# Bulletin Board

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

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## **Regulatory Update**

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### **ASIA PACIFIC**

#### Australia has completed the transition to GHS 7

#### 2023-06-28

GHS 7 is now the only system to classify newly manufactured and imported hazardous chemicals and prepare their labels and safety data sheets (SDS) across Australia.

Thank you to all manufacturers and importers of hazardous chemicals for adopting GHS 7 over the transition period. This change will ensure that labels and SDS use up-to-date hazard classification and communication, and align Australia with our key international trading partners.

Safe Work Australia has updated the Model Code of Practice: Managing risks of hazardous chemicals in the workplace, Model Code of Practice: Labelling of workplace hazardous chemicals, Model Code of Practice: Preparation of a safety data sheets for hazardous chemicals and the Classifying hazardous chemicals – National guide, as well as other fact sheets on hazardous chemicals to reflect Australia's adoption of GHS 7.

For more information visit. https://www.safeworkaustralia.gov.au/safetytopic/hazards/chemicals/classifying-chemicals/transition-ghs7

#### Safe Work Australia, 28-06-23

https://www.safeworkaustralia.gov.au/safety-topic/hazards/chemicals/ classifying-chemicals/transition-ghs7

#### Notice of completed evaluations - 29 June 2023

#### 2023-06-29

We have published 18 evaluations about the human health and environmental risks associated with the use of certain chemicals on the Australian Inventory of Industrial Chemicals (Inventory). The status of these evaluations has been updated in our Rolling Action Plan.

These evaluations are issued by the AICIS Executive Director under section 78 of the Industrial Chemicals Act 2019 and are listed below. The draft versions of these evaluation statements were open for public consultation that closed on the 19th of May 2023 (for 17 Evaluations) and on the 7th of December 2022 (for EVA00091).

# **Regulatory Update**

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| ID       | Subject of evaluation                                      | CAS<br>number                  | Public<br>comment<br>received | Public  | Evaluation<br>outcome                                  |
|----------|--|--------------------------------|-------------------------------|---|--|
| EVA00041 |  | 13560-89-9                     | No                            | -   |  |
| EVA00091 | 1-methoxy-<br>4-(2-<br>propenyl)<br>benzene<br>(estragole) | 140-67-0                       | Yes –<br>hazard               | A variation<br>to the<br>evaluation<br>statement<br>was<br>required.<br>The<br>evaluation<br>statement<br>has been<br>amended<br>to include |  |
| EVA00093 | Chemicals<br>not<br>considered                             | See<br>evaluation<br>statement | No                            | -   | No new<br>means of<br>managing<br>risk are<br>proposed |
| EVA00096 |  | 100-52-7                       | No                            | -   |  |

#### Read More

AICIS, 29-06-23

https://www.industrialchemicals.gov.au/news-and-notices/noticecompleted-evaluations-29-june-2023

#### China to Revise the Rules for Classification and **Labelling of Chemicals**

#### 2023-06-29

On June 14, China Ministry of Industry and Information Technology (MIIT) has opened up a public consultation on GB 30000.1 Rules for classification and labelling of chemicals - Part I: General specifications. Comments are welcomed before August 15, 2023.

GB 30000.1 is to replace GB 13690-2009 - General rule for classification and hazard communication of chemicals. After the standard takes effect, the chemical classifications in China will more align the UN GHS Rev. 8.

GB 30000.1 comprises of six parts, these are:

Part I Scope



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- Part II Normative References
- Part III Terms & Definitions
- Part IV Classification
- **Part V** Hazard Communication: Labels
- Part VI Hazard Communication: SDS

#### Part I prescribes the scope of application.

- Pharmaceuticals, food additives, cosmetics, and pesticide residues in food are not subject to label requirements in GB 30000.1 when ingested intentionally. However, if workers are likely to be exposed to or will potentially contact these substances during transportation, then GB 30000.1 prevails. Where there are other provisions stipulated by laws and regulations, those provisions shall apply.
- Labels in the package shall give priority to the requirements of the Recommendations on the Transport of Dangerous Goods, Model Regulations (hereinafter referred to as the "Model Regulations").

#### Read More

CIRS, 29-06-23

https://www.cirs-group.com/en/chemicals/china-to-revise-the-rules-forclassification-and-labelling-of-chemicals

### AMERICA

#### MAINE AMENDS PFAS REPORTING, INCLUDING START DATE

#### 2023-06-09

On June 8, the Maine Legislature passed "An Act to Support Manufacturers" Whose Products Contain Perfluoroalkyl and Polyfluoroalkyl Substances." This Act provides amendments to the PFAS reporting law originally passed in July 2021 as Public Law c. 477, An Act To Stop Perfluoroalkyl and Polyfluoroalkyl Substances Pollution. This Law received numerous comments from all over the consumer product industry via public hearings on rulemakings and the proposed amendments process. Most notably, the amendment pushes the reporting start date out to January 1, 2025.

#### Amendments to the Law:

## **Regulatory Update** Start date moves back to January 1, 2025 (was originally January 1,

- 2023)
- Changes reporting requirements (new parts underlined):
- Brief description of the product;

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- Estimate of total number of units sold annually in the State or nationally;E
- urpose of the use of PFAS in any product component;
- Amount of each of the PFAS in the product,

- Each PFAS listed by its chemical abstracts service registry (CAS) number or, in the absence of this number,

a description approved by the department,

- Reported as an exact quantity, or as the amount of total organic fluorine if the amount of each

PFAS compound is not known;

- Quantities determined using commercially available analytical methods or based on information

provided by a supplier as falling within a range approved for reporting purposes by the department;

- Name and address of the manufacturer, and the name, address and phone number of a contact person for the manufacturer; and
- Any additional information established by department rule as necessary to implement the requirements.
- Requirements no longer apply to companies that have 25 employees or less.
- Clarifies packaging that is exempt and notes that if packaging is the product being manufactured it is not exempt.

#### Read More

Bureau Veritas, 09-06-23

https://www.cps.bureauveritas.com/newsroom/maine-amends-pfasreporting-including-start-date



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## **Regulatory Update**

### MINNESOTA SIGNS LEAD AND CADMIUM BILL INTO LAW

#### 2023-06-05

Minnesota has enacted Chapter 60 – H.F. No. 2310 into law. As part of the Environmental Omnibus bill it establishes lead and cadmium requirements for certain consumer products under section 24 – Lead and Cadmium in Consumer Products: Prohibition. These requirements become effective August 1, 2023.

#### **Product Scope**

A person must not import, manufacture, sell, hold for sale, or distribute or offer for use in the state of Minnesota any of the following covered products containing lead or cadmium exceeding the limits established by the state:

- Jewelry
- Toys
- Cosmetics and personal care products
- Puzzles, board games, card games, and similar games
- Play sets and play structures
- Outdoor games
- School supplies
- Pots and pans
- Cups, bowls, and other food containers
- Craft supplies and jewelry-making supplies
- Chalk, crayons, paints, and other art supplies
- Fidget spinners
- Costumes, costume accessories, and children's and seasonal party supplies
- Keys, key chains, and key rings,
- Clothing, footwear, headwear, and accessories

#### Limits

- No more than 90 ppm (0.009%) total lead, and
- No more than 75 ppm (0.0075%) total cadmium

The requirements do not apply to the above products if preempted by federal law.

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# **Regulatory Update**

When requested, must furnish to the commissioner or attorney general any relevant information or documentation that is available or that can be reasonably obtained to show compliance with the requirement.

#### Read More

JUL. 07, 2023

Bureau Veritas, 05-06-23

https://www.cps.bureauveritas.com/newsroom/minnesota-signs-lead-and-cadmium-bill-law

# Regulators announce stricter rules for trains carrying hazardous materials

#### 2023-06-25

Nearly four months after a train carrying hazardous materials derailed in Ohio, federal officials are proposing a requirement for railroads to maintain real-time updates about hazmat shipments that can be accessed by first responders.

The U.S. Department of Transportation's Pipeline and Hazardous Materials Safety Administration announced the proposed regulation on Wednesday, hoping to prevent environmental impacts from crashes and improve public safety.

"When railroads transport hazardous materials, they must do so safely and responsibly," Transportation Secretary Pete Buttigieg said in a press release. "Our proposal would improve rail safety and help protect communities across the country by requiring railroads to maintain detailed, real-time information about trains carrying hazardous materials."

The regulation would require railroads to proactively provide information about hazardous materials to local first responders as soon as it is aware of any accident. The real-time information would include the quantity and position of shipments, details on origin and destination and a designated emergency contact.

"On-demand access to key information about hazmat shipments coupled with proactive information sharing will enable first responders to better prepare for the risks present at the scene of an incident before they arrive on scene," PHMSA Deputy Administrator Tristan Brown said in the release. "This will improve safety for firefighters and first responders, and the communities they so courageously serve."



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## **Regulatory Update**

#### Read More

Courthouse News, 25-06-23

https://www.courthousenews.com/regulators-announce-stricter-rules-fortrains-carrying-hazardous-materials/

#### EPA Requests Comments for Implementation of PRIA **5 Bilingual Labeling Requirements for Agricultural Pesticides**

#### 2023-06-29

On June 20, 2023, the U.S. Environmental Protection Agency (EPA) announced that it is seeking input from stakeholders on ways to make bilingual pesticide labeling accessible to farmworkers and to implement a plan to ensure that farmworkers have access to the bilingual pesticide labeling by December 2025, as required by the Pesticide Registration Improvement Act of 2022 (PRIA 5). 88 Fed. Reg. 39845. PRIA 5 requires EPA to begin to seek stakeholder input on ways to make bilingual pesticide labeling accessible to farmworkers by June 30, 2023. Comments are to be submitted in docket EPA-HQ-OPP-2023-0270 and are due on or before August 21, 2023.

PRIA 5, enacted on December 29, 2022, amended the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) requiring Spanish language translation for sections of the end-use pesticide product labels where translation is available in the EPA Spanish Translation Guide for Pesticide Labeling. According to EPA, the Spanish Translation Guide for Pesticide Labeling contains translations of the health and safety portions of pesticide product labels. The Spanish Translation Guide for Pesticide Labeling is available here. Specifically, it has Spanish translations of the following statements:

- "Keep out of reach of children";
- **Restricted Use Pesticide Statements;**
- Signal Word;
- First Aid; ٠
- Precautionary Statements;
- Personal Protective Equipment;
- Misuse Statement; and
- Storage and Disposal Instructions Statements.

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## **Regulatory Update**

The Spanish Translation Guide for Pesticide Labeling also has examples of pesticide product label language for the agricultural use requirements section that includes restricted entry interval information and precautionary statements.

#### Read More

FIFRA Blog, 29-06-23

https://pesticideblog.lawbc.com/entry/epa-requests-comments-forimplementation-of-pria-5-bilingual-labeling-requirements-for-agriculturalpesticides

#### FPF comments on US EPA draft plastics strategy 2023-06-23

Members of the Food Packaging Forum (FPF) submitted feedback highlighting aspects of food packaging and chemical safety for the US Environmental Protection Agency (EPA) to consider during development of the draft national strategy to prevent plastic pollution. A shortened version of the comment follows.

Plastic packaging makes up 28% of municipal solid waste in the US (according to EPA figures from 2018), and food packaging strongly contributes to plastic pollution (FPF reported). The creation of a plastics strategy is therefore an important opportunity for effective measures to curtail problematic food packaging.

FPF research has demonstrated 509 chemicals in repeat-use FCMs made of plastic, and 853 chemicals in recycled PET FCMs (FPF reported). Some of these chemicals and chemical families are known to create long term effects that add up to potentially billions of dollars in public health costs (FPF reported also here).

#### Read More

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FPF, 26-06-23

https://www.foodpackagingforum.org/news/fpf-comments-on-us-epadraft-plastics-strategy



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## **Regulatory Update**

JUL. 07, 2023

### **EUROPE**

#### EU proposes comprehensive new outlook on threats of climate change and environmental degradation on peace, security and defence

#### 2023-06-28

Today, the European Commission and the High Representative adopted a Joint Communication laying out how the EU will address the growing impact of climate change and environmental degradation in the fields of peace, security, and defence.

Recurrent climate extremes, rising temperatures and sea levels, desertification, water scarcity, threats to biodiversity, environmental pollution and contamination are threatening the health and well-being of humanity, and can create greater displacement, migratory movements, pandemics, social unrest, instability and even conflicts. Europe's armed forces are also confronted with the changing and challenging operational conditions due to climate change. These new threats have already prompted allies and partners to update their policies too.

The Joint Communication offers a new outlook and sets the EU framework for responding to these challenges as they regard our society and our security operations, as well as the intensifying geopolitical competition for the resources and technologies necessary for the green transition.

New outlook on the climate and security nexus

With this Joint Communication, the EU aims to better integrate the climate, peace and security nexus in the EU's external policies, with a set of concrete actions across the entire spectrum of data, policies, missions, defence, and cooperation with third partners to ensure that the impacts are accounted for at all levels of external policymaking, planning and operations. It sets out the EU's plan for the Union and its partners to become more resilient and secure as the climate crisis intensifies, and improves connections between different policies to ensure that external action and capabilities are fit to tackle these challenges.

The Joint Communication sets out four main priorities:

Strengthening planning, decision-making and implementation, through reliable and accessible evidence-based analysis on the climate and security nexus;

# **Regulatory Update**

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- Operationalising the response to climate and security challenges in EU external action, inter alia through integrating the climate and security nexus in regional and national conflict analyses;
- Enhancing the climate adaptation and mitigation measures of Member States' civilian and military operations and infrastructure to lower costs, carbon footprints, while ensuring that operational effectiveness is maintained;
- Reinforcing international partnerships through multilateral fora and with partners such as NATO, in line with the EU's climate change and environment agenda.

#### Read More

#### FPF, 29-06-23

https://ec.europa.eu/commission/presscorner/detail/en/ip\_23\_3492

#### **Report highlights needs for reuse systems, consumer** demand grows

#### 2023-06-29

A report published on June 16, 2023, by UK-based civil society organization City to Sea outlines how innovations in packaging could improve reuse systems on the market. Specifically, City to Sea cited consumer confusion surrounding refill and reuse options as a driving factor in conducting the research that went into this report.

The goal of the project was to provide recommendations for brands and retailers on maximizing the potential of reusable packaging. Specifically, by identifying consumer groups most likely to change their behavior and facilitating a trial of prefilled returnable packaging.

Three crucial factors for turning intention into reality were identified: (i) a convenient and frictionless user experience, (ii) price parity with existing options, and (iii) receptive demographics. The three main consumer groups ready to adopt reuse extensively make up over three-quarters of the population (FPF reported).

The text discusses the significant opportunity for refillable, reusable, and returnable packaging with insights from behavior-change consultants, campaigners, supply chain specialists, retail brands, and grocery brands in the UK.

Other efforts in the sustainable packaging world have often focused on recycling and reducing single-use packaging rather than rethinking



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## **Regulatory Update**

packaging circulation (FPF reported and here). Overcoming structural barriers such as commercial viability, packaging standardization, and industrial standards for cleaning reusable packaging is necessary to enable efficient reuse systems. Existing research has identified gaps between consumer perceptions and behaviors, as well as the need to balance factors like convenience, cost, and product availability (FPF reported and here). But the demand for reusable packaging exists, and consumers are expressing frustration over the lack of provisions in place, according to the report.

News outlet Circular reported on June 16, 2023, that the Chartered Institution of Waste Management (CIWM) together with ResourceFutures, has urged the UK to take the lead in adopting reuse and refill packaging systems to establish a circular economy. They recommend a long-term strategy to bridge the policy gap on reuse, extending beyond consumer packaging to various sectors. In a policy comment, CIWM emphasized the need to reduce overall material consumption and consider end-of-life pathways. They also stressed cautious design and adequate support for regulators and local authorities. Furthermore, the organization urges the government and stakeholders to prioritize reuse for waste reduction and plastic pollution prevention.

#### Read More

FPF, 29-06-23

https://www.foodpackagingforum.org/news/report-highlights-needs-forreuse-systems-consumer-demand-grows

### **INTERNATIONAL**

#### How to avoid the next PFAS crisis

2023-06-29

About a decade ago, researchers at the German Environment Agency noticed a hole in chemical regulation.

There was lots of talk about protecting people from chemicals that build up in the human body. "But what is there that protects water?" Sarah Hale, an environmental chemist from the German Water Center, remembers discussing with colleagues.

Questions like hers sparked a movement to regulate chemicals based partly on their mobility, meaning their ability to move easily with water.

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Such substances escape most traditional water purification. If they're also slow to break down, that means they'll build up in the water supply, where many can cause health problems for humans and ecosystems.

The current poster-children for such chemicals are certain per- and polyfuoroalkyl substances, or PFAS — but other high-profile examples include melamine, which is sometimes used to make wooden dishware and plywood feel smooth, and dapsone, a drug used to treat skin problems. Mobile substances are in many other widely used materials, from household cleaners to construction materials. There's been a recent surge in regulation aimed at chemicals that build up in the human body, but regulations based on mobility are in their infancy.

This spring, the European Chemicals Agency took a first step toward recognizing the dangers posed by some mobile substances. But the U.S. has yet to follow suit.

For Hale, the European move is a major victory. Some mobile substances are poised to become serious health risks to future generations, but if recent and upcoming regulations limit how widespread these chemicals become in the environment, "it will really change things," she told Environmental Health News (EHN).

#### Read More

JUL. 07, 2023

EHN, 29-06-23

https://www.ehn.org/persistent-mobile-chemicals-2661211633.html





# Bulletin Board

## **REACH Update**

#### New EU chemicals enforcement project to focus on products sold online

#### 2023-06-20

ECHA's Enforcement Forum agreed to launch an EU-wide project to check that products sold online comply with REACH restrictions and the requirements of the Classification, Labelling and Packaging (CLP) Regulation. Its subgroup on Biocidal Products Regulation, BPRS, agreed to launch a project on labelling of biocidal products.

Inspections in this REACH-EN-FORCE (REF)-13 project will take place in 2025. The objective is to check that products, such as toys, common household goods or chemicals, sold online comply with REACH restrictions. Inspectors will also check that mixtures are classified, labelled and packaged in line with CLP and that online offers include the required information about the hazards of the mixture. Inspectors may also check compliance with restrictions under the Persistent Organic Pollutants (POPs) Regulation and the Restriction of Hazardous Substances (RoHS) Directive.

The online sale of chemicals is an area of high non-compliance. In a previous Forum project (REF-8), inspectors often found that mixtures and articles sold online contained restricted hazardous substances, including those causing cancer. The project found that 78 % of controlled mixtures or articles did not fulfil the conditions of REACH restrictions.

In the upcoming project, inspectors can rely on stricter rules governing online sales, such as the Digital Services Act and General Product Safety Regulation. These new laws are expected to make enforcement stronger.

The Forum's subgroup on Biocidal Products Regulation (BPRS), agreed that the next major enforcement project on biocides (BEF-3) will focus on controlling the correctness of product labels for biocidal products. Inspectors will check that the information on the labelling of biocides corresponds to that what has been authorised and included in the Summary of Product Characteristics. Inspectors may also check the presence and quality of information in the Safety Data Sheets, where it is required for biocidal products.

Both REF-13 and BEF-3 projects will be prepared in 2024, inspections are planned for 2025 and reports are expected to be published in 2026.

During the meeting, the Forum members elected a new chair and vice chair. Henrik Hedlund (SE) will start as the Forum chair and Katja vom Hofe

#### **REACH Update** JUL. 07, 2023

(DE) and Maria Orphanou (CY) will be the vice chairs as of 21 June 2023. Its biocides subgroup elected Helmut de Vos (BE) as chair and Jenny Karlsson (SE) and Eugen Anwander (AT) as vice chairs.

#### Read More

ECHA, 20-06-23

CHEMWATCH

https://echa.europa.eu/-/new-eu-chemicals-enforcement-project-tofocus-on-products-sold-online



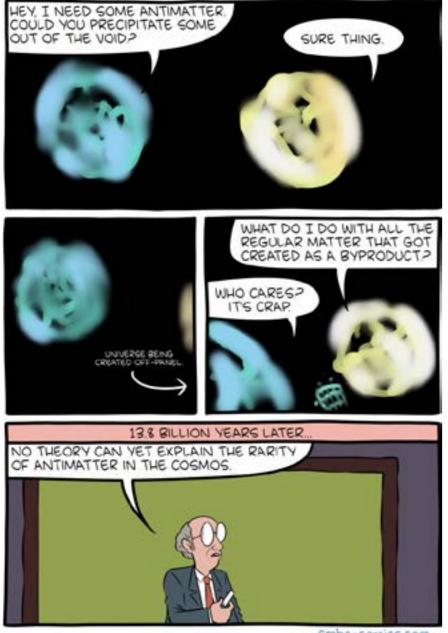


# **Bulletin Board**

## **Janet's Corner**

JUL. 07, 2023

## 2023-07-07



smbc-comics.com

(https://www.smbc-comics.com/comic/antimatter)

## **Hazard Alert**

CHEMWATCH

Sodium hydroxide

2023-07-07

#### **USES** [2]

Sodium hydroxide is used across a range of applications in various industries. It is used in soap-making and other cleaning products and disinfectants. Sodium hydroxide is used in a variety of pharmaceutical products, and in the energy industry, it is used in fuel cell production. The chemical is also used in the water and food industries for various applications, including water treatments and curing, respectively. Sodium hydroxide is used in the textile industry and in the treatment of wood and paper products.

#### **ROUTES OF EXPOSURE [4,5]**

The main routes of exposure to sodium hydroxide are skin and eye contact.

People can also be exposed to sodium hydroxide dust through inhalation.

Higher levels of sodium hydroxide in the air are found nearer the ground. This means that children are potentially more likely to exposed to higher rates than adults because they are closer to the higher source.

#### **HEALTH EFFECTS** [4]

#### **Acute Health Effects**

Severity of symptoms depend on the level and type of exposure.

Acute exposure from skin contact to the chemical can result in red, burning, blistering and painful skin, which can lead to permanent scarring. Burns from the chemical may not be immediately painful; the onset of pain could be delayed. Acute eye contact to sodium hydroxide can result in swelling, pain, blurred vision and redness in the eye. It can also cause permanent blindness. If the chemical is ingested, it can cause nausea, vomiting, diarrhoea, stomach cramps and death.



JUL. 07, 2023

Sodium hydroxide, aka lye and caustic soda, is an alkaline chemical known for its causticity. It is a coproduct of chlorine, and in its raw form, it can be found in flakes, crystals or chips. Its chemical formula is NaOH. [1,2,3]

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## **Hazard Alert**

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#### SAFETY

#### First Aid Measures [6]

Ingestion: If swallowed, contact a medical professional immediately. DO NOT INDUCED VOMITING. If vomiting occurs, place patient in the recovering position. If the person is conscious (and not showing signs of signs of sleepiness), they are able to have water to rinse out their mouth. They are then allowed to drink it slowly—and as much as they can comfortably drink.

Skin contact: Remove all contaminated clothing, footwear and accessories. Do not re-wear clothing until it has been thoroughly decontaminated. Immediately rinse affected areas with plenty of water. Contact a doctor immediately.

Eye contact: Flush eyes (including under the eyelids), with water for at least 15 minutes. Removal of contact lenses should only be done by skilled personnel. Contact a medical professional immediately.

Inhalation: Take victim away from the contaminated area to the nearest fresh air source and monitor their breathing. Prosthesis that could block the airway, such as false teeth, should be removed. Keep the victim warm. If the victim is not breathing, and you are gualified, you may perform CPR with a one-way valve or protective mask. Immediately contact a medical professional.

**General:** Never administer anything by mouth to an unconscious, exposed person.

#### Workplace Controls & Practices [6]

Engineering controls: Emergency eyewash fountains and guick-drench areas should be accessible in the immediate area of the potential exposure. Ensure there is adequate ventilation. Use a local exhaust ventilation or process enclosure, to limit the amount of chemical dust in the air.

#### **Personal Protection**

Personal protection: Safety glasses, protective and dustproof clothing, gloves, an apron and an appropriate mask or dusk respirator. Wear impervious shoes. Do not wear contact lenses. For specifications regarding other PPE, Follow the guidelines set in your jurisdiction.

## **Hazard Alert**

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#### REGULATION

#### **United States** [7]

The Occupational Safety and Health Administration (OSHA) has set a permissible exposure limit (PEL) concentration limit for sodium hydroxide of 2mg/m3.

#### Australia [8]

Safe Work Australia has set an 8-hour time-weighted average (TWA) for sodium hydroxide of 2mg/m3 has been set.

#### REFERENCES

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- 5. https://assets.publishing.service.gov.uk/government/uploads/system/ uploads/attachment\_data/file/337689/hpa\_hydrogen\_chloride\_ toxicological\_overview\_v1.pdf
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# Bulletin Board

## Gossip

Chinese scientists push lithium batteries up to a record 711 Wh/kg

#### 2023-06-19

The current cells, frankly, are good enough for most electric car use cases. But in other areas – such as high-powered mobile devices, highperformance electric motorcycles, and above all, electric aircraft and eVTOLs – manufacturers are crying out for batteries that can pack more energy into significantly less weight.

There are some pretty impressive new cells beginning to trickle onto the market - CATL's 500 Wh/kg "condensed battery," for one. But in terms of single-purpose cells designed purely to max out specific energy, the previous highest figure ever reported was a 575 Wh/kg anode-free pouch cell tested by Dalhousie University professor Jeff Dahn and his team.

This has now been smashed by a team from the Institute of Physics at the Chinese Academy of Sciences. A small team developed a rechargeable 10-Ah pouch cell using an ultra-thin lithium metal anode, and a lithium-rich, manganese oxide-based cathode.

The team expanded the charge/discharge voltage range, and studied the structural stability of the cathode, as well as how modifications to the surface of the lithium anode affected the way in which lithium ions deposit onto the electrode and dissolve away from it as the battery charges and discharges.

The battery tested at 711.3 Wh/kg, and it also offered an exceptional volumetric energy density of 1,653.65 Wh/liter.

Naturally, it's just a research-grade lab cell, and a long way off any form of commercialization. Building this prototype required "extremely advanced process technologies such as high-loading electrode preparation and lean electrolyte injection," so they'd likely be very expensive.

And since the team went in targeting extreme density above all else, there are surely compromises. There's no mention of how much power the cell is capable of putting out or taking in at a time, or what its lifespan is like, or how it performs at different temperatures, or whether it maintains a strong output as it comes close to running out, or whether it has a tendency to cause a fireball when something goes wrong. All of these points and many more will need to be solved before these kinds of things hit the market.

The researchers say there's still room for improvement even on the density metrics, so it'll be interesting to see if they best their own record from here.

#### Tesla's 4680 cells, for comparison, measure somewhere between 244-296 Wh/kg. So the extreme-density cells recently tested in Beijing represent a huge leap forward from the status quo even if they're solely focused on maximizing a single metric.

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The paper is available in the "rapid publication" journal Chinese Physics Letters.

New Atlas, 19 June 2023

https://newatlas.com

### Droplets that can spot cancer and improve DNA testing: the new field of micro elastofluidics

2023-07-05

That's the theory of Professor Nam-Trung Nguyen, director of the Queensland Micro and Nanotechnology Centre at Griffith University, who is in a new field called micro elastofluidics.

Nguyen gave a plenary talk at the First Australian Conference on Green and Sustainable Chemistry and Engineering, being held in Cairns this week and also just received an ARC Laureate Fellowship to make wearable devices that can connect with the body chemically.

Nguyen tells Cosmos that he first became interested in micro elastofluidics after looking at wearable medical devices, which for the moment are mostly solid.

Because liquids can be more flexible, small devices made from them could be more effective at providing medical care.

Micro elastofluidics looks at how fluids flow in solid structures, at the scale of molecules and devices.

This means drops of fluids somewhere on the scale of micrometres to nanometres (or human hairs to molecules).

It also concerns things that happen within a fraction of a fraction of a second, meaning that, even though the distances are very short, the speed is very quick.

"With high speed, and short distance, you get a lot of energy," said Nguyen at the talk.

"This energy can help your reaction happen faster."

What's the catch?

"Liquid is formless: you cannot control it easily."

Nguyen and colleagues have figured out some ways to manage this.



Fluids behave differently at microscopic and nanoscopic levels. If their behaviour can be manipulated, they could be used to deliver medicines to the body, spot diseases, and grow cells that become vital medical treatments.

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One is to coat micrometre-sized drops of liquid with a solid, such as a gel, making liquid marbles.

These tiny beads have a number of applications. One could be to fill them with medicine, for targeted drug delivery without needles.

"If I can make this type of small capsule, micrometre-sized, and use kinetic energy to ballistically pierce the skin, I can deliver the same liquid into the skin without pain," says Nguyen.

They could also be used to grow and deliver stem cells to treat injuries, and make PCR testing - the best way to sequence DNA - more accurate, being able to show the concentration of DNA as well as its presence.

Another technique can both mix together, and separate, fluids at the microscale.

"Mixing is a problem at the microscale," says Nguyen.

"We solve that by [adding] small, long, flexible molecules to make [fluid] elastic."

This allows researchers to mix fluids like sweat, which can help them figure out its contents.

Nguyen and colleagues have shown that this method can be used to separate cancer cells from ordinary blood cells, potentially allowing for faster and more accurate diagnoses.

Ellen Phiddian's airfare to Cairns was paid by the Royal Australian Chemical Institute, which is managing the First Australian Conference on Green and Sustainable Chemistry and Engineering.

Originally published by Cosmos as Droplets that can spot cancer and improve DNA testing: the new field of micro elastofluidics

Cosmos, 5 July 2023

https://cosmosmagazine.com

#### **Recreation of Ediacaran 'death masks' offers chemical** explanation for fossils' formation

#### 05-07-2023

Dating back to between 635–538.8 million years ago, the Ediacaran is often described as a period of evolutionary experimentation, one that occurred before the first appearances of the major branches in the tree of

#### For the first time, researchers have convincingly recreated in the lab the conditions that preserved the enigmatic fossils of the Ediacaran biota - which represent the earliest-known examples of complex multicellular life.

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life that we would recognise today. Examples of life from this time include Dickinsonia - a mysterious blob with a quilted body - and the frond-like Charnia.

Beyond their strange forms, what is unusual about the Ediacaran biota is that it is made up of soft-bodied creatures whose fossils have been found all across the globe. This suggests that they weren't preserved by a fluke of local conditions - as is the case for the soft-bodied fossils of the iconic, younger Burgess Shale – but by something systemic.

While multiple preservation pathways have been proposed for the Ediacaran biota, the leading hypothesis is the pyritic 'death mask' model, first proposed by James Gehling in 1999. The idea is that the unique taphonomic processes of the Ediacaran were mediated by the microbial mats that coated the seafloors of this period, before the evolution of burrowing organisms. When the dead Ediacaran creatures were buried by storms, these mats rapidly colonised the overlying sediments, creating anoxic conditions that both slowed decay and allowed bacteria to reduce seawater sulfate to bisulfide, which would in turn react with iron to form pyrite on the external surfaces of the buried organisms. Little is known, however, about the exact chemical constraints on this preservation process.

Chemistry World, 5 July 2023

https://chemistryworld.com

### Hand-built caesium-based 'artificial atoms' used to create 'synthetic' benzene

#### 2023-06-14

The scanning tunneling microscope's ability to manipulate individual atoms was famously demonstrated in 1989 when Don Eigler and Erhard Schweizer at IBM Almaden in California spelt out 'IBM' using 35 xenon atoms on a nickel substrate. In 1993, Eigler and two colleagues then looked at guantised electronic resonances from iron atoms arranged in a circle on copper, and others have subsequently created more complex 2D arrangements akin to atoms and molecules. However, ubiquitous metal substrates have proved a problem. 'You do create something like an artificial molecule on the surface,' explains Daniel Wegner of Radboud University in Nijmegen, 'but it is still strongly coupled to the substrate, and that basically kills a lot of the properties that are intrinsic to what you actually build.' Removing the conductive substrate, however, is



'Artificial atoms' that form molecular orbitals reminiscent of those in well-known organic molecules have been produced by researchers in the Netherlands using strategically positioned caesium atoms on the surface of a semiconductor. The artificial atoms should allow researchers to measure the energies of molecular systems that would be unstable in real life, and thereby potentially gain greater insights into chemical energetics.

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tricky because scanning tunnelling microscopy works by measuring the variation in the quantum tunnelling of electrons between the tip and the surface under an applied bias voltage. If the substrate itself does not conduct electrons, the tunnelling current becomes zero, which makes the tip unable to detect the substrate and thus renders scanning tunnelling microscopy impossible.

In the new work, Wegner and Radboud University colleagues led by Alexander Khajetoorians used the narrow-bandgap semiconductor indium antimonide as a substrate. This has just enough conductivity to allow them to detect a background tunnelling current provided the voltage was high enough. They then added highly electropositive caesium, which released electrons into a bound state in the semiconductor bandgap, forming a '2D electron gas' that did not couple to the bulk material. The researchers arranged the remaining caesium cations into what Wegner describes as 'an atom without a nucleus' – a ring that had an electromagnetic potential analogous to that between atoms. 'There seem to be s- and p-orbitals like for a real atom,'Wegner says.

The group went on to arrange these 'artificial atoms' into artificial molecules such as cis and trans butadienes and even artificial benzene – finding energetic evidence of sp2 hybridisation even in their 2D model, which Wegner explains is due to the projection of the pz orbitals into the xy-plane.

Cosmos Magazine, 14 June 2023

https://cosmosmagazine.com

## Scientists make common pain killers from pine trees instead of crude oil

#### 2023-07-05

It is perhaps not widely known that many common pharmaceuticals are manufactured using chemical precursors derived from crude oil, presenting a niche sustainability challenge as the world targets Net Zero.

The research team from Bath has developed a method of creating a range of pharmaceutical precursors from biorenewable  $\beta$ -pinene, a component of turpentine which is a waste by-product from the paper industry (annual production >350,000 tons).

A team of scientists, from the University of Bath's Department of Chemistry and **Institute for Sustain**ability have found a way to create two of the world's most common painkillers, paracetamol and ibuprofen, out of a compound found in pine trees, one which is also a waste product from the paper industry.

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They successfully converted  $\beta$ -pinene into two everyday painkillers, paracetamol and ibuprofen, which are produced on ~100,000 ton scales annually.

They also successfully synthesized a range of other precursor chemicals from turpentine, including 4-HAP (4-hydroxyacetophenone), which is the precursor of drugs including beta-blockers and the asthma inhaler drug, salbutamol, as well as others widely used for perfumes and in cleaning products.

They hope that this more sustainable "biorefinery" approach could replace the need for crude oil products in the chemical industry.

Dr. Josh Tibbetts, Research Associate in the University's Department of Chemistry, said, "Using oil to make pharmaceuticals is unsustainable—not only is it contributing to rising CO2 emissions, but the price fluctuates dramatically as we are greatly dependent on the geopolitical stability of countries with large oil-reserves, and it is only going to get more expensive."

"Instead of extracting more oil from the ground, we want to replace this in the future with a 'bio-refinery' model."

"Our turpentine-based biorefinery model uses waste chemical by-products from the paper industry to produce a spectrum of valuable, sustainable chemicals that can be used in a wide range of applications from perfumes to paracetamol."

Instead of putting chemicals in a large reactor to create separate batches of product, the method uses continuous flow reactors, meaning production can be uninterrupted and easier to scale up.

While the process in its current form may be more expensive than using oil-based feedstocks, consumers may be prepared to pay a slightly higher price for more sustainable pharmaceuticals that are completely plant-derived.

The findings are published in the journal ChemSusChem.

Phys Org, 5 July 2023

https://phys.org



The profile of scent compounds from a person's hand can be used to predict their sex, according to a new study led by Kenneth Furton of Florida International University, and published in the journal PLOS ONE.

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#### Hand odor can reveal a person's sex, study shows 2023-07-05

In criminal investigations, dogs have long been used to reliably identify and track people based on their odor. But while human scent evidence from the field is well established, researchers have made little progress in analyzing human scent profiles in the lab.

In the new study, researchers used an analysis technique called mass spectrometry to analyze the volatile scent compounds present on the palms of 60 individuals—half male and half female. After identifying the compounds in each sample, the team performed a statistical analysis to see if they could determine the individual's sex based on their profile of scents. The analysis successfully predicted a person's sex with a 96.67% accuracy rate.

Robberies, assaults and rape are all crimes that are often executed with a perpetrator's hands, and thus have the potential to leave behind valuable trace evidence at a crime scene.

The new study shows that it is possible to predict a person's sex based on hand scents, and existing human odor research indicates scent compounds can also reveal a person's age and racial or ethnic group. With further validation, the chemical and statistical analyses presented in this paper could be used to uncover many details about a potential perpetrator solely through their hand scent profiles.

The authors add, "This approach to analyzing hand odor volatiles can be applied when other discriminatory evidence such as DNA is lacking and allow for differentiation or class characterization such as sex, race and age."

Phys Org, 5 July 2023

https://phys.org

#### The future of recycling could one day mean dissolving plastic with electricity

#### 2023-07-05

The researchers described their new approach to chemical recycling in the journal Chem Catalysis.

The study tackles the mounting problem of plastic trash around the world. According to the Environmental Protection Agency, the United

#### Chemists at CU Boulder have developed a new way to recycle a common type of plastic found in soda bottles and other packaging. The team's method relies on electricity and some nifty chemical reactions, and it's simple enough that you can watch the plastic break apart in front of your eyes.

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States alone produced nearly 36 million tons of plastic products in 2018. A majority of the waste winds up in landfills, said study co-author Oana Luca.

"We pat ourselves on the back when we toss something into the recycling bin, but most of that recyclable plastic never winds up being recycled," said Luca, assistant professor in the Department of Chemistry. "We wanted to find out how we could recover molecular materials, the building blocks of plastics, so that we can use them again."

In the new research, she and her colleagues got one step closer to doing just that.

The group focused on a type of plastic called polyethylene terephthalate (PET), which consumers encounter every day in water bottles, blister packs and even some polyester fabrics. In small-scale lab experiments, the researchers mixed bits of that plastic with a special kind of molecule then applied a small electric voltage. Within minutes, the PET began to disintegrate.

The team has a lot more work to do before its recycling tool can take a realistic bite out of the world's plastic trash problem. But it was still fun to watch the waste, which can stick around in garbage piles for centuries, disappear in a matter of hours or days, said study lead author Phuc Pham.

"It was awesome to actually observe the reaction progress in real time," said Pham, a doctoral student in chemistry. "The solution first turns a deep pink color, then becomes clear as the polymer breaks apart."

#### One person's trash

Luca said it's a whole new way of thinking about the possibilities of trash. Recycling bins, she noted, may look like a good solution to the world's plastics problem. But most municipalities around the world have struggled to collect and sort the small mountain of rubbish that people produce every day. The result: Less than one-third of all PET plastic in the U.S. comes close to being recycled (other types of plastic lag even farther behind). Even then, methods like melting plastic waste or dissolving it in acid can alter the material properties in the process.

In a lab on campus, Phuc Pham applies electricity to a solution containing ground up PET plastic. The solution turns pink as the plastic begins to dissolve. The final step in the proccess is exposing the solution to oxygen, which turns it yellow and eventually back to clear as the plastic fully breaks down. Credit: University of Colorado at Boulder



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"You end up changing the materials mechanically," Luca said. "Using current methods of recycling, if you melt a plastic bottle, you can produce, for example, one of those disposable plastic bags that we now have to pay money for at the grocery store."

She and her team, in contrast, want to find a way to use the basic ingredients from old plastic bottles to make new plastic bottles. It's like smashing your Lego castle so that you can retrieve the blocks to create a whole new building.

#### Another's treasure

To achieve that feat, the group turned to a process called electrolysis—or using electricity to break apart molecules. Chemists, for example, have long known that they can apply a voltage to beakers filled with water and salts to split those water molecules into hydrogen and oxygen gas.

But PET plastic is a lot harder to divide than water. In the new study, Pham ground up plastic bottles then mixed the powder into a solution. Next, he and his colleagues added an extra ingredient, a molecule known as [N-DMBI]+ salt, to the solution. Pham explained that in the presence of electricity, this molecule forms a "reactive mediator" that can donate its extra electron to the PET, causing the grains of plastic to come undone. Think of it like the chemistry equivalent of delivering a karate chop to a wooden board.

The researchers are still trying to understand how exactly these reactions take place, but they were able to break down the PET into its basic building blocks—which the group could then recover and, potentially, use to make something new.

Deploying only tabletop equipment in their lab, the researchers reported that they could break down about 40 milligrams (a small pinch) of PET over several hours.

"Although this is a great start, we believe that lots of work needs to be done to optimize the process as well as scale it up so it can eventually be applied on an industrial scale," Pham said.

Luca, at least, has some big-picture ideas for the technology.

"If I were to have my way as a mad scientist, I would use these electrochemical methods to break down many different kinds of plastic at once," Luca said. "That way, you could, for example, go to these massive

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garbage patches in the ocean, pull all of that waste into a reactor and get a lot of useful molecules back."

Phys Org, 5 July 2023

https://phys.org

#### From atoms to materials: Algorithmic breakthrough unlocks path to materials for sustainable technologies 2023-07-05

In the paper, "Optimality Guarantees for Crystal Structure Prediction," published in the journal Nature, the Liverpool researchers have shown that a mathematical algorithm can guarantee to predict the structure of any material just based on knowledge of the atoms that make it up.

Developed by an interdisciplinary team of researchers from the University of Liverpool's Departments of Chemistry and Computer Science, the algorithm systematically evaluates entire sets of possible structures at once, rather than considering them one at a time, to accelerate identification of the correct solution.

This breakthrough makes it possible to identify those materials that can be made and, in many cases, to predict their properties. The new method was demonstrated on quantum computers that have the potential to solve many problems faster than classical computers and can therefore speed up the calculations even further.

Our way of life depends on materials—"everything is made of something." New materials are needed to meet the challenge of net zero, from batteries and solar absorbers for clean power to providing low-energy computing and the catalysts that will make the clean polymers and chemicals for our sustainable future.

This search is slow and difficult because there are so many ways that atoms could be combined to make materials, and in particular so many structures that could form. In addition, materials with transformative properties are likely to have structures that are different from those that are known today, and predicting a structure that nothing is known about is a tremendous scientific challenge.

Professor Matt Rosseinsky, from the University's Department of Chemistry and Materials Innovation Factory, said, "Having certainty in the prediction of crystal structures now offers the opportunity to identify from the whole of the space of chemistry exactly which materials can be synthesized and



New research by the University of Liverpool could signal a step change in the quest to design the new materials that are needed to meet the challenge of net zero and a sustainable future.

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**New University of** 

is fluttering closer

to turning chicken

feathers into an ef-

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fective filter for water

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Alberta research

the structures that they will adopt, giving us for the first time the ability to define the platform for future technologies.

"With this new tool, we will be able to define how to use those chemical elements that are widely available and begin to create materials to replace those based on scarce or toxic elements, as well as to find materials that outperform those we rely on today, meeting the future challenges of a sustainable society."

Professor Paul Spirakis, from the University's Department of Computer Science, said, "We managed to provide a general algorithm for crystal structure prediction that can be applied to a diversity of structures. Coupling local minimization to integer programming allowed us to explore the unknown atomic positions in the continuous space using strong optimization methods in a discrete space."

"Our aim is to explore and use more algorithmic ideas in the nice adventure of discovering new and useful materials. Joining efforts of chemists and computer scientists was the key to this success."

The research team includes researchers from the University of Liverpool's Departments of Computer Science and Chemistry, the Materials Innovation Factory and the Leverhulme Research Center for Functional Materials Design, which was established to develop new approaches to the design of functional materials at the atomic scale through interdisciplinary research.

Phys Org, 5 July 2023

https://phjys.org

#### Researchers take a step forward in turning chicken feathers into water filters

#### 2023-07-05

Experiments using two chemical agents have improved how keratin from the feathers adsorbs—or sticks to—heavy metals usually found in surface, well or dugout water used by poultry producers for their stock.

The research shows that for the first time, the bio-based filter can remove up to 99% of eight heavy metals simultaneously—the highest numbers yet, says Muhammad Zubair, who conducted the work to earn a Ph.D. in bioresource technology from the Faculty of Agricultural, Life & **Environmental Sciences.** 

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That finding increases the throwaway poultry byproduct's potential as a low-cost, sustainable way to solve a larger global problem, he says.

"Access to clean drinking water is a key to building a healthy and sustainable society, yet many countries, like in South Asia, have groundwater that is contaminated with heavy metals. Arsenic alone has affected 137 million people in 70 countries."

Zubair's work, supervised by professors Aman Ullah and Roopesh Syamaladevi Mohandas, contributes to ongoing research into biobased sorbents, led by Ullah through the U of A's Future Energy Systems program.

#### 'An exciting step forward'

To help improve adsorption of the protein found in the feathers, Zubair used graphene oxide and nanochitosan in separate experiments, to modify the properties of the keratin. Treating the feathers with the chemical agents created more surface area in the adsorbent-which looks like a black powder-to capture contaminants.

Both chemical agents proved effective at removing arsenic, cadmium, chromium, cobalt, lead, nickel, selenium and zinc from small samples of simulated wastewater, Zubair's research showed.

All of the toxins are also commonly found in wastewater used in processing industries such as oil, gas and mining. Boosting the capacity of the adsorbent "is an exciting step forward for greater efficiency," he adds.

Working with the two chemicals also built a better understanding of the interaction between keratin and heavy metals during adsorption, he says. "That may help us to further modify the keratin's properties, to adsorb other heavy metals beyond the eight types we worked with."

#### Potential for global impact

Though only tested in simulated synthetic water for poultry use, the adsorbent technology has potential tobe used in wastewater from oil and gas processing and other chemical-related industries as well, he suggests.

"This technology could go beyond Alberta and have a global impact."

The chemically treated keratin will now be tested in larger volumes of wastewater, part of the process aimed at eventually bringing it to industrial scale.



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The research is published in the journal Chemosphere.

Phys Org, 5 July 2023

https://phys.org

#### Researchers create highly conductive metallic gel for 3D printing

#### 2023-07-05

"3D printing has revolutionized manufacturing, but we're not aware of previous technologies that allowed you to print 3D metal objects at room temperature in a single step," says Michael Dickey, co-corresponding author of a paper on the work and the Camille & Henry Dreyfus Professor of Chemical and Biomolecular Engineering at North Carolina State University. "This opens the door to manufacturing a wide range of electronic components and devices."

To create the metallic gel, the researchers start with a solution of micronscale copper particles suspended in water. The researchers then add a small amount of an indium-gallium alloy that is liquid metal at room temperature. The resulting mixture is then stirred together.

As the mixture is stirred, the liquid metal and copper particles essentially stick to each other, forming a metallic gel "network" within the aqueous solution.

"This gel-like consistency is important, because it means you have a fairly uniform distribution of copper particles throughout the material," Dickey says. "This does two things. First, it means the network of particles connect to form electrical pathways. And second, it means that the copper particles aren't settling out of solution and clogging the printer."

The resulting gel can be printed using a conventional 3D printing nozzle and retains its shape when printed. And, when allowed to dry at room temperature, the resulting 3D object becomes even more solid while retaining its shape.

However, if users decide to apply heat to the printed object while it is drying, some interesting things can happen. The researchers found that the alignment of the particles influences how the material dries.

For example, if you printed a cylindrical object, the sides would contract more than the top and bottom as it dries. If something is drying at room temperature, the process is sufficiently slow that it doesn't create

#### **Researchers have de**veloped a metallic gel that is highly electrically conductive and can be used to print three-dimensional (3D) solid objects at room temperature. The paper, "Metallic **Gels for Conductive** 3D and 4D Printing," has been published in the journal Matter.

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structural change in the object. However, if you apply heat—for example, put it under a heat lamp at 80° Celsius—the rapid drying can cause structural deformation. Because this deformation is predictable, that means you can make a printed object change shape after it is printed by controlling the pattern of the printed object and the amount of heat the object is exposed to while drying.

"Ultimately, this sort of four-dimensional printing—the traditional three dimensions, plus time—is one more tool that can be used to create structures with the desired dimensions," Dickey says. "But what we find most exciting about this material is its conductivity.

"Because the printed objects end up being as much as 97.5% metal, they are highly conductive. It's obviously not as conductive as conventional copper wire, but it's impossible to 3D print copper wire at room temperature. And what we've developed is far more conductive than anything else that can be printed. We're pretty excited about the applications here.

"We're open to working with industry partners to explore potential applications and are always happy to talk with potential collaborators about future directions for research," Dickey says.

Phys Org, 5 July 2023

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## **Curiosities**

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# Next Big Thing: Catalysts can change the world 2023-06-29

We now have more cars in Sydney's CBD then we had in the 1970s, yet our air quality is radically better. Why? Because today we have catalytic converters installed in our vehicles to reduce emissions. In fact, about 90% of the world's chemicals and organic materials are touched by catalysts during their production.

Catalysts can change the world. They already have. But there are big challenges ahead.

#### **Fast facts: Catalysts**

- A catalyst speeds a chemical reaction up by offering an alternative way for chemicals to react.
- They can also allow reactions to happen at lower temperatures, and direct the results of a reaction to favour certain products.
- Catalysts can take many forms, from the complicated and highly specific enzymes in your body to organocatalysts, simple soluble organic molecules that are taking the world by storm.
- Transition metals, are of particular interest as metal catalysts in chemistry and are foundational to the modern life.

Early on in my career, I became fascinated by the process of designing catalytic sites to influence the progress of chemical reactions. To be able to draw up a concept for a catalyst and then physically make it, to see it in action, to generate new molecules with it – this was just so exciting for me.

I also realised that if I want to help make our world more sustainable, I had to turn my attention to improving our chemical processes. Catalysis and catalysts are the obvious tools to do it.

For a start, I want to help create a future characterised by dramatic changes to the way we generate, distribute and use power. It's generally agreed that our energy sources must be fully renewable. Less well understood is how this transition to renewable energy has the potential to also power what we call the "circular economy", where clever re-purposing, re-using and recycling dramatically extends the lifetime of the raw materials we use.

I had to turn my attention to improving our chemical processes. Catalysis and catalysts are the obvious tools to do it.

It is possible to step towards a sustainable world – you just have to be clever with the chemistry, says PM Innovation Prizewinner Professor Thomas Maschmeyer.

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Many years ago I was involved in the development of some of the views that are now commonly referred to as the "12 Principles of Green Chemistry" – for example, how we should think about processing using non-toxic materials, low energy inputs, low waste/no waste, high atom efficiency etc. These ideas join beautifully with our need to preserve the materials that we are using – plastics, for example.

The idea of a circular economy is simply a rational response to the fact that we are currently using just under two planets' worth of resources to maintain the lifestyle of the one planet's people. (If everybody lived the kind of lifestyle we enjoy in Australia, we actually would need around five planets!) We only have one – so the rational response is to use what we have over and over again. Hence, the term "circular economy".

But the circular economy needs to be powered. And this power has to come from renewable energy. Such energy, like wind and solar, is often intermittent. Therefore, it needs buffers to interact with grid systems that have not been designed for this intermittent input.

Everyone agrees that batteries are the buffers that will be the backbone of our future energy grid. What used to be supplied by carbon-intensive fossil fuels will be supplied by reversible energy storage based on carbon neutral battery chemistries to ensure high-quality power for 24 hours a day. These power systems will give rise to largely untapped opportunities for wealth and job creation in a non-polluting power industry.

From my laboratory at the University of Sydney we spun out (2016) and successfully listed in London (2021) Gelion, a battery company with exciting technologies in zinc-based, and lithium-sulfur based, batteries.

The zinc-based systems have their origin in using gels to control the flow of ions inside the battery. Highlighting the importance of basic science in generating impact breakthroughs, these gels were based on an effectively failed experiment exploring the fundamental science of gels, the insights of which were put to good use here.

We are excited about pursuing our aim to bring much higher power zinc-based batteries to applications traditionally dominated by lead acid technology, using similar production methods and lowering hurdles to production.

Our work on lithium sulfur batteries is targeted at delivering a sulfur platform cathode technology that can be paired to a range of lithium anode types, namely lithium/graphite, lithium/silicon (with and without

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carbon), and lithium metal. Such systems will yield batteries that are less than half the weight of the current best-in-class batteries for the same amount of energy stored. A revolution for the mobility sector, be it drones, cars, trucks or even short-range aeroplanes. Our recent acquisition of a broad IP portfolio from Johnson Matthey in the UK (82 patent families and 420 patents) perfectly complements Gelion's proprietary IP in polysulfide management, making us a player with global relevance.

These power systems will give rise to largely untapped opportunities for wealth and job creation in a non-polluting power industry.

Plastic waste is another huge problem for the planet, but my company Licella's catalytic hydrothermal reactor technology (Cat-HTR) can convert mixed end-of-life plastics that currently end up in landfill back into usable material. Our reactor system enables us to convert any organic polymer, be it biological or synthetic in origin, into gases, oils and waxes, as well as bitumen additives. For plastics, the efficiency of the process is such that 98.5% of all the carbon in the feedstock ends up in products leaving our reactor. We make about 15% gas, which is used to run the process. We also have been certified for sustainable Jet A fuel.

The breakthrough moment came when we confirmed our understanding that the transfer of hydrogen from the aqueous process medium into the products generated would just about stop cross-linking of these products. Therefore, we had a suite of materials that did not need expensive hydrogen gas for their stabilisation. This transformed the economics of the process, leading to its global roll-out with partners/licensees including Dow, Shell, Mitsubishi Chemicals, LGChem, Chevron Phillips and Canfor.

Our next great challenge? We are working to generate ammonia from sunshine and air via electrolysis that can compete with the traditional Haber-Bosch process, which feeds the world by making fertiliser but creates approximately 3% of all CO2 emissions. Our initial reactor looks promising!

As told to Graem Sims for Cosmos Weekly.

Cosmos, 29 June 2023

https://cosmosmagazine.com

From plastics, to pharmaceuticals, to fertilisers, most industrial chemicals are made with catalysts.

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Getting precious metals out of green energy with catalysts (and putting carbon back in) 2023-07-05

Catalysts don't get consumed in the manufacturing process - they just make the reactions possible.

But the world is going to need more catalysts as we decarbonise, particularly to use in making hydrogen fuel and capturing carbon.

According to Professor Liming Dai, director of the new ARC Centre of Excellence for Carbon Science and Innovation, and a researcher at the University of New South Wales, to be genuinely sustainable we're going to need to update our catalyst science - and get rid of some metals.

Cosmos spoke to Dai at the First Australian Conference on Green and Sustainable Chemistry and Engineering, being held in Cairns this week.

"Now, people use metal-based catalysts, particularly for clean and renewable energy technologies," he says.

Noble metals (not the same as noble gases), including silver, platinum, palladium and gold, are particularly good catalysts.

These metals are all expensive, and difficult to mine in large quantities.

"Critical minerals, including noble metals and some precious metals, are concentrated in several countries only. So, due to geopolitical risks, the price of noble metals will increase further," says Dai.

"So, we need to find cheaper, abundant materials to use in catalysts for many things. That's why metal-free catalysts can play important roles in clean energy technologies."

Dai's research group started working on metal-free catalysts 12 years ago and has helped spur researchers around the country and the rest of the world to follow suit.

"We opened the metal-free catalyst research field," he says.

They've found particular success with carbon-based materials, many of which have been derived from graphite and carbon nanotubes.

"We found that carbon catalysts are really good to replace platinum, say, for fuel cell technologies to generate clean electricity with hydrogen," says Dai.



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Carbon is abundant on Earth - and there's flexibility in the feedstocks people can use.

"Carbon catalysts can be made from carbon dioxide, which reduces carbon dioxide emissions," points out Dai.

They can also be made from biomass and other agricultural sources – even grasses or plants.

The new Centre of Excellence has received \$35 million in funding across seven years.

With this funding, Dai is confident they'll find better chemicals to use in climate change solutions. "We will develop new carbon catalysts for clean energy production and storage without any carbon dioxide emissions, and also, clean production of chemicals to reduce carbon dioxide emissions."

Ellen Phiddian's airfare to Cairns was paid by the Royal Australian Chemical Institute, which is managing the First Australian Conference on Green and Sustainable Chemistry and Engineering.

Cosmos, 05 July 2023

https://cosmosmagazine.com

### Researchers grow bio-inspired polymer brains for artificial neural networks

2023-07-04

Now, researchers from Osaka University and Hokkaido University plan to change this by creating neuromorphic "wetware." The work is published in the journal Advanced Functional Materials.

While neural-network models have achieved remarkable success in applications such as image generation and cancer diagnosis, they still lag far behind the general processing abilities of the human brain. In part, this is because they are implemented in software using traditional computer hardware that is not optimized for the millions of parameters and connections that these models typically require.

Neuromorphic wetware, based on memristive devices, could address this problem. A memristive device is a device whose resistance is set by its history of applied voltage and current. In this approach, electropolymerization is used to link electrodes immersed in a precursor solution using wires made of conductive polymer. The resistance of each The development of neural networks to create artificial intelligence in computers was originally inspired by how biological systems work. These "neuromorphic" networks, however, run on hardware that looks nothing like a biological brain, which limits performance.

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wire is then tuned using small voltage pulses, resulting in a memristive device.

"The potential to create fast and energy-efficient networks has been shown using 1D or 2D structures," says senior author Megumi Akai-Kasaya. "Our aim was to extend this approach to the construction of a 3D network."

The researchers were able to grow polymer wires from a common polymer mixture called "PEDOT:PSS," which is highly conductive, transparent, flexible, and stable. A 3D structure of top and bottom electrodes was first immersed in a precursor solution. The PEDOT:PSS wires were then grown between selected electrodes by applying a square-wave voltage on these electrodes, mimicking the formation of synaptic connections through axon guidance in an immature brain.

Once the wire was formed, the characteristics of the wire, especially the conductance, were controlled using small voltage pulses applied to one electrode, which changes the electrical properties of the film surrounding the wires.

"The process is continuous and reversible," explains lead author Naruki Hagiwara, "and this characteristic is what enables the network to be trained, just like software-based neural networks."

The fabricated network was used to demonstrate unsupervised Hebbian learning (i.e., when synapses that often fire together strengthen their shared connection over time). What's more, the researchers were able to precisely control the conductance values of the wires so that the network could complete its tasks.

Spike-based learning, another approach to neural networks that more closely mimics the processes of biological neural networks, was also demonstrated by controlling the diameter and conductivity of the wires.

Next, by fabricating a chip with a larger number of electrodes and using microfluidic channels to supply the precursor solution to each electrode, the researchers hope to build a larger and more powerful network. Overall, the approach determined in this study is a big step toward the realization of neuromorphic wetware and closing the gap between the cognitive abilities of humans and computers.

Phys Org, 04 July 2023

https://phys.org



**Researchers at the Max Planck Institute** of Colloids and Interfaces (MPICI) have designed a carbohydrate sequence capable of folding into a stable secondary structure.

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#### New discovery toward sugar origami 2023-07-04

Until now, such self-folding biopolymers had only been developed for DNA and proteins, and sugars were previously considered too flexible to assume a stable conformation. Folded carbohydrates could open up completely new perspectives in biomedicine and materials science.

Carbohydrates make up about 80% of the earth's biomass—half on land and half in the sea. Yet, their material properties are still quite poorly understood. The researchers led by Dr. Martina Delbianco, from the Department of Biomolecular Systems, are interested in how polysaccharides, or long chains of sugars, fold and assemble into materials. For example, they have discovered how individual glucose chains come together to generate cellulose, the main component of plants.

Using this knowledge, they are now designing non-natural carbohydrates. Their work is inspired by peptide research (short proteins). Knowledge about natural proteins, was used to design synthetic peptide sequences that could adopt programmable 3D shapes and perform specific functions. This approach opened up many possibilities, for example in drug production and nanotechnology. Carbohydrates hold even more opportunities owing to their higher abundance and diversity when compared with peptides.

In their paper published in the journal Nature Chemistry, Dr. Delbianco and her team demonstrated that it is possible to design glycans that adopt a specific stable conformation in aqueous solution. They linked together natural sugar motives to generate a shape that does not exist in nature, a hairpin. In a Lego-like approach, they connected two linear cellulose rods (in blue) to a rigid glycan turn (in green) to obtain a new non-natural shape.

"Carbohydrates can be generated with programmable shapes, which opens up the possibility of endowing glycans with new properties and functions," says Dr. Martina Delbianco. The structure was quickly prepared using "Automated Glycan Assembly" (AGA), a process in which monosaccharides are connected in an automated synthesizer to generate tailor-made polysaccharide sequences. To reveal the 3D structure, Dr. Delbianco's group used a plethora of analytical techniques.

Furthermore, international researchers like Prof. Jesús Jiménez-Barbero from CIC BioGUNE collaborated with Dr. Martina Delbianco. "The 3D structure of a biomolecule determines its function. This could mean,

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for example, that in the future we might use folded sugars as drugs, as catalysts for chemical transformations, or as structural units for the creation of nanomaterials," says Dr. Martina Delbianco.

Phys.Org, 04 July 2023

https://phys.org

### Planting seeds: Researchers dig into how chemical gardens grow

#### 2023-07-03

Until now, researchers have been unable to model how these deceptively simple tubular structures—called chemical gardens—work and the patterns and rules that govern their formation.

In a paper published in the Proceedings of the National Academy of Sciences, Florida State University researchers lay out a model that explains how these structures grow upward, form different shapes and how they go from a flexible, self-healing material to a more brittle one.

"In a materials context, it's very interesting," said FSU Professor of Chemistry and Biochemistry Oliver Steinbock. "They don't grow like crystals. A crystal has nice sharp corners and grows atom layer by atom layer. And when a hole occurs in a chemical garden, it's self-healing. These are really early steps in learning how to make materials that can reconfigure and repair themselves."

Typically, chemical gardens form when metal salt particles are put in a silicate solution. The dissolving salt reacts with the solution to create a semipermeable membrane that ejects upward in the solution, creating a biological-looking structure, similar to coral.

Scientists observed chemical gardens for the first time in 1646 and for years have been fascinated with their interesting formations. The chemistry is related to the formation of hydrothermal vents and the corrosion of steel surfaces where insoluble tubes can form.

"People realized these were peculiar things," Steinbock said. "They have a very long history in chemistry. It became more like a demonstration experiment, but in the past 10-20 years, scientists became interested in them again."

Inspiration for the mathematical model developed by Steinbock, along with postdoctoral researcher Bruno Batista and graduate student Amari



Since the mid-1600s, chemists have been fascinated with brightly colored, coral-like structures that form by mixing metal salts in a small bottle.

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Morris, came from experiments that steadily injected a salt solution into a larger volume of silicate solution between two horizontal plates. These showed distinct growth modes and that the material starts off as stretchy, but as it ages, the material becomes more rigid and tends to break.

The confinement between two layers allowed the researchers to simulate a number of different shape patterns, some looking like flowers, hair, spirals and worms.

In their model, the researchers described how these patterns emerge over the course of the chemical garden's development. Salt solutions can vary a lot in chemical makeup, but their model explains the universality in formation.

For example, the patterns can consist of loose particles, folded membranes, or self-extending filaments. The model also validated observations that fresh membranes expand in response to microbreaches, demonstrating the material's self-healing capabilities.

"The good thing we got is we got into the essence of what is needed to describe the shape and growth of chemical gardens," Batista said.

Phys.Org, 03 July 2023

https://phys.org

#### Chemists discover why photosynthetic light-harvesting is so efficient

#### 2023-07-03

This transfer of energy through the light-harvesting complex occurs with extremely high efficiency: Nearly every photon of light absorbed generates an electron, a phenomenon known as near-unity quantum efficiency.

A new study from MIT chemists offers a potential explanation for how proteins of the light-harvesting complex, also called the antenna, achieve that high efficiency. For the first time, the researchers were able to measure the energy transfer between light-harvesting proteins, allowing them to discover that the disorganized arrangement of these proteins boosts the efficiency of the energy transduction.

"In order for that antenna to work, you need long-distance energy transduction. Our key finding is that the disordered organization of the light-harvesting proteins enhances the efficiency of that long-distance

When photosynthetic cells absorb light from the sun, packets of energy called photons leap between a series of light-harvesting proteins until they reach the photosynthetic reaction center. There, cells convert the energy into electrons, which eventually power the production of sugar molecules.

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energy transduction," says Gabriela Schlau-Cohen, an associate professor of chemistry at MIT and the senior author of the new study.

MIT postdocs Dihao Wang and Dvir Harris and former MIT graduate student Olivia Fiebig Ph.D. are the lead authors of the paper, published in the Proceedings of the National Academy of Sciences. Jianshu Cao, an MIT professor of chemistry, is also an author of the paper.

#### **Energy capture**

For this study, the MIT team focused on purple bacteria, which are often found in oxygen-poor aquatic environments and are commonly used as a model for studies of photosynthetic light-harvesting.

Within these cells, captured photons travel through light-harvesting complexes consisting of proteins and light-absorbing pigments such as chlorophyll. Using ultrafast spectroscopy, a technique that uses extremely short laser pulses to study events that happen on timescales of femtoseconds to nanoseconds, scientists have been able to study how energy moves within a single one of these proteins. However, studying how energy travels between these proteins has proven much more challenging because it requires positioning multiple proteins in a controlled way.

To create an experimental setup where they could measure how energy travels between two proteins, the MIT team designed synthetic nanoscale membranes with a composition similar to those of naturally occurring cell membranes. By controlling the size of these membranes, known as nanodiscs, they were able to control the distance between two proteins embedded within the disks.

For this study, the researchers embedded two versions of the primary light-harvesting protein found in purple bacteria, known as LH2 and LH3, into their nanodiscs. LH2 is the protein that is present during normal light conditions, and LH3 is a variant that is usually expressed only during low light conditions.

Using the cryo-electron microscope at the MIT.nano facility, the researchers could image their membrane-embedded proteins and show that they were positioned at distances similar to those seen in the native membrane. They were also able to measure the distances between the light-harvesting proteins, which were on the scale of 2.5 to 3 nanometers.



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A new online platform

to explore computa-

tionally calculated

chemical reaction

ing and design of

chemical reactions.

pathways has been

released, allowing for

in-depth understand-

#### **Disordered is better**

Because LH2 and LH3 absorb slightly different wavelengths of light, it is possible to use ultrafast spectroscopy to observe the energy transfer between them. For proteins spaced closely together, the researchers found that it takes about 6 picoseconds for a photon of energy to travel between them. For proteins farther apart, the transfer takes up to 15 picoseconds.

Faster travel translates to more efficient energy transfer, because the longer the journey takes, the more energy is lost during the transfer.

"When a photon gets absorbed, you only have so long before that energy gets lost through unwanted processes such as nonradiative decay, so the faster it can get converted, the more efficient it will be," Schlau-Cohen says.

The researchers also found that proteins arranged in a lattice structure showed less efficient energy transfer than proteins that were arranged in randomly organized structures, as they usually are in living cells.

"Ordered organization is actually less efficient than the disordered organization of biology, which we think is really interesting because biology tends to be disordered. This finding tells us that that may not just be an inevitable downside of biology, but organisms may have evolved to take advantage of it," Schlau-Cohen says.

Now that they have established the ability to measure inter-protein energy transfer, the researchers plan to explore energy transfer between other proteins, such as the transfer between proteins of the antenna to proteins of the reaction center. They also plan to study energy transfer between antenna proteins found in organisms other than purple bacteria, such as green plants.

Phys.Org, 03 July 2023

https://phys.org

# A user-friendly platform for virtual exploration of chemical reactions

#### 2023-07-03

Advances in computational chemistry have lead to the discovery of new reaction pathways for the synthesis of high-value compounds. Computational chemistry generates much data, and the process of organizing and visualizing this data is vital to be able to utilize it for future research.

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A team of researchers from Hokkaido University, led by Professor Keisuke Takahashi at the Faculty of Chemistry and Professor Satoshi Maeda at the Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), have developed a centralized, interactive, and user-friendly platform, Searching Chemical Action and Network (SCAN), to explore reaction pathways generated by computational chemistry. Their research was published in the journal Digital Discovery.

"From a computational viewpoint, chemical reactions can be considered as extremely complex networks that consist of numerous molecular interactions," explains Takahashi. "Many tools have been developed to calculate these networks, such as the AFIR method we use at WPI-ICReDD. However, tools to explore these calculated networks are also needed, which led us to the current study."

Broadly, all the raw data from AFIR calculations form a "data lake." This data is then subjected to a pre-processing step, creating a "data warehouse." Finally, the "data mart" accesses and retrieves data from the data warehouse and provides tools to visualize, analyze, and share the retrieved data.

"The pre-processing step is crucial," Maeda elaborates. "The raw data form AFIR contains an immense amount of information, from which the key data required for the SCAN platform must be extracted. This key data is sufficient to allow the creation of an interactive reaction pathway map which can be searched and viewed."

SCAN is accessible on the internet at https://scan.sci.hokudai.ac.jp/. The source code for SCAN is also publicly available.

"We have developed SCAN with a user-friendly graphic user interface," concludes Takahashi. "Users can search and explore the chemical reaction path network generated by the first principle calculation (AFIR). It will aid in achieving a detailed understanding of complex chemical reaction pathways."

Phys.Org, 03 July 2023

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**Researchers have** demonstrated a new material for singlemolecule electronic switches, which can effectively vary current at the nanoscale in response to external stimuli. The material for this molecular switch has a unique structure created by locking a linear molecular backbone into a ladder-type structure. A new study finds that the ladder-type molecular structure greatly enhances the stability of the material, making it highly promising for use in single-molecule electronics applications.

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### **Researchers demonstrate single-molecule electronic** 'switch' using ladder-like molecules

#### 2023-06-30

Reported in the journal Chem, the study shows that the ladder-type molecule serves as a robust and reversible molecular switch over a wide range of conductivity levels and different molecular states.

"Our work provides a significant step forward towards the development of functional molecular electronic devices," says Charles Schroeder, who is the James Economy Professor of Materials Science and Engineering and Professor of Chemical and Biomolecular Engineering at the University of Illinois Urbana-Champaign.

To enhance the chemical and mechanical stability of the molecule, the team used new strategies in chemical synthesis to lock the molecular backbone to prevent the molecule from rotating, like converting a rope ladder into something more stable like metal or wood.

"Imagine a light switch that we turn on and off every day, but instead of flipping an actual switch, we add chemical or electrochemical stimuli to turn the electrical signal from the material on and off," says lead author and former graduate student Jialing (Caroline) Li. Compared to bulk inorganic materials, organic single molecules can be made into basic electrical components, like wires and transistors, and will help enable the ultimate goal of shrinking electrical circuits.

Single-molecule electronic devices are constructed as junctions with a single molecule bridge that is generally anchored to two terminal groups connected to metal electrodes. These devices can be made programmable by using a stimuli-responsive element in the bridge that can be switched on and off by using an array of stimuli such as pH, optical fields, electric fields, magnetic fields, mechanical forces and electrochemical control.

"The molecular scale switch has been a very popular subject in studies of single molecule electronics," Li explains. "But realizing a multi-state switch on a molecular scale is challenging because we require a material that is conductive and has several different molecular charge states, and we require the material to be very stable so it can be switched on and off for many cycles."

Though Li explored many other organic materials, the drawback of those materials was that they were not stable in ambient conditions and could break down easily when exposed to oxygen. After searching for the ideal

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material for a long time, Li struck gold when she stumbled upon a material from a research group at Texas A&M University (collaborators on this project) and immediately identified it as ideal for her purposes.

Modifying the structure by locking the backbone of the molecule prevents hydrolysis, chemical breakdown due to reaction with water, and other degradation reactions from occurring, and makes characterization of the material easier since it cannot rotate and change forms.

This rigid, coplanar form enhances the electronic properties of the molecule, making the flow of electrons through the material easier. The ladder-type structure allows for stable molecular charge states when external stimuli are applied that give rise to significantly different levels of conductivity—making multi-state switching possible.

This material meets almost all of the requirements needed to serve in single-molecule electronic devices: it is stable in ambient conditions, can be cycled on/off many times, is conductive (although not as conductive as metal) and has different molecular states accessible to be utilized.

"Researchers have been struggling to minimize the size of the transistor to fit as many as possible on chips for semiconductors, usually using inorganic materials like silicon," Li says. "An alternative way of doing that is using organic materials like a single-molecule material to conduct the electrons and replace the inorganic counterparts." The ladder-type structure used in this research shows promise to be used as functional materials for single-molecule transistors.

For now, only one unit of the molecule is used for single-molecule electronics, but it is possible to extend the length to include many repeating units to make a longer molecular wire. The team believes that the material will still be highly conductive, even over a longer distance.

Phys.Org, 30 June 2023

https://phys.org

#### Potent new compound has breakthrough potential for parasitic sleeping sickness and Chagas treatment 2023-06-30

The findings—published in the journal Science and led by researchers at the University of Glasgow and Novartis Global Health (formerly Novartis Institutes for Tropical Diseases)—reveal potent compounds discovered



Scientists have discovered a new class of compound that is potentially active against trypanosome parasites that cause human African trypanosomiasis (or sleeping sickness) and Chagas disease.

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for the two separate types of trypanosomiases, showing potential for development as new medicines for these diseases.

The study demonstrated that the compounds were able to cure a mouse model of sleeping sickness with just a single dose, and a short course of daily doses across five days cured Chagas disease in the same models.

African trypanosomiasis (or sleeping sickness) is a major killer disease that puts around 70 million people at risk in sub-Saharan African countries and is invariably fatal if untreated or inadequately treated. Meanwhile, around 7 million people are currently infected by Chagas disease, which can cause irreversible damage to the heart and digestive tract.

There are currently no drugs available that effectively cure Chagas disease; while for sleeping sickness, there have been some steps toward new therapies in recent years.

The researchers also show in the study exactly how the compounds, called cyanotriazoles (or CTs for short), kill parasites without adversely affecting host cells. These compounds selectively bind to a parasite enzyme (called topoisomerase II) that is essential for the replication and maintenance of DNA, which carries the genetic blueprint vital for life. By binding to and inhibiting this enzyme, the compounds introduce breaks into the DNA that are lethal to the parasites.

The Glasgow group, led by Professor Mike Barrett from the Wellcome Center for Integrative Parasitology in the University's School of infection & Immunity, made inroads into finding that mechanism of action using a technique known as metabolomics, through the Glasgow Polyomics facility, which showed how DNA was being degraded in the cells. Parasites resistant to the drugs had changed their topoisomerase protein structure such that they no longer bound the drug.

The Novartis team, led by Srini Rao, worked out the three-dimensional structure of the trypanosome's topoisomerase, revealing how CTs bind to a particular part of the trypanosome's enzyme that is absent from the human version.

Mike Barrett, Professor of Biochemical Parasitology at the University of Glasgow, said, "Compounds with this degree of potency, working through a newly discovered mechanism, represent a major breakthrough. If they are proven to be safe in humans and retain the levels of activity seen in

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mice, they could offer the first effective therapy of Chagas disease which afflicts millions of people in Latin America."

Phys.Org, 30 June 2023

https://phys.org

#### Scientists designed new enzyme using Antarctic bacteria and computer calculations 2023-06-30

The type of cold-adapted enzymes used by the researchers for their study can be found in bacteria and fish that live in icy water, for example. Evolution has shaped them to be able to function even at very low temperatures at which other enzymes are normally stone dead. These enzymes also always have a lower optimum temperature and melting point than enzymes from warm-blooded animals and organisms that live at higher temperatures.

The researchers wondered whether computer simulations of the catalyzed chemical reaction could predict a small number of mutations in the Antarctic enzyme that could result in an increase in its optimum temperature. The results of the calculation showed that this would be possible if 16 mutations were inserted from the corresponding pig enzyme into the bacterial variant.

The researchers then produced this hybrid enzyme and measured its catalytic activity as a function of temperature, and it was indeed found that the new variant had a 6°C higher optimum than the original variant and was faster than both the Antarctic and pig enzymes at 50°C. They also solved the three-dimensional structure of the hybrid enzyme by X-ray crystallography and showed that the necessary structural changes predicted by the computer calculations had indeed taken place.

Computer-based enzyme design has become a major and hotly pursued research area in recent years. The goal is to create enzymes with new properties and to do so with the help of computer calculations instead of labor-intensive experiments.

"For example, this may involve creating new enzymes that catalyze chemical reactions not found in nature or changing their properties so that they can better cope with heat, cold, high pressure, increased salinity and so on. This area is therefore the subject of great biotechnological



For the first time, researchers have succeeded in predicting how to change the optimum temperature of an enzyme using large computer calculations. A cold-adapted enzyme from an Antarctic bacterium was used as a basis. The study was published in the journal Science Advances and is a collaboration between researchers at Uppsala University and the University of Tromsø.



# **Technical Notes**

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