether ALPHA-003 would have the same protective effect on tau. Our studies showed that it does, to the extent of blocking the ability of tau to form sheets of oligomers that comprise the 'tau neurofibrillary tangles.'"

But it wasn't just the need to fill a treatment niche that drove the drug's development. Kelly explained to New Atlas that experiencing the devastating effects of dementia first-hand was also a motivating factor.

"The personal angle has been the confronting experience of seeing a very good friend who has always been a bundle of energy and force of nature deteriorate into a tragic, sunken, shell of a woman who has lost all recognition of friends and family," he said.

But does ALPHA-003 work? Pre-clinical studies strongly suggest that it does. Importantly, the drug has been found to cross the blood-brain barrier in mammals, meaning it can exert a direct effect on brain cells. The team at Filamon were so happy with the results that they announced them prior to journal publication.

"The announced news is literally freshly generated," Kelly told New Atlas. "We considered it to be of such importance to warrant being released pre-publication. More studies are underway, and the results of those studies will be the subject of journal submissions."

Kelly foresees ALPHA-003 being used to treat dementia at the time of diagnosis.

"We see dementia as a two-step process involving (i) creation of an ongoing neuroinflammatory trigger, and (ii) the consequences of that trigger," he told New Atlas. "ALPHA-003 is aiming at blocking the latter, but that requires accepting that the underlying neuroinflammation trigger continues unabated. ALPHA-003 simply is aiming to mitigate the effects of the trigger. Another Filamon experimental drug program underway with another drug technology aims to deactivate this trigger."

Filamon aims to have ALPHA-003 approved for clinical trial use in 2026. It's expected that the drug will treat tauopathies other than the two major forms of dementia – Alzheimer's disease and frontotemporal dementia – such as progressive supranuclear palsy, an uncommon Parkinson's-like disorder, and CTE, caused by repeated concussions.

New Atlas, 4 December 2024

https://newatlas.com

Incorrect pKa values have slipped into chemical databases and could distort drug design

2024-12-10

Inconsistencies have been uncovered in how acid dissociation constants for zwitterionic compounds are recorded in chemical databases, as well as how they are used in modelling.1 This could have a significant impact on areas like drug design or environmental chemistry where pKa values play a crucial role. 'We found that the ChEMBL database, one of the largest data repositories for biochemicals – and frequently used as a data corpus for training pKa models – includes many incorrect pKa values due to this nomenclature issue,' says Jonathan Zheng from the Massachusetts Institute of Technology who participated in the study.

The pKa of a molecule describes how that molecule behaves at different pH values, influencing important properties such as its solubility in water and other media or its ability to penetrate cell membranes. In pharmaceutical chemistry, this property can indicate whether a compound is suitable for medical applications or not. 'Drug molecules often form zwitterions – molecules that have distinct charged centres while being neutral overall,' explains Zheng. 'Our results could therefore help to avoid confusion during drug development efforts, as well as in the broader literature.'

Kai Leonhard from RWTH Aachen University in Germany, who wasn't involved in the research, agrees that the errors discovered by the US team might affect areas such as drug discovery. 'Candidates for new medicines, even if active in vitro, are screened with respect to several properties like their solubility in blood. So, it could happen that an effective drug candidate isn't brought into clinical studies just because the misinterpreted pKa data suggests it's not soluble in blood, although it actually is.'

The scientists realised that something was wrong when they weren't able to reconcile the values obtained from pKa prediction models with experimental data that had been previously compiled by the International Union of Pure and Applied and Chemistry (Iupac). After discovering the mismatch between experimental data and that on ChEMBL, Zheng and colleagues noticed that a popular machine-learning model called QupKake,2 which was trained on ChEMBL data, was less accurate for zwitterionic compounds too.

These discrepancies result from confusion about what the terms acidic and basic mean when describing pKa values, points out Zheng. He explains that for compounds that can form zwitterions, these designations are ambiguous because of the presence of different isomers (uncharged and dipolar) in solution.

'While it may seem simple to tell what a dissociation constant is, matters can become complex for molecules with multiple acidic and basic functional groups,' comments Leonhard. 'In this case, the pKa value of one group may depend on the protonation states of the others.'

That's why, decades ago, chemists thought it would be reasonable to label the lower pKa for zwitterion-forming compounds as acidic and the higher pKa values as basic, while the opposite convention is used for compounds that don't really form zwitterions, notes Zheng. But he adds that this difference in nomenclature isn't widely known, or if known, it isn't handled consistently. 'Modellers and data curators typically use one of these conventions, applying it broadly to all species, which leads to incorrect applications of the data.'

Zheng says that to fix this, data curators may have to re-examine many compounds for which errors have been identified and use more precise labels and metadata in future. He suggests avoiding the use of acidic or basic as pKa labels and either use pKa to only refer to acidic phenomena or use proton gain and proton loss instead. He also recommends introducing the tags 'macroscopic' and 'microscopic' whenever possible to indicate whether the reported pKa values refer to the ensemble of multiple isomeric forms of an acid or a specific isomer.

The magnitude of the mismatch between experimental data and modelling that has made its way into databases depends on the molecule and the type of error made. However, it can be significant. For example, the values the team calculated for glycine showed that modelling errors could put dissolved ion concentrations out by two orders of magnitude,

while errors where proton gain was used when the user wanted proton loss or vice versa led to values out by as much as five orders of magnitude.

'In general, we believe that researchers should spend more time in carefully examining and curating data for any chemical property,' concludes Zheng. 'Based on our experience, it is very likely that systematic issues are pervasive in other physicochemical property data as well.'

Chemistry World, 10 December 2024

https://chemistryworld.com

Hot Cocoa Could Protect Against the Vasculature Stress of Fatty Foods

2024-11-20

Food choices made during periods of stress can influence the effect of stress on cardiovascular health. For example, recent research from the University of Birmingham found that high-fat foods can negatively affect vascular function and oxygen delivery to the brain, meanwhile flavanol compounds found in abundance in cocoa and green tea can protect vascular function during periods of everyday stress.

Now, in a new study, the same research team has found that drinking cocoa high in flavanols in combination with a fatty meal can counteract some of the impact of fatty food and protect the vascular system from stress.

The research has been published today (18th November) in the journal Food and Function.

Dr Catarina Rendeiro, Assistant Professor in Nutritional Sciences at the University of Birmingham, and leading author said: "We know that when people are stressed, they tend to gravitate towards high-fat foods. We have previously shown that fatty food can impair the body's vascular recovery from stress. In this study, we wanted to see if adding a high-flavanol food to the fatty meal would alleviate the negative impact of stress in the body"

Rosalind Baynham, first author on the paper, explained: "Flavanols are a type of compound that occur in different fruits, vegetables, tea and nuts including berries and unprocessed cocoa. Flavanols are known to have health benefits, particularly for regulating blood pressure and protecting cardiovascular health.

"We took a group of young healthy adults and gave them two butter croissants with 10 g salted butter, 1.5 slices of cheddar cheese and 250 ml whole milk as breakfast, and either a high-flavanol cocoa or a low-flavanol cocoa drink. Following a rest period, we asked the participants to complete a mental maths test which increased in speed for eight minutes, alerting them when they got an answer wrong. During the 8 minute rest period and 8 minute mental maths test, we measured forearm blood flow, cardiovascular activity and prefrontal cortex (PFC) tissue oxygenation. We also measured vascular function using Brachial Flow-mediated dilatation (FMD), which is a prognostic measure for future risk of cardiovascular disease. This stress task induced significant increases in heart rate and blood pressure, similar to the stress you may encounter in daily life."

The cocoa beverages were prepared by dissolving 12 g cocoa powder into 250 ml of whole milk. The low-flavanol powder was an alkalized cocoa powder which was processed to reduce total flavanols to 5.6 mg per serving; and the high-flavanol cocoa powder was a non-alkalized powder, delivering 695.0 mg total flavanols per serving. Alkalization is a process typically used in chocolate making to enhance flavour, but unfortunately it reduces the amount of flavanols.

The team confirmed that consuming fatty foods with the low-flavanol drink when mentally stressed reduced vascular function (by 1.29% FMD) and lasted up to 90 minutes after the stressful event was over. The findings also showed that the cocoa drink high in flavanols was effective at preventing the decline in vascular function following stress and fat consumption. Brachial flow-mediated dilatation was significantly higher following high-flavanol cocoa compared to low-flavanol cocoa 30 and 90 minutes after the stressful period. The team had also found in their previous work, that eating high-fat foods attenuated cerebral oxygenation in the pre-frontal cortex, during stress. However, cocoa flavanols did not improve cerebral oxygenation or impact mood.

Dr Catarina Rendeiro, Assistant Professor in Nutritional Sciences at the University of Birmingham, added: "This research shows that drinking or eating a food high in flavanols can be used as a strategy to mitigate some of the impact of poorer food choices on the vascular system. This can help us make more informed decisions about what we eat and drink during stressful periods."

In the supermarket look for a minimally processed cocoa powder, and if cocoa isn't quite your beverage of choice, there are other ways you can get a higher dose of flavanols, such as green tea, black tea and berries. Recent

published guidelines for flavanol intake recommend between 400 to 600 mg/day, which can be achieved for example, by consuming two cups of black or green tea, or a combination of berries, apples and high-quality cocoa.

Jet Veldhuijzen van Zanten, Professor of Biological Psychology at the University of Birmingham, and author of this paper added: "Modern life is stressful and the impact of stress on our health and the economy has been well documented, so any changes we can make to protect ourselves from some of the symptoms of stress is positive. For those who tend to reach for a treat when stressed or depend on convenient food because they work high-pressure jobs or are time-poor, incorporating some of these small changes could make a real difference."

Technology Networks, 20 November 2024

https://technologynetworks.com

Catalyst 'breathes' new life into acrylonitrile production

2024-12-12

A team of engineers is reimagining one of the essential processes in modern manufacturing. Their goal? To transform how a chemical called acrylonitrile (ACN) is made—not by building world-scale manufacturing sites, but by using smaller-scale, modular reactors that can work if they let the catalyst, in a sense, "breathe."

Their article, titled "Propene Ammoxidation over an Industrial Bismuth Molybdate-Based Catalyst Using Forced Dynamic Operation," is published in Applied Catalysis A: General.

ACN is everywhere, from carbon fibers in sports equipment to acrylics in car parts and textiles. Traditionally, producing it requires a continuous, energy-intensive process. But now, researchers at the University of Virginia and the University of Houston have shown that by pausing to "inhale" fresh oxygen, a chemical catalyst can produce ACN more efficiently. This discovery could open the door to smaller, versatile production facilities that adapt to fluctuating needs.

William Epling, a professor and chair of the Department of Chemical Engineering at UVA, calls the technique "forced dynamic operation," or FDO. Picture a machine cycling through work and rest periods, using short breaks to recharge and perform at its best.

This is what Epling's team has done with an industrial bismuth molybdate-based catalyst, alternating between two phases: one containing the full mixture of ingredients needed to make ACN, and another containing only oxygen. This rhythmic approach allows the catalyst to regenerate its lattice oxygen—the source of the key reactant in driving the transformation into ACN.

"FDO is essentially like giving the catalyst a breather, letting it work harder and more effectively in each cycle," said Zhuoran Gan, a Ph.D. candidate in Epling's lab. When the catalyst "rests" with just oxygen, it regains strength to tackle the next cycle of production. The results were surprising: ACN production was exceeded by as much as 30% over traditional, continuous methods.

The impact could be transformative. Smaller production facilities that use this method could meet the demand for ACN growth without the need for world-scale, capital-intensive plants. Such facilities could also operate closer to end-users, like manufacturers of high-performance carbon fibers, reducing transportation costs and making production more adaptable.

Epling envisions a future where chemical manufacturing can be more flexible and efficient, with small, scalable production units that meet demand exactly where and when it arises.

The UVA team's work underscores how sometimes, a catalyst just needs a breath of fresh air to become a powerful tool for innovation.

Phys Org, 12 December 2024

https://phys.org

Novel zeolite structure demonstrates superior heavy oil cracking efficiency

2024-12-12

Researchers have developed a new aluminosilicate zeolite, ZMQ-1, which features a unique intersecting meso-microporous channel system that is expected to enhance catalytic processes in the petrochemical industry.

The study, published in Nature, highlights ZMQ-1 as the first aluminosilicate zeolite with interconnected intrinsic 28-ring mesopores. This breakthrough overcomes long-standing challenges related to zeolite pore size limitation, stability, and catalytic efficiency.

Curiosities

DEC. 13, 2024

Zeolites are crystalline materials renowned for their applications in ion exchange, adsorption, and catalysis. However, their microporous structure limits their use in processing larger molecules. Researchers have addressed this limitation by developing a zeolite with intrinsic mesopores—pores larger than 20 Å—while maintaining stability and acidity.

Previous attempts to create mesoporous zeolites faced challenges such as structural instability and reduced acidity, making them unsuitable for industrial applications. However, the newly developed ZMQ-1 has shown the potential to address these issues.

The researchers employed a phosphonium-based organic structure-directing agent (OSDA), which was instrumental in forming the mesoporous framework. Compared to traditional ammonium-based OSDAs, this phosphonium-based OSDA possesses a stronger positive charge and greater stability, enabling the synthesis of stable mesoporous structures.

The crystallization of ZMQ-1 was achieved through hydrothermal synthesis with tunable silicon-to-aluminum (Si/Al) ratios, allowing for customization in specific applications.

"ZMQ-1 is the first aluminosilicate zeolite with an intrinsic meso-microporous channel system," said co-corresponding author Prof. Lu Peng from the Qingdao Institute of Bioenergy and Bioprocess Technology (QIBEBT) of the Chinese Academy of Sciences. "Unlike previously reported mesoporous materials that often lacked structural stability after the removal of organic templates, the interconnected 28-ring channels in ZMQ-1 mark a significant advancement in zeolite design."

The unique structure of ZMQ-1 was elucidated using three-dimensional electron diffraction (3D ED) and scanning transmission electron microscopy (STEM). The analysis revealed that the 28-ring mesopores were interconnected by 10-ring microporous windows, forming an efficient channel system.

This design enables the diffusion of both large and small molecules, addressing the diffusion limitations of traditional zeolites. Consequently, ZMQ-1 proves particularly effective for catalytic cracking of heavy oil.

To evaluate the performance of ZMQ-1, the researchers conducted catalytic cracking experiments with vacuum gasoil (VGO), an essential feedstock in petroleum refining. The results showed that ZMQ-1 achieved a high VGO conversion rate comparable to commercial USY and Beta

zeolites. Moreover, it significantly outperformed MCM-41, a well-known mesoporous molecular sieve, in both conversion efficiency and stability.

Notably, phosphorus-containing ZMQ-1 demonstrated twice the selectivity for diesel production and significantly reduced coke formation compared to its commercial counterparts. This combination of higher diesel yield and lower coke generation resulted in an impressive overall fuel selectivity (gasoline and diesel combined) of 80%, a marked improvement over conventional zeolites.

These results highlight the ability of phosphorus-containing ZMQ-1 to efficiently convert heavy hydrocarbons into valuable fuels, leveraging its unique meso-microporous structure to maximize the yield of target products while minimizing undesirable by-products.

With its demonstrated potential in catalytic applications, ZMQ-1 represents a breakthrough in developing more efficient and sustainable chemical processes. By overcoming persistent challenges in zeolite research, such as pore size limitations and structural stability, ZMQ-1 creates new opportunities for applications in heavy oil cracking and green energy conversion.

Phys Org, 12 December 2024

https://phys.org

From sunlight to hydrogen: Researchers unveil structure of photosynthetic catalyst

2024-12-12

Photosynthesis is one of the most efficient natural processes for converting light energy from the sun into chemical energy vital for life on earth. Proteins called photosystems are critical to this process and are responsible for the conversion of light energy to chemical energy.

Combining one kind of these proteins, called photosystem I (PSI), with platinum nanoparticles, microscopic particles that can perform a chemical reaction that produces hydrogen—a valuable clean energy source—creates a biohybrid catalyst. That is, the light absorbed by PSI drives hydrogen production by the platinum nanoparticle.

In a recent breakthrough, researchers at the U.S. Department of Energy's (DOE) Argonne National Laboratory and Yale University have determined the structure of the PSI biohybrid solar fuel catalyst. Building on more than 13 years of research pioneered at Argonne, the team reports the first high-

resolution view of a biohybrid structure, using an electron microscopy method called cryo-EM.

The results of the research were published in Nature Communications.

With structural information in hand, this advancement opens the door for researchers to develop biohybrid solar fuel systems with improved performance, which would provide a sustainable alternative to traditional energy sources.

PSI is a large protein complex that is found in plants, algae and photosynthetic bacteria. This protein plays a critical role in capturing and converting sunlight into energy.

Uniquely, PSI is able to very efficiently convert sunlight into energy—for every one photon that is absorbed by the protein, one electron is almost always generated. These electrons can then be transferred to the bound platinum nanoparticles of the biohybrid, which facilitates the production of hydrogen gas.

In earlier work, Argonne chemist Lisa Utschig was able to use PSI to manipulate photosynthesis and produce hydrogen fuel. Now, she and her team have been able to see the structure of the PSI biohybrid in detail. "It's been really exciting to now directly look at the system we've worked at for 13 years," Utschig said.

Although a few studies have explored the properties of PSI biohybrid catalysts, researchers have not known where the platinum nanoparticles attach to the protein. Using high-resolution cryo-EM, the researchers were able to more thoroughly study the structure of the biohybrid and found exactly where the nanoparticles bind to PSI.

"We assumed the nanoparticles were binding where PSI's electron transfer partners connect," Utschig said. "But the structure shows there's actually two sites. And that was very much a surprise."

With this structural information, researchers can now begin to optimize how the nanoparticles attach and interact to further enhance catalytic efficiency. They can engineer the biohybrid by altering the protein properties and by adjusting the nanoparticles.

"It's amazing to see bioenergy at the molecular level and to see how a man-made particle and a natural protein come together to create energy," said Utschig.

Other contributors to this work include Christopher J. Gisriel, Tirupathi Malavath, Tianyin Qiu, Jan Paul Menzel, Victor S. Batista and Gary W. Brudvig.

Phys Org, 12 December 2024

https://phys.org

Faster organic phosphorescence for better display tech

2024-12-09

Screens for TVs, smartphones or other displays could be made with a new kind of organic LED material developed by an international team, co-led by University of Michigan engineers. The material maintains sharp color and contrast while replacing the heavy metal with a new hybrid material.

Curiously, the material also seemed to break a quantum rule.

OLED devices currently on the market include heavy metal components like iridium and platinum, which improve the efficiency, brightness and color range of the screen. But they come with drawbacks -- significantly higher cost, a shorter device lifetime and increased health and environmental hazards.

In OLEDs, light emission through the more energy-efficient phosphorescence is preferred over fluorescence, but phosphorescence happens more slowly, taking milliseconds or longer without the heavy metal component. Speeding up phosphorescence to happen in microseconds is necessary to keep up with modern displays, which operate at 120 frames per second, without producing a lingering "ghost" image. This is a key role of the heavy metals.

"We found a way to make a phosphorescent organic molecule that can emit light on the microsecond scale, without including heavy metals in the molecular framework," said Jinsang Kim, U-M professor of materials science and engineering and co-corresponding author of the study published in Nature Communications.

Dong Hyuk Park, professor of chemical and biomedical science and engineering at Inha University, and Sunkook Kim, professor of advanced materials science and engineering at Sungkyunkwan University, both in the Republic of Korea, are also co-corresponding authors.

The speed difference between fluorescence and phosphorescence is driven by what happens after electrons from the electrical current running

through the OLED material slide into the high energy level within the molecule's available electron orbitals, known as an excited state -- sort of like jumping onto a rung of a ladder. In fluorescence, they can immediately release the energy as light, jumping back down to the ground state. But in phosphorescence, they have to make a conversion first.

The conversion has to do with the electron's spin. Each electron has a partner in its ground state, and a quantum mechanical rule -- Pauli Exclusion Principle -- demands that they spin in opposite directions. But when an electron slides into that higher rung, it can end up spinning in either direction because each electron is now alone in its orbital. It only remains opposite its partner a quarter of the time, and this is the case that results in fluorescence.

Phosphorescence is three times more efficient because it harnesses the other 75% of excited electrons too, but it requires the electron to flip its spin before it can come back down. In conventional phosphorescent materials, the large atomic nucleus of the heavy metal generates a magnetic field that forces the same spin direction excited electron to turn quickly, resulting in faster light emission as it returns to its ground state.

The new material positions a 2D layer of molybdenum and sulfur near a similarly thin layer of the organic light emitting material, achieving the same effect by physical proximity without any chemical bonding. This hybrid construction sped up light emission by 1,000 times, achieving speeds fast enough for modern displays.

Light emission happens entirely within the organic material without having the weak metal-organic ligand bonding, helping the material last longer. Phosphorescent OLEDs that rely on heavy metals also use the metals to help produce the color, and the weaker chemical bonds between the metal and organic material can break apart when two excited electrons come into contact, dimming out the pixel.

Pixel burnout is a particular problem for high energy blue light that has yet to be solved, but the research team hopes their new design approach can help work towards stable, blue phosphorescent pixels. Current OLEDs use phosphorescent red and green pixels and fluorescent blue pixels, avoiding blue pixel burnout at the expense of lower energy efficiency.

Beyond the potential applications, analysis of this molecular hybrid system measured something once thought to be impossible -- paired electrons sharing an orbital seemed to have a combined spin under dark conditions,

suggesting a forbidden 'triplet' state when instead their spins should cancel one another out.

"We don't yet fully understand what causes this triplet character in the ground state because this violates the Pauli Exclusion Principle. That is very impossible, but looking at the measurement data, yes, that seems to be the case," Kim said. "That's why we have a lot of questions about what really makes that happen."

The research team will explore how the material achieves triplet character ground states while also pursuing potential spintronics device applications.

The team has applied for patent protection with the assistance of U-M Innovation Partnerships and is seeking partners to create devices using this new type of material.

This work was supported by the National Research Foundation of Korea grant funded by the Korea government and START grant from the U-M College of Engineering.

Collaborators from the University of California, Berkeley and Dongguk University contributed to the study. Jinsang Kim is also a director of academic programs for macromolecular science and engineering and a professor of chemistry.

Science Daily, 9 December 2024

https://scienecedaily.com

MIT Unveils a Biodegradable Alternative to Microplastic Beads

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MIT researchers have developed an environmentally friendly alternative to the harmful microbeads used in some health and beauty products.

These new polymers break down into harmless sugars and amino acids and could also encapsulate nutrients for food fortification, showing promise in both cosmetic and nutritional applications.

Biodegradable Solutions by MIT

Microplastics are tiny plastic particles that pose a major environmental threat and are found almost everywhere on Earth. They come from the breakdown of everyday items like tires, clothing, and plastic packaging.

Another key source is the tiny plastic beads commonly added to cleansers, cosmetics, and other beauty products.

To tackle this growing problem, chemical engineers at MIT have developed biodegradable materials designed to replace these plastic beads in beauty products. These eco-friendly polymers naturally break down into safe byproducts like sugars and amino acids.

The Importance of Future-Focused Solutions

"One way to mitigate the microplastics problem is to figure out how to clean up existing pollution. But it's equally important to look ahead and focus on creating materials that won't generate microplastics in the first place," says Ana Jaklenec, a principal investigator at MIT's Koch Institute for Integrative Cancer Research.

These particles could also find other applications. In the new study, Jaklenec and her colleagues showed that the particles could be used to encapsulate nutrients such as vitamin A. Fortifying foods with encapsulated vitamin A and other nutrients could help some of the 2 billion people around the world who suffer from nutrient deficiencies.

Jaklenec and Robert Langer, an MIT Institute Professor and member of the Koch Institute, are the senior authors of the paper, which was published on December 6 in Nature Chemical Engineering. The paper's lead author is Linzixuan (Rhoda) Zhang, an MIT graduate student in chemical engineering.

Research and Development Challenges

In 2019, Jaklenec, Langer, and others reported a polymer material that they showed could be used to encapsulate vitamin A and other essential nutrients. They also found that people who consumed bread made from flour fortified with encapsulated iron showed increased iron levels.

However, since then, the European Union has classified this polymer, known as BMC, as a microplastic and included it in a ban that went into effect in 2023. As a result, the Bill and Melinda Gates Foundation, which funded the original research, asked the MIT team if they could design an alternative that would be more environmentally friendly.

Innovative Material Design

The researchers, led by Zhang, turned to a type of polymer that Langer's lab had previously developed, known as poly(beta-amino esters). These polymers, which have shown promise as vehicles for gene delivery and

other medical applications, are biodegradable and break down into sugars and amino acids.

By changing the composition of the material's building blocks, researchers can tune properties such as hydrophobicity (ability to repel water), mechanical strength, and pH sensitivity. After creating five different candidate materials, the MIT team tested them and identified one that appeared to have the optimal composition for microplastic applications, including the ability to dissolve when exposed to acidic environments such as the stomach.

Nutrient Protection and Delivery

The researchers showed that they could use these particles to encapsulate vitamin A, as well as vitamin D, vitamin E, vitamin C, zinc, and iron. Many of these nutrients are susceptible to heat and light degradation, but when encased in the particles, the researchers found that the nutrients could withstand exposure to boiling water for two hours.

They also showed that even after being stored for six months at high temperature and high humidity, more than half of the encapsulated vitamins were undamaged.

Potential in Food Fortification

To demonstrate their potential for fortifying food, the researchers incorporated the particles into bouillon cubes, which are commonly consumed in many African countries. They found that when incorporated into bouillon, the nutrients remained intact after being boiled for two hours.

"Bouillon is a staple ingredient in sub-Saharan Africa, and offers a significant opportunity to improve the nutritional status of many billions of people in those regions," Jaklenec says.

In this study, the researchers also tested the particles' safety by exposing them to cultured human intestinal cells and measuring their effects on the cells. At the doses that would be used for food fortification, they found no damage to the cells.

Safety and Efficacy in Cleansing Applications

To explore the particles' ability to replace the microbeads that are often added to cleansers, the researchers mixed the particles with soap foam. This mixture, they found, could remove permanent marker and waterproof eyeliner from skin much more effectively than soap alone.

Soap mixed with the new microplastic was also more effective than a cleanser that includes polyethylene microbeads, the researchers found. They also discovered that the new biodegradable particles did a better job of absorbing potentially toxic elements such as heavy metals.

"We wanted to use this as a first step to demonstrate how it's possible to develop a new class of materials, to expand from existing material categories, and then to apply it to different applications," Zhang says.

Ongoing Research and Future Directions

With a grant from Estée Lauder, the researchers are now working on further testing the microbeads as a cleanser and potentially other applications, and they plan to run a small human trial later this year. They are also gathering safety data that could be used to apply for GRAS (generally regarded as safe) classification from the U.S. Food and Drug Administration and are planning a clinical trial of foods fortified with the particles.

The researchers hope their work could help to significantly reduce the amount of microplastic released into the environment from health and beauty products.

"This is just one small part of the broader microplastics issue, but as a society we're beginning to acknowledge the seriousness of the problem. This work offers a step forward in addressing it," Jaklenec says. "Polymers are incredibly useful and essential in countless applications in our daily lives, but they come with downsides. This is an example of how we can reduce some of those negative aspects."

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