

(click on page numbers for links)

	1 -	$\boldsymbol{c}$	ш		Λ-		$\neg$	Ю	W		D	П	V٨	٠.	
N.	1-1	ч	u	Щ,	н	ш	U)	м	Y	U	P	L	J.	М	15

AS	IΛ	DI	1	1
$\boldsymbol{\Lambda}$	$\mathbf{I}$	T /	~	 •

Nepalese government cracks down on unsafe food4
Guidance on obtaining harmonised veterinary medicine labels in
Australia and New Zealand4

#### **AMERICA**

ACC's High Phthalates Panel Statement on EPA's Draft Risk Evaluation for DIDP and Draft Hazard Assessments for DINP	5
NOTICE OF PROPOSED RULEMAKING TITLE 27, CALIFORNIA CODE OF REGULATIONS, DIVISION 4, CHAPTER 1, ARTICLE 7	
Notice of intent to amend the Domestic Substances List, adding the	0
letter "P" to the identifiers of 264 reduced regulatory requirement polymers	7
Canada Assessment - Aldehydes group	9

### **EUROPE**

Switzerland Amends Chemical Ordinance to Align with EU Regulations1	0
EU Parliament backs revision of Toys Safety directive1	1
73 EU candidates pledge a toxic-free future ahead of EU-elections1	1

#### **INTERNATIONAL**

EU and Australia Sign Partnership on Sustainable Critical and
Strategic Minerals12
IARC marks World No Tobacco Day 202413

## **REACH UPDATE**

European Commission decisions on applications for authorisation	.15
Assessment of regulatory needs reports published	.15
Consultations on harmonised classification and labelling	.15

### JANET'S CORNER

ppendix1	7
DDENGIX	
PP = 1 G // C	•

## **CONTACT US**

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

1227 Glen Huntly Rd Glen Huntly Victoria 3163 Australia

\* 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.

## CHEMWATCH

# Bulletin Board

## **Contents**

HAZARD ALERT
Phenanthrene18
COSCID
GOSSIP
New material puts eco-friendly methanol conversion within reach26
New material puts eco-friendly methanol conversion within reach28
New Seashell-Inspired Building Material Is 17 Times Tougher Than
Cement29
Chemists develop technique for extending nitrene reactions to
three days31
Dark Chocolate May Pose Slight Heavy Metal Risk to Children32
"Cocktail Effect" Explains How Tin Toughens Titanium Alloy Medical
Implants34
Old drugs new tricks—novel approach shows 'enormous potential'
for rapid antibiotic discovery36
Eating Small Fish May Prolong Life in Women38
Intermediate considered 'too reactive to isolate' finally tamed40
CURIOCITIES
CURIOSITIES
Inherited Traits Determine Your Coffee Intake42
Tough new pineapple leather is 60X stronger than other materials44
Spectroscopic technique that singles out water molecules lying on
the surface reveals how they relax after being excited46
Much of the Nord Stream gas remained in the sea47
Drugs Commonly Used To Treat Enlarged Prostate May Also
Decrease Dementia Risk49
Great British Bake Off finalist discusses the parallels between
chemistry and baking51
The US abortion drugs regulation challenge has stalled, but it will return 52
Researchers Invent 100% Biodegradable "Barley Plastic"54

### **TECHNICAL NOTES**

Revolutionizes Hydrogen Production.....

(Note: Open your Web Browser and click on Heading to link to section)...64

Researchers create new class of materials called 'glassy gels'....

Cutting Costs and Increasing Efficiency: New Catalyst

## **CHEMWATCH**

# **Bulletin Board**

## **Contents**

JUN. 21, 2024

JUIN. 21, 202

CHEMICAL EFFECTS	64
ENVIRONMENTAL RESEARCH	64
PHARMACEUTICAL/TOXICOLOGY	64
OCCUPATIONAL	64



## ASIA PACIFIC

## Nepalese government cracks down on unsafe food

2024-05-09

The Nepalese government has amended the law relating to food (the Food Quality and Hygiene Laws - 2081 BS), imposing up to five years in prison for the production and sale of inedible products that pose a threat to human health. While amending the Food Act, 2023, the government has included provisions to regulate the production, processing, export, import, transportation, sale, distribution or storage of food products, with fines of up to Rs 500,000 (roughly 5500 euros). The Department of Food Technology and Quality Control (DFTQC) has stated that action will be taken against any unlicensed food business, unauthorized imports of food or production, processing, export, import, storage, transportation, or sale of contaminated food.

#### Read More

Food Compliance International, 09-05-24

https://na.parliament.gov.np/uploads/attachments/mungsyv2vzzvhkjz.pdf

# **Guidance on obtaining harmonised veterinary medicine labels in Australia and New Zealand**

2024-06-13

The New Zealand Ministry for Primary Industries (MPI) Agricultural Compounds and Veterinary Medicines (ACVM) and the Australian Pesticides and Veterinary Medicines Authority (APVMA) allow harmonised labels for veterinary medicines registered in both countries.

Registrants of veterinary medicine products registered in both New Zealand and Australia can benefit from one common label to sell and market in both countries.

Guidance has been issued to clarify the harmonised labelling requirements for industry.

Harmonised labels must be formatted in line with APVMA requirements, with a separate section on the label to provide regulatory statements and other specific content required by New Zealand's ACVM Act.

CHEMWATCH

# Bulletin Board

# **Regulatory Update**

JUN. 21, 2024

Harmonised labels can be considered if the Australia-specific information regarding the claims and use of the product do not jeopardise the risk areas managed under the ACVM Act.

The main part of the label must be written to comply with both the Australian and New Zealand requirements for registration, other than content clearly identified as New Zealand-specific information.

Additionally, New Zealand-specific information must not contradict, confuse, appear misleading or deceptive, or affect the meaning of the relevant particulars approved by the APVMA.

The APVMA does not approve marketed labels, therefore harmonised labels must not be submitted to the APVMA for approval. Marketed labels must comply with the requirements of the Veterinary Labelling Code and other statutory conditions.

#### Read More

JUN. 21, 2024

APVMA, 13-06-24

https://www.apvma.gov.au/

## **AMERICA**

## ACC's High Phthalates Panel Statement on EPA's Draft Risk Evaluation for DIDP and Draft Hazard Assessments for DINP

2024-05-21

Today, the American Chemistry Council's High Phthalates Panel issued the following statement on the U.S. Environmental Protection Agency's (EPA) completion of a draft manufacturer-requested risk evaluation for DIDP and the release of draft hazard assessments for DINP:

We recognize the effort by EPA to generate a comprehensive risk evaluation for DIDP and appreciate the opportunity to evaluate the application of best-available science in the draft risk evaluation. We're still reviewing the draft documents in detail.

"EPA did not find evidence to determine that DIDP causes cancer, which is similar to the findings of other regulatory agencies like the U.S. Consumer Product Safety Commission, Health Canada, the European Chemicals



Agency, and Australia's National Industrial Chemicals Notification and

"EPA concluded that 46 of the 47 industrial/commercial uses for DIDP are safe and requested further clarification on the single use identified as posing unreasonable risk. EPA determined that DIDP does not pose unreasonable risk of injury to human health for consumers, the general population or to the environment. We look forward to continuing engagement with EPA and the Science Advisory Committee on Chemicals (SACC) to clarify any uncertainties and demonstrate the safety of DIDP in all current uses.

"We appreciate EPA releasing the hazard assessments for DINP for peer review. Based on initial review, EPA's conclusions are in line with those made by other regulatory agencies including that the weight of scientific evidence supports a peroxisome proliferator activated receptor alpha (PPAR $\alpha$ ) MOA for liver tumors observed in rats and mice. The consensus of the scientific community is that this is a non-human relevant mode of action.

#### **Read More**

American Chemistry, 21-05-24

Assessment Scheme.

https://www.americanchemistry.com/chemistry-in-america/news-trends/press-release/2024/acc-s-high-phthalates-panel-statement-on-epa-s-draft-risk-evaluation-for-didp-and-draft-hazard-assessments-for-dinp

## NOTICE OF PROPOSED RULEMAKING TITLE 27, CALIFORNIA CODE OF REGULATIONS, DIVISION 4, CHAPTER 1, ARTICLE 7

2024-05-10

NOTICE IS HEREBY GIVEN that the Office of Environmental Health Hazard Assessment (OEHHA) proposes to adopt a Proposition 65 No Significant Risk Level (NSRL) for titanium dioxide (airborne, unbound particles of respirable size) by amending Title 27, California Code of Regulations, section 25705(c)(2).1 OEHHA is proposing an NSRL of 440 micrograms per day for airborne, unbound titanium dioxide particles with diameters of 10 micrometers or less, and an NSRL of 44 micrograms per day for airborne, unbound titanium dioxide particles with diameters of 0.8 micrometers or less. Both parts of the NSRL must be met before it applies. SUBMISSION OF PUBLIC COMMENTS All written comments must be submitted to OEHHA by electronic submission, mail, or hand-delivery, by June 24,

CHEMWATCH

# Bulletin Board

# **Regulatory Update**

JUN. 21, 2024

2024, as indicated below. OEHHA strongly recommends that comments be submitted electronically through our website at https://oehha.ca.gov/comments rather than in paper form. Alternatively, comments can be submitted in paper form, by either mail or delivered in person.

#### Read More

JUN. 21, 2024

OEHHA, 10-05-24

https://oehha.ca.gov/media/downloads/crnr/tio2nsrlnprm051024.pdf

# Notice of intent to amend the Domestic Substances List, adding the letter "P" to the identifiers of 264 reduced regulatory requirement polymers

2024-05-11

#### Description

The notice of intent is an opportunity for the public to comment on the proposed amendments to the Domestic Substances List (DSL), pursuant to subsection 66(1) of the Canadian Environmental Protection Act, 1999 (CEPA), adding the letter "P" to the identifiers of 264 polymers, as the form of those polymers that were assessed met the reduced regulatory requirement (RRR) polymer criteria.

### Background

The DSL provides an inventory of substances manufactured in or imported into Canada on a commercial scale. A substance not on the DSL is therefore a new substance in Canada. Under CEPA, no new substances can be imported into or manufactured in Canada above the prescribed thresholds before an assessment of their potential impacts on human health and the environment has been performed. Reporting requirements for new chemicals and polymers are set out in the New Substances Notification Regulations (Chemicals and Polymers) [the Regulations].

Substances on the DSL are not subject to notification under the Regulations; however, when a substance identifier on the DSL is followed by a regulatory flag (that is the letter "S," "S prime" or "P"), this substance is subject to notification under certain circumstances.

The letter "P" after a substance identifier indicates that the substance assessed and added to the DSL met the RRR polymer criteria in the Regulations. Substances that meet the RRR polymer criteria are considered of low concern, which allows for fewer regulatory information



requirements under the Regulations than for non-reduced regulatory requirement (non-RRR) polymers. Typically, a substance synthesized in a form that meets the RRR polymer criteria can also be synthesized in a form that does not meet these criteria.

The purpose of the letter "P" is to indicate that any person who intends to manufacture in or import into Canada the polymer in a form that does not meet the RRR polymer criteria in a quantity above prescribed thresholds must submit the information prescribed in the Regulations. Please consult section 4.7 of the Guidance document for the New Substances Notification Regulations (Chemicals and Polymers) for help determining the applicable notification schedule.

#### **Project scope**

Environment and Climate Change Canada identified substances assessed as RRR polymers and added to the DSL prior to the introduction of the letter "P" in 2003.footnote3Any form of these polymers that does not meet the RRR polymer criteria currently does not require notification. Therefore, it is proposed to add the letter "P" to the identifiers of these polymers to clarify that only the RRR forms of these polymers are on the DSL, as per their assessment, and not the non-RRR forms. The addition of the letter "P" would allow for the environmental and human health risk assessment of any form of these polymers that does not meet the RRR polymer criteria prior to their import or manufacture in Canada.

#### **Next steps**

Within 120 days of publication of the notice of intent, any person may submit comments on the proposed amendments, which will be taken into consideration during the development of the final order. The final order will be published in the Canada Gazette, Part II. Amendments to the DSL are not in force until the order is published in the Canada Gazette, Part II.

#### **Read More**

Government of Canada, 11-05-24

https://www.canadagazette.gc.ca/rp-pr/p1/2024/2024-05-11/html/notice-avis-eng.html



# Bulletin Board

# **Regulatory Update**

JUN. 21, 2024

## **Canada Assessment - Aldehydes group**

2024-05-30

JUN. 21, 2024

Pursuant to section 77 of the Canadian Environmental Protection Act, 1999 (CEPA), the Minister of the Environment and the Minister of Health have conducted an assessment of 5 substances referred to collectively under the Chemicals Management Plan as the Aldehydes Group. The 5 substances are listed in the table below along with their Chemical Abstracts Service Registry Numbers, their Domestic Substances List (DSL) names and their common names.

Benzaldehyde, octanal, nonanal, and methylbenzaldehyde are reported to naturally occur in a variety of foods. Vanilla oils are also naturally occurring and are defined as the extractives and physically modified derivatives of Vanilla planifolia. All 5 substances in the Aldehydes Group were included in surveys issued pursuant to section 71 of CEPA. According to information submitted, octanal and methylbenzaldehyde were not imported or manufactured in Canada above the reporting threshold of 100 kg in 2011. Benzaldehyde, nonanal and vanilla oils were imported into Canada with quantities ranging from 123 kg to 9075 kg, while 3086 kg of benzaldehyde was manufactured in the same year. Reported uses include air care, cleaning and furnishing care, lubricants and greases, and personal care products.

In Canada, the substances in the Aldehydes Group have uses as ingredients in cosmetics, as formulants in pest control products, as non-medicinal ingredients in natural health products, and may be used as food flavouring agents and as components in the manufacture of certain food packaging materials. In addition, substances in the Aldehydes Group are present in various other products available to consumers, including air fresheners.

The ecological risks of the substances in the Aldehydes Group were characterized using the ecological risk classification of organic substances (ERC), which is a risk-based approach that employs multiple metrics for both hazard and exposure, with weighted consideration of multiple lines of evidence for determining risk classification. Hazard profiles are based principally on metrics regarding mode of toxic action, chemical reactivity, food web-derived internal toxicity thresholds, bioavailability, and chemical and biological activity. Metrics considered in the exposure profiles include potential emission rate, overall persistence, and long-range transport potential. A risk matrix is used to assign a low, moderate or high level of potential concern for substances on the basis of their hazard and exposure



profiles. Based on the outcome of the ERC analysis, the substances in the Aldehydes Group are considered unlikely to be causing ecological harm.

Read More

Government of Canada, 30-05-24

https://www.canada.ca/en/environment-climate-change/services/evaluating-existing-substances/assessment-aldehydes-group.html

## **EUROPE**

# **Switzerland Amends Chemical Ordinance to Align with EU Regulations**

2024-06-05

The revision takes into account the new developments in the EU, OECD and UN.

Switzerland has notified the WTO on May 27, 2024 of its intention to modify Annexes 2 and 3 of the Chemical Ordinance (ChemO), with the objective of enhancing the protection of the environment and human health and safety, as well as reducing trade barriers and facilitating trade. The proposed revision is expected to be adopted on August 2, 2024, and will come into effect on September 1, 2024.

The major changes are outlined in brief as follows:

#### Annex 2

- 28 substances or groups of substances are listed in the List of harmonized classifications and labeling of dangerous substances, and 24 existing entries are modified to align with 21st ATP of the EU CLP regulation;
- Introduce new EU hazard classes of endocrine disruptors, persistent chemicals, bioaccumulative chemicals, which will become mandatory in stages, first for substances, then for preparations;
- Incoporate latest developments in test methods (OECD, UN Manual of Test and Criteria) into Swiss legislation.

#### Annex 3

Add 7 entries to Annex 3 ChemO (List of Candidate Substances). In addition, one entry is updated.



# Bulletin Board

# **Regulatory Update**

JUN. 21, 2024

#### Read More

JUN. 21, 2024

Chemlinked, 05-06-24

https://chemical.chemlinked.com/news/chemical-news/switzerland-amends-chemical-ordinance-to-align-with-eu-regulations

## **EU Parliament backs revision of Toys Safety directive**

2024-03-21

Toxic chemicals do not belong in children's toys – and last week, the European Parliament took a strong position on making this a reality. With 603 votes in favour, 5 against and 15 abstentions, the Members of the European Parliament decided to support the revision of the current EU Toys Safety Directive.

Last week saw the European Parliament vote almost unanimously to improve toys legislation, which will update the directive that dates back to 2009. We now have greater knowledge of the harms that lurk in some children's toys and this move will bring toy safety up to date with what the science is telling us.

The legislation is set to ban the most harmful chemicals in toys, such as endocrine disruptors, the forever chemicals PFAS and bisphenols. It would also broaden the scope for restricting potentially harmful chemicals that bioaccumulate, persist and are toxic. Some of these chemicals have been linked to reduced immunity and increased risk of developing certain cancers, and even at low doses some can harm a child's development.

#### Read More

Chemtrust, 21-03-24

https://chemtrust.org/eu-parliament-backs-revision-toys-safety-directive/

# 73 EU candidates pledge a toxic-free future ahead of EU-elections

2024-06-04

In a move to prioritise public health and environmental sustainability, 19 leading environmental and health organisations have united to call on EU candidates to commit to a toxic-free Europe. This critical pledge comes just ahead of the upcoming EU elections, with 73 candidates from 23 national parties in 14 countries, including 16 heads of lists, vowing to address



the pervasive threat of chemical pollution. The Pledge remains open for

Today, chemical pollution is still a persistent menace in the EU. Harmful chemicals, including pesticides, are increasingly present in our food, water, air, soil, products, and even our bodies. The consequences are dire, with numerous health effects such as premature death, illness, infertility and cognitive impairments. Vulnerable groups, including children, pregnant women, the elderly and those facing health inequalities are particularly at risk.

The Toxic-free Pledge, developed by a coalition of experts from various health and environmental NGOs, outlines key actions for the next five years to combat the significant impact of harmful chemicals on health and the environment. There is still much work to be done to fully complete the ambition of the EU Chemicals Strategy for Sustainability. With 84% of EU citizens believing that EU environmental legislation is essential and 92% stating that companies should bear the costs of cleaning up pollution, swift action is crucial. This initiative aims to enhance health protection, drive innovation, and transition to safer, sustainable chemicals, ensuring a competitive EU industry.

Read More

EEB, 04-06-24

endorsement.

https://eeb.org/73-eu-candidates-pledge-a-toxic-free-future-ahead-of-eu-elections/

## **INTERNATIONAL**

# **EU and Australia Sign Partnership on Sustainable Critical and Strategic Minerals**

2024-05-28

The EU and Australia signed today a Memorandum of Understanding (MoU) for a bilateral partnership to cooperate on sustainable critical and strategic minerals.

The MoU was signed on behalf of the EU by Executive Vice-President and Commissioner for Trade Valdis Dombrovskis, and Commissioner for Internal Market, Thierry Breton. The signatories for Australia were Resources and Northern Australia Minister Madeleine King, and Minister for Trade and Tourism Don Farrell.

CHEMWATCH

# Bulletin Board

# **Regulatory Update**

JUN. 21, 2024

This partnership aims to support several common objectives, while based on mutual benefits. In particular, it seeks to enable the EU to diversify its supplies of materials necessary for the green and digital transitions, whilst contributing to the development of Australia's domestic critical minerals sector. The partnership covers the entire critical and strategic minerals value chain: exploration, extraction, processing, refining, recycling, and processing of extractive waste.

In addition to jointly developing projects along the entire value chain in the EU and in Australia, the partnership will also explore cooperation in countries where the EU and Australia have mutual interests, focusing on reducing environmental impacts and benefiting local communities. Additionally, it promotes innovative and digital technologies and services for mining, and other projects along the critical minerals value chain.

#### Areas of cooperation

JUN. 21, 2024

This MoU enhances cooperation between Australia and the EU in the following areas:

- Integration of sustainable raw materials value chains, including networking, joint facilitation of projects (e.g., via joint ventures), creation of new business models and promotion and facilitation of trade and investment linkages, ensuring the well-functioning, sustainability, and resilience of these critical supply chains.
- Cooperation on research and innovation along the raw materials value chains, including on minerals knowledge and the minimisation of environmental and climate footprint.
- Cooperation to promote high environmental, social, and governance standards and practices, as well as improved policy alignment, driven by full respect of worker's conditions and safety, and by the need of a sustainable and secure production of critical minerals.

#### Read More

Delegation of the European Union to Australia, 28-05-24

https://www.eeas.europa.eu/delegations/australia/eu-and-australia-sign-partnership-sustainable-critical-and-strategic-minerals\_en?s=163

## **IARC marks World No Tobacco Day 2024**

2024-05-31

Tobacco smoking remains the most important avoidable cause of cancer worldwide. Smokeless tobacco products are also an important

# Bulletin Board

## **Regulatory Update**

contributor to the global cancer burden. On World No Tobacco Day 2024, the International Agency for Research on Cancer (IARC) is supporting the World Health Organization (WHO) #TobaccoExposed campaign and highlighting the Agency's research on the impact of tobacco on the global burden of cancer.

To mark the day, IARC has released videos of IARC scientists Dr Isabelle Soerjomataram and Dr Béatrice Lauby-Secretan speaking about the contribution of tobacco use to the global cancer burden, how IARC tracks the impact of tobacco control policies, and how IARC evaluates approaches to prevent tobacco-related cancers. IARC is also making available social media tiles with a message from IARC scientist Dr Mahdi Sheikh: it's never too late to quit smoking, even after a cancer diagnosis.

In addition, IARC scientists Dr Béatrice Lauby-Secretan and Dr Hilary Robbins are presenting their research on prevention and screening for lung cancer and oral cancer at the Seventy-seventh World Health Assembly during a World No Tobacco Day side event on 31 May 2024.

IARC research shows that tobacco smoking causes at least 20 different types of cancer. The use of smokeless tobacco products is among the leading causes of oral cancer in countries where they are commonly used. Quitting smoking after a cancer diagnosis, even with a late-stage cancer, can reduce the risk of cancer progression or cancer death by half.

#### **Read More**

WHO, 31-05-24

https://www.iarc.who.int/news-events/iarc-marks-world-no-tobacco-day-2024/

CHEMWATCH

# Bulletin Board

# **REACH Update**

JUN. 21, 2024

# **European Commission decisions on applications for authorisation**

2024-06-07

IUN. 21, 2024

The Commission has granted an authorisation for one use of Chromium trioxideand refused an authorisation for two uses of Sodium dichromate.

Find the substances and all details on the Commission website.

Read More

ECHA, 07-06-24

https://ec.europa.eu/docsroom/documents/60075

## Assessment of regulatory needs reports published

2024-06-13

Reports for the following substance groups are now available on our website:

- Benzophenones not alkyl- nor p-amino, and other hydroxy substituted
- Hydroxyphenyl benzotriazoles

Read More

ECHA, 13-06-24

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

# Consultations on harmonised classification and labelling

2024-06-13

We are looking for comments on the harmonised classification and labelling (CLH) proposals for:

- O-isopropyl ethylthiocarbamate (EC 205-517-7, CAS 141-98-0);
- 1-ethoxy-2-(2-methoxyethoxy)ethane (EC 213-690-5, CAS 1002-67-1);
- Silica, amorphous, fumed, cryst.-free; Pyrogenic, synthetic amorphous silica, nano [1]
- Silica gel, pptd., cryst.-free; Precipitated silica, silica gel, colloidal silica, amorphous, nano [2] (EC -[1]; -[2], CAS 112945-52-5 [1]; 112926-00-8
   [2]); and
- flonicamid (ISO); N-(cyanomethyl)-4-(trifluoromethyl)pyridine-3carboxamide (EC -, CAS 158062-67-0).

# Bulletin Board

# **REACH Update**

The flonicamid (ISO); N-(cyanomethyl)-4-(trifluoromethyl)pyridine-3-carboxamideproposal format combines the draft (renewal) assessment report prepared according to the Plant Protection Products Regulation and the proposal for CLH under the CLP regulation. For additional information, consult the European Commission's Guidelines on Active Substances and Plant Protection Products.

For more information on this active substance and on the studies included in the CLH report, consult the draft assessment report on the European Food Safety Authority's consultation website.

Have your say until 9 August 2024.

Read More

ECHA, 13-06-24

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

**CHEMWATCH** 

# Bulletin Board

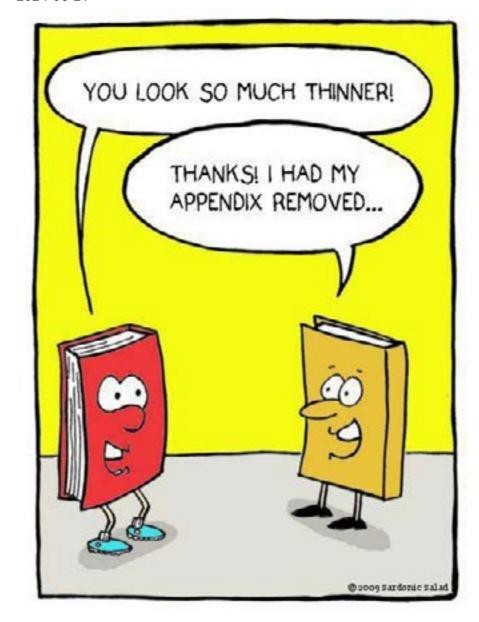
## Janet's Corner

JUN. 21, 2024

**Appendix** 

2024-06-21

JUN. 21, 2024



https://sardonicsalad.blogspot.com/2009/

# **CHEMWATCH** Bulletin Board UN. 21, 2024

**Hazard Alert** 

## **Phenanthrene**

2023-05-12

#### **USES [2,3]**

2-Hexanone was used in the past in paint and paint thinner, to make other chemical substances, and to dissolve oils and waxes. It is no longer made or used in the United States because it has harmful health effects. It is formed as a waste product resulting from industrial activities such as making wood pulp and producing gas from coal, and in oil shale operations.

#### **EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]**

### **Exposure Sources**

- Breathing contaminated air;
- Drinking contaminated water;
- Absorbing it through your skin if you touch liquid or soil that contains
- Eating some foods that naturally contain low levels of 2-hexanone;
- Using products manufactured before 1982 that contain 2-hexanone (such as paint thinners);
- Working in coal gasification, oil shale processing, or wood pulping
- Living near hazardous waste sites where it is found, or if you breathe the contaminated air.

#### **Routes of Exposure**

Inhalation is the primary route of exposure to 2-hexanone; however, dermatologic exposure can lead to skin irritation and this absorption may contribute to chronic exposure and polyneuropathy. Ingestion has rarely been reported.

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

#### **Acute Health Effects**

- Contact with 2-hexanone can irritate the skin and eyes;
- Inhalation can cause coughing and wheezing;

2-Hexanone is the organic compound with the formula C4H9COCH3. This colourless to pale yellow liquid has a sharp odour. It is a ketone and often known either as MBK (methyl butyl ketone) or 2-hexanone. It has moderate water solubility, and can evaporate easily into the air as a vapour. [1,2]

CHEMWATCH

# Illetin Board

## **Hazard Alert**

JUN. 21, 2024

Exposure can cause headache, dizziness, light-headedness, and fainting

#### **Carcinogenicity**

The Department of Health and Human Services has not classified 2-hexanone as to human carcinogenicity. In addition, the International Agency for Research on Cancer and the Environmental Protection Agency (EPA) have not classified 2-hexanone as to human carcinogenicity. There is no information available on the potential carcinogenic effects of 2-hexanone in people or in experimental animals.

#### **Other Effects**

In animal studies, there was evidence that 2-hexanone damaged the male (testes) reproductive system and pregnant rats inhaled it did not gain as much weight during their pregnancy, had fewer babies, and had babies that were smaller and less active than the rats that were not exposed. It is unknown if breathing 2-hexanone affects human reproduction or causes birth defects.

#### **SAFETY**

#### First Aid Measures [5]

- **Eye Contact:** Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.
- **Skin Contact:** After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cold water may be used. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.
- Serious Skin Contact: Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek medical attention.
- **Inhalation:** Allow the victim to rest in a well-ventilated area. Seek immediate medical attention.
- Serious Inhalation: Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If

# Bulletin Board

## **Hazard Alert**

breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

• **Ingestion:** Do not induce vomiting. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

#### **Workplace Controls & Practices [4]**

The following work practices are also recommended:

Exhaust ventilation or other engineering controls should be used to keep the airborne concentrations of vapours below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

#### **Personal Protective Equipment [5]**

The following personal protective equipment is recommended when handling 2-hexanone:

- Splash goggles;
- Lab coat;
- Vapour respirator (be sure to use an approved/certified respirator or equivalent);

#### Gloves.

Personal Protection in Case of a Large Spill:

- Splash goggles;
- Full suit;
- Vapour respirator;
- Boots;
- · Gloves;
- A self contained breathing apparatus should be used to avoid inhalation of the product.
- Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

#### **REGULATION**

#### **United States**

The following exposure limits are for Coal Tar Pitch Volatiles:

## CHEMWATCH

# Bulletin Board

## **Hazard Alert**

JUN. 21, 2024

- OSHA: The Occupational Safety and Health Administration has set a limit of 5 ppm (5 parts of 2-hexanone in 1 million parts of air) as an average exposure level to this chemical over a 40-hour work week.
- ACGIH: The American Conference of Governmental Industrial Hygienists has made the same recommendation.
- NIOSH: The National Institute for Occupational Safety and Health recommends an even lower limit, 1 ppm, as an average exposure during a 10-hour period.

#### **REFERENCES**

IUN. 21, 2024

- 1. <a href="http://www.atsdr.cdc.gov/toxfaqs/tfacts44.pdf">http://www.atsdr.cdc.gov/toxfaqs/tfacts44.pdf</a>
- 2. <a href="http://www.atsdr.cdc.gov/ToxProfiles/tp44-c1-b.pdf">http://www.atsdr.cdc.gov/ToxProfiles/tp44-c1-b.pdf</a>
- 3. <a href="http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=11583">http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=11583</a>
- 4. <a href="http://nj.gov/health/eoh/rtkweb/documents/fs/1280.pdf">http://nj.gov/health/eoh/rtkweb/documents/fs/1280.pdf</a>
- 5. <a href="http://www.sciencelab.com/msds.php?msdsId=9924258">http://www.sciencelab.com/msds.php?msdsId=9924258</a>
- 6. <a href="http://www.safeworkaustralia.gov.au/sites/swa/search/results?k=2-hexanone">http://www.safeworkaustralia.gov.au/sites/swa/search/results?k=2-hexanone</a>

# Bulletin Board Gossip JUN. 21, 2024

Is Plant-Based "Fake" Meat Good for Your Health?

2024-06-19

Fake burgers. Fake bacon. Fake sausages. Even fake chicken and sweetcorn sandwiches. These days, there doesn't seem to be a meat product that doesn't have its own ersatz vegan doppelgänger, and consumers are lovin' it; in the US alone, the size of the plant-based food market more than doubled between 2017 and 2023, growing from \$3.9 billion to \$8.1 billion.

In parallel, the research field supporting the health benefits of plant-based diets has also bloomed in recent years. According to a meta-review published in PLOS One this year, the health benefits of vegetarianism and veganism are unmistakable; compared to meatier diets, plant-based ones were firmly associated with better health outcomes regarding blood pressure, blood sugar management and body mass index scores, as well as lower incidences of ischemic heart disease and gastrointestinal and prostate cancers.

The two phenomena seem like the perfect match. More people turning to plant-based diets just as more promising plant-based research is published? Time to crack open the plant-based party sausages and celebrate healthy living!

There's a catch, though: nearly every study demonstrating the health benefits of plant-based diets examined the effects of actual plant-derived ingredients, like vegetables, legumes and nuts; fabricated food items like "lamb kebabs" made from pea protein and emulsifiers were not considered.

So, based off this mounting plant-based research alone, there's no guarantee that that plant-based chicken shawarma is any good for you. It could even pose some health risks of its own...

After all, such manufactured fake meats meet the definition of ultraprocessed foods – the very class of artificially altered food thought to contribute to the rise of obesity, cardiovascular disease and cancers seen in the Western world.

Which is it, then? Are fake meats the healthy, greener alternative to the fatty flesh of cows and pigs? Or are they just another counterfeit component of the West's new detrimental diet?

Let's dig into the few relevant studies on plant-based meat substitutes to find out.

## CHEMWATCH

# Bulletin Board

Gossip

JUN. 21, 2024

#### What does the research say?

Perhaps unsurprisingly, only a handful of studies investigating the nutritional qualities of plant-based "meats" have been conducted so far. Nonetheless, a consensus is already building.

According to these studies, when compared to their meaty counterparts, plant-based alternatives are generally lower in saturated fat, higher in sugars and lacking in nutrients like vitamin B12 and iron.

In a paper published in Nutrients in 2019, researchers from Australia's Grains & Legumes Nutrition Council found that less than a quarter of purchased meat alternatives (24%) were fortified with B12. Only 20% were fortified with iron and 18% were packed with zinc. Most of the 137 fake meat products tested were also lower in kilojoules(kJ) and total fat and saturated fat, but higher in carbohydrates and dietary fiber when compared with actual meat. The majority of the products (96%) were also high in sodium.

This last finding in particular led the researchers to conclude that alternative meats may pose their own health concerns, given that salt is "the leading dietary factor in terms of the global burden of disease."

Other researchers (who may or may not be less biased towards grains and legumes) have produced slightly different results when testing plant-based "meats".

In a paper published in Nutrition & Dietetics in 2023, researchers from the University of Sydney found their tested alternative meats to be lower in sodium than the real meats. Like the Grains & Legumes researchers, though, they found that the 132 plant-based foods they analyzed were lower in saturated fats and higher in sugars than the foods' fleshy counterparts. Similarly, only 12.1% of the meat analogs were fortified with iron, B12 and zinc.

Another study published in the Journal of Food Composition and Analysis last year found that, out of 216 meat alternatives, most had an average energy content similar to that of meatier versions. The range of these energy values, however, varied to a greater degree (ranging from 267-1,796 kJ per 100 g) than the range of the meat products.

Fake sausages had the highest average sodium content (494 mg per 100 g), but this value was still lower than the average sodium content for real sausages (611 mg). These bogus bangers also had similar levels of protein and saturated fat to the real sausages.

Copyright Chemwatch 2024 © Copyright Chemwatch 2024 © Copyright Chemwatch 2024 © 23

# Bulletin Board Gossip JUN. 21, 2024

Foods made from tempeh (fermented soybeans) were typically lower in energy and fat than foods made from mycoprotein and tofu, but higher in

Ultimately, these studies tend to come to the same general conclusion: meat substitutes may offer convenience and familiarity, but they are likely to be less healthy, less sustainable and more costly than actual plant-derived foods like legumes and vegetables.

#### What do the experts say?

sugar and dietary fiber.

For the sake of our health, should we be cutting down on our plant-based meat as well as the real thing?

Not completely, say some experts. When it comes to choosing our next meal, it's best to measure meat substitutes on the same principles we measure other foods on: their levels of salt, sugar, fat, protein and nutrients, they say. After all, not all fake meats are equal in nutrition.

"If you're looking at sausages, there's a tendency for plant-based sausages to be high in salt – something for consumers to be aware of," Dr. Duane Mellor, a registered dietician and spokesperson for the British Dietetic Association, says.

Other than minimizing one's intake of synthetic bangers, Mellor says a health-minded plant-based dieter could also benefit from keeping their shopping basket as "naked" as possible.

"In terms of health effects, they're [plant-based "meats"] going to be minus some of the nutrients," he says. "Possibly they're going to be a low fat, low salt, protein alternative to meat. If you start wrapping it in breadcrumbs, if you start wrapping it in pastry, if you start adding it to a creamy, rich sauce – it might be slightly better than the meat alternative – but it's not going to be a healthy option. A sausage roll is still a sausage roll. A chicken Kyiv is still a Kyiv. You've still got all that fat in there, that salt."

"If it's closer to the naked meat version, it might be technically ultraprocessed," he continued, "but it hasn't got all those things that bind it together," he adds. "Is it going to have any negative health benefits? Probably not, apart from you needing to replace those key vitamins and minerals you might be missing out on."

Unsurprisingly, producers of plant-based meat alternatives have a slightly different outlook on the position such foods should have in our diets.

CHEMWATCH

# Bulletin Board

Gossip

JUN. 21, 2024

Like Mellor, Andy Shovel, founder of THIS, the third largest meat substitute manufacturer the UK, acknowledges that fake meats can have their unhealthier qualities when compared to plant products like vegetables and legumes. However, he says, THIS's products aren't substituting vegetables and legumes – they're substituting meat.

"It's funny, because some people say, 'Well, they're not healthy products.' And you're like, 'Well, are you comparing them to an aubergine [eggplant], or a salad? Or are you comparing them to the meat products that we're trying to substitute out?" Shovel told Technology Networks during an Ask Me Anything webinar held earlier this year.

"You can't compare our plant-based bacon to ratatouille. You have to compare it to pork bacon, because that's what we're trying to substitute. And when you do that – our plant-based bacon and bacon – it's like night and day in terms of health," he said. "We've got, like, five percent of the fat, two percent of the saturated fat, [and] we've got half the salt. So, I think it's always important that people make really fair comparisons with absolute parity between the meat version and our version when thinking about nutrition."

### So, is fake meat healthy?

Based off existing research, it appears meat alternatives made from mycoprotein and soy can come with some unwholesome properties. Many products are high in sugars and lacking in the essential nutrients like B12 that their fleshier counterparts offer. And while most meat analogs are lower in saturated fats than the fleshy foods they're aping, these fat values have a wide range over different products and brands; veggie sausages, in particular, appear to recreate the unhealthy qualities of their meaty lookalikes more than most substitutes.

And yet, by several measures, many of these products are still healthier than the real-deal fleshy foods. With a little B12 and iron supplementation, they could offer a healthier option for those wanting to eat less meat, which is the exact kind of substitution the manufacturers say their products are intended for.

The consensus is clear that diets filled with plant products, cooked from scratch, offer bountiful benefits to human health. If such a diet included the odd veggie burger rather than the odd genuine burger, it's hard to imagine any substantial harm to health, accounting for adequate B12 and zinc intake, too.

**G0331**P

#### **About the interviewees**

Dr. Duane Mellor is an award-winning registered dietitian and science communicator.

Andy Shovel is an entrepreneur and influential figure in the sphere of sustainable food innovation in the UK.

Technology Networks, 19 June 2024

https://technologynetworks.com

# New material puts eco-friendly methanol conversion within reach

2024-06-17

Griffith University researchers have developed innovative, eco-friendly quantum materials that can drive the transformation of methanol into ethylene glycol.

Ethylene glycol is an important chemical used to make polyester (including PET) and antifreeze agents, with a global production of over 35 million tons annually with strong growth.

Currently, it's mainly produced from petrochemicals through energy-intensive processes.

Methanol (CH3OH) can be produced sustainably from CO2, agricultural biomass waste, and plastic waste through various methods such as hydrogenation, catalytic partial oxidation, and fermentation. As a fuel, methanol also serves as a circular hydrogen carrier and a precursor for numerous chemicals.

Led by Professor Qin Li, the Griffith team's method uses solar-driven photocatalysis to convert methanol into ethylene glycol under mild conditions.

This process uses sunlight to drive chemical reactions, which minimises waste and maximises the use of renewable energy.

While previous attempts at this conversion have faced challenges -- such as the need for toxic or precious materials -- Professor Li and the research team have identified a greener solution.

"Climate change is a major challenge facing humanity today," Professor Li said.

CHEMWATCH

# Bulletin Board

Gossip

JUN. 21, 2024

"To tackle this, we need to focus on zero-emission power generation, lowemission manufacturing, and a circular economy. Methanol stands out as a crucial chemical that links these three strategies.

"What we have created is a novel material that combines carbon quantum dots with zinc selenide quantum wells."

"This combination significantly enhances the photocatalytic activity more than four times higher than using carbon quantum dots alone, demonstrating the effectiveness of the new material," Lead author Dr Dechao Chen said.

The approach has also shown high photocurrent, indicating efficient charge transfer within the material, crucial for driving the desired chemical reactions.

Analyses confirmed the formation of ethylene glycol, showcasing the potential of this new method. It's worth noting that the by-product of this reaction is green hydrogen.

This discovery opens up new possibilities for using eco-friendly materials in photocatalysis, paving the way for sustainable chemical production.

As a new quantum material, it also has the potential to lead to further advancements in photocatalysis, sensing, and optoelectronics.

"Our research demonstrates a significant step towards green chemistry, showing how sustainable materials can be used to achieve important chemical transformations," Professor Li said.

"This could transform methanol conversion and contribute significantly to emissions reduction."

The findings 'Colloidal Synthesis of Carbon Dot-ZnSe Nanoplatelet Vander Waals Heterostructures for Boosting PhotocatalyticGeneration of Methanol-Storable Hydrogen' have been published in the journal Small.

Science Daily, 17 June 2024

https://sciencedaily.com

# New material puts eco-friendly methanol conversion within reach

2024-06-17

Griffith University researchers have developed innovative, eco-friendly quantum materials that can drive the transformation of methanol into ethylene glycol.

Ethylene glycol is an important chemical used to make polyester (including PET) and antifreeze agents, with a global production of over 35 million tons annually with strong growth.

Currently, it's mainly produced from petrochemicals through energy-intensive processes.

Methanol (CH3OH) can be produced sustainably from CO2, agricultural biomass waste, and plastic waste through various methods such as hydrogenation, catalytic partial oxidation, and fermentation. As a fuel, methanol also serves as a circular hydrogen carrier and a precursor for numerous chemicals.

Led by Professor Qin Li, the Griffith team's method uses solar-driven photocatalysis to convert methanol into ethylene glycol under mild conditions.

This process uses sunlight to drive chemical reactions, which minimises waste and maximises the use of renewable energy.

While previous attempts at this conversion have faced challenges -- such as the need for toxic or precious materials -- Professor Li and the research team have identified a greener solution.

"Climate change is a major challenge facing humanity today," Professor Li said.

"To tackle this, we need to focus on zero-emission power generation, lowemission manufacturing, and a circular economy. Methanol stands out as a crucial chemical that links these three strategies.

"What we have created is a novel material that combines carbon quantum dots with zinc selenide quantum wells."

"This combination significantly enhances the photocatalytic activity more than four times higher than using carbon quantum dots alone, demonstrating the effectiveness of the new material," Lead author Dr Dechao Chen said.

CHEMWATCH

# Bulletin Board

Gossip

JUN. 21, 2024

The approach has also shown high photocurrent, indicating efficient charge transfer within the material, crucial for driving the desired chemical reactions.

Analyses confirmed the formation of ethylene glycol, showcasing the potential of this new method. It's worth noting that the by-product of this reaction is green hydrogen.

This discovery opens up new possibilities for using eco-friendly materials in photocatalysis, paving the way for sustainable chemical production.

As a new quantum material, it also has the potential to lead to further advancements in photocatalysis, sensing, and optoelectronics.

"Our research demonstrates a significant step towards green chemistry, showing how sustainable materials can be used to achieve important chemical transformations," Professor Li said.

"This could transform methanol conversion and contribute significantly to emissions reduction."

The findings 'Colloidal Synthesis of Carbon Dot-ZnSe Nanoplatelet Vander Waals Heterostructures for Boosting PhotocatalyticGeneration of Methanol-Storable Hydrogen' have been published in the journal Small.

Science Daily, 17 June 2024

https://sciencedaily.com

# New Seashell-Inspired Building Material Is 17 Times Tougher Than Cement

2024-06-12

Inspired by the material that makes up oyster and abalone shells, engineers at Princeton have created a new cement composite that is 17 times more crack-resistant than standard cement and 19 times more able to stretch and deform without breaking. The findings could eventually help increase the crack resistance of a wide range of brittle ceramic materials, from concrete to porcelain.

"If we can engineer concrete to resist crack propagation, we can make it tougher, safer and more durable," said researcher Shashank Gupta, a graduate student in Reza Moini's lab in the Department of Civil and Environmental Engineering.

# Bulletin Board Gossin Jun. 21, 2024

In an article published June 10 in the journal Advanced Funct

In an article published June 10 in the journal Advanced Functional Materials, the research team led by Moini, an assistant professor of civil and environmental engineering, reported that creating alternating layers of tabulated cement paste and thin polymer can significantly increase crack resistance and the ability to deform without completely breaking (ductility).

Moini's lab often looks to biology for inspiration in its work on building materials. In this case, the team developed a composite inspired by a natural material called nacre, or mother of pearl, which is found inside certain shells. Gupta said that at the microscopic level, nacre consists of hexagonal tablets of the hard mineral aragonite glued together by a soft biopolymer.

The aragonite tablets contribute significantly to nacre's strength, while the biopolymer adds flexibility and crack resistance. The toughening mechanism involves the aragonite tablets sliding under stress, which, along with other mechanisms, allows the nacre to dissipate energy. This sliding action, combined with the crack deflection and biopolymer deformation, enables nacre to endure substantial mechanical stress while maintaining its structural integrity, making it both strong and resilient.

"This synergy between the hard and soft components is crucial to nacre's remarkable mechanical properties," Gupta said.

The Princeton team has developed innovative composites inspired by nacre, utilizing conventional construction materials like Portland cement paste combined with a limited amount of polymer. They alternated layers of cement paste sheets with a highly stretchable polymer, polyvinyl siloxane. The researchers created multi-layered small beams by alternating cement paste sheets with thin layers of polymer. These beams were then subjected to a notched three-point bending test, where each beam was tested under flexure to evaluate crack resistance (or fracture toughness).

In the experiment, the researchers produced three types of beams. The first type consisted of alternating layers of cement paste sheets and thin polymer. For the second type, they used a laser to engrave hexagonal grooves into the cement paste sheets. These grooved sheets were then stacked with thin polymer layers in between. The third type was similar to the third, but the researchers cut through the cement completely, creating separated hexagonal tablets connected by the polymer layer. These cement-paste tablets lay atop the polymer layer similarly to how aragonite lies on the biopolymer layer in nacre. These three types were compared against a reference solid (monolithic) cast cement paste counterpart.

CHEMWATCH

# Bulletin Board

Gossip

JUN. 21, 2024

The experiments revealed that the failure of the reference beams was brittle — meaning that the beams broke suddenly and completely upon reaching their failure point, with no ductility. The beams with alternating layers, both grooved and non-grooved, demonstrated increased ductility and resistance to cracking.

The most significant results were observed in the beams with completely separated hexagonal tablets, which are similar to nacre. These beams exhibited 19 times the ductility and 17 times the fracture toughness while retaining nearly the same strength as the solid cement paste beam.

"Our bio-inspired approach is not to simply mimic nature's microstructure but to learn from the underlying principles and use that to inform the engineering of human-made materials. One of the key mechanisms that makes a nacreous shell tough is the sliding of the tablet at the nanometer level. Here, we focus on the mechanism of tablet sliding by engineering the built-in tabulated structure of cement paste in balance with the properties of the polymer and the interface between them." Moini said. "In other words, we intentionally engineer defects in the brittle materials as a way to make them stronger by design."

The researchers noted that the findings are based on lab conditions and that it would take additional work and research to develop the techniques for use in the field. They are working to determine whether the structures' fracture toughness and ductility apply to other ceramic materials beyond cement paste, such as concrete.

"We are only scratching the surface; there will be numerous design possibilities to explore and engineer the constitutive hard and soft material properties, the interfaces, and the geometric aspects that play into the fundamental size effects in construction materials," Moini said.

Technology Networks, 12 June 2024

https://technologynetworks.com

# Chemists develop technique for extending nitrene reactions to three days

2024-06-20

A team of chemists at the University of Bremen, in Germany has developed a new type of nitrene capable of slow reactions that can last for up to three days. Their paper is published in the journal Science.

# Bulletin Board Gossip JUN. 21, 2024

Nitrenes (reactive intermediates and analogs of carbenes) are types of electrophile molecules that have a neutral atom bonded to a single other substituent. Because they have just six electrons in their valence level, they have brief reaction times, generally measured in the nanoseconds. That

has made it difficult for chemists to use them in commercial applications.

In this new study, the researchers have found a way to dramatically slow nitrene reactions, by synthesizing a slow-reacting nitrene, possibly allowing for a whole new class of nitrenes that could be used in a wide variety of applications.

To achieve this feat, the research team employed the use of a MSFluind—a type of chemical scaffolding first built back in 2011 by another team. It has been used in other recent research efforts to stabilize other molecules, some of which are similar to nitrenes.

Using the scaffolding, the researchers were able to separate the components in a reaction from accessing the nitrogen atom, allowing for a much slower process. More specifically, they shone an ultraviolet light on a sample of MSFluindN3(an azide precursor), which reduced it to MSFluindN.

The researchers then subjected the newly synthesized nitrene to X-ray crystallography to learn more about its characteristics, followed by electron paramagnetic resonance spectroscopy and then superconducting quantum interference device magnetometry.

They confirmed that it had kept its spin-triplet ground state and persisted for up to three days. They also note that such imaging techniques are not normally possible with nitrene due to their fast reaction times.

The research team suggests their newly developed technique should allow for the synthesis of new transition metal complexes.

Phys Org, 20 June 2024

https://phys.org

# **Dark Chocolate May Pose Slight Heavy Metal Risk to Children**

2024-06-05

Most dark chocolate bars don't pose a heavy metal health risk to adults or children, according to a new study.

CHEMWATCH

# Bulletin Board

Gossip

JUN. 21, 2024

A minority of bars (4 out of 155) tested by researchers, however, did contain levels of cadmium unsafe for children to consume in excess (more than 2 bars per week).

The findings appear to stand in contrast to the well-publicized results of a 2023 Consumer Report, which concluded that a third of chocolate products tested contained harmful levels of lead and cadmium.

The results of the new study were published in Food Research International.

### **Heavy handed**

Cocoa crops can absorb heavy metals, particularly cadmium, from surrounding soil. The harvested cocoa beans can then become contaminated with lead during handling and processing.

To help determine the level of heavy metals in chocolate in the US, Tulane University researchers first went out to stores and bought 155 chocolate bars, 101 of which were dark chocolate, all made from cocoa sourced from 5 major regions: Asia Pacific, West Africa, East Africa, South America and Central America.

Samples from bars were tested for 16 heavy metals, ranging from the toxic (lead and cadmium) to the essential (copper, iron, zinc).

To gauge the safety of eating the bars, the researchers modeled the risk of eating 1 ounce (28 grams) of the chocolates per day, which is equivalent to consuming more than 2 whole chocolate bars a week.

For every respective heavy metal, the average level found in the 155 bars was within acceptable, safe-to-consume limits for adults.

Only 1 brand of Colombian dark chocolate exceeded the international limit for cadmium in bars (800 micrograms per kilogram) set by the European Commission Regulation. Four dark chocolate bars contained cadmium levels that could pose a risk to children weighing 33 pounds (15 kilograms) or less, the average weight of a 3-year-old in the US.

"For adults there is no adverse health risk from eating dark chocolate, and although there is a slight risk for children in 4 of the 155 chocolate bars sampled," said lead author Dr. Tewodros Godebo, assistant professor of environmental health sciences at Tulane University School of Public Health and Tropical Medicine.

Copyright Chemwatch 2024 © Copyright Chemwatch 2024 © Copyright Chemwatch 2024 ©



Gossip

Godebo tempered the concerning finding, however, saying that a child would need to consume at least two bars of dark chocolate a week to be at significant risk.

"It is not common to see a three-year-old regularly consume more than two bars of chocolate per week," she added. "What we've found is that it's quite safe to consume dark chocolate and milk chocolates."

Cacao originating from West African countries tended to contain lower cadmium and lead levels than those sourced from Central and South America.

Two chocolate bars contained lead levels above California's interim standards for dark chocolates, but neither bar was determined by the researchers to pose adverse risks to children or adults.

All essential heavy metals (magnesium, calcium, etc.) were more present in the dark chocolate bars than the milk chocolate ones. Several of the bars provided more than 50% of the daily requirement for children and adults – a health benefit of dark chocolates that shouldn't be overshadowed by the study's few unsavory findings, said Godebo.

"Not only is it [dark chocolate] packed with these essential minerals, but they can potentially reduce the absorption of toxic metals in the intestine since these metals compete for the same site," Godebo said.

This article is a rework of a press release issued by Tulane University. Material has been edited for length and content.

Technology Networks, 05 June 2024

https://technologynetworks.com

# "Cocktail Effect" Explains How Tin Toughens Titanium Alloy Medical Implants

2024-06-07

Beta( $\beta$ )-type titanium (Ti) alloys are renowned for their strength, formability and resistance to harsh environments. This, along with their excellent biocompatibility, has made them adequately suited for implants and prosthetics, from joint replacement to stents.

However, under certain conditions a brittle omega phase can form, making the material prone to breaking. Whilst it is known that adding tin

CHEMWATCH

# Bulletin Board

Gossip

JUN. 21, 2024

(Sn) negates this, and makes  $\beta$ -type Ti alloys stronger, the exact mechanics behind this has continued to puzzle scientists. That is until now.

A research team led by Norihiko Okamoto and Tetsu Ichitsubo from Tohoku University's Institute for Materials Research (IMR) has revealed how this occurs. Their revelation came via a systematic investigation using model titanium-vanadium (Ti-V) alloys, which included a combination of experiments and theoretical analyses.

"Our findings reveal that the multi-element interaction between Ti, V, and Sn, coupled with the anchoring effect of Sn atoms, work together to completely suppress the formation of the detrimental omega phase, exemplifying the so-called cocktail effect," explained Ichitsubo.

Just like skillfully blending various drinks often results in a cocktail that is more delicious than imagined, the cocktail effect in the metallurgical field refers to the phenomenon where mixing multiple elemental components in a well-balanced ratio can lead to superior properties beyond expectations.

"This cocktail effect is a prime example of the phenomena observed in high-entropy materials, highlighting the importance of considering multi-element interactions in alloy design," adds Okamoto. "This discovery underscores the significance of accounting for multi-element interactions not just for biomaterials but also in the broader context of alloy design."

Understanding the finite details of strengthening  $\beta$ -type Ti alloys will help improve biomedical titanium implants, which provide invaluable support for people suffering from degenerative bone condition or aging populations.

The study, which was published in the journal Acta Materialia on April 29, 2024, drew heavy inspiration from the pioneering work by Shuji Hanada and Naoya Masahashi, emeritus professors at IMR.

Technology Networks, 07 June 2024

https://technologynetworks.com

Gossip

# Old drugs new tricks—novel approach shows 'enormous potential' for rapid antibiotic discovery

2024-06-19

An innovative project to re-purpose existing drugs for their potential as antibiotics has uncovered a highly promising candidate with a potent and unique way of killing drug resistant bacteria.

A research collaboration between the University of Leiden, the Netherlands and the John Innes Centre, UK screened a chemical library of 352 small molecules for antimicrobial activity. These molecules have found uses in human therapies for cancer but had not been tested for their ability to kill harmful bacteria like Escherichia coli.

The screen identified 12 compounds that inhibited bacterial growth. The most potent of these, a representative of a class of compounds called isoquinoline sulfinamides, was chemically optimized by researchers at the University of Leiden.

The enhanced compound, LEI-800, exhibited antimicrobial activity against E. coli and K. pneumoniae, two gram-negative bacteria that often cause hospital acquired infections.

To find out why the compounds were able to kill these harmful bacteria, researchers selected naturally occurring resistant strains. They discovered that all the resistant strains contained mutations in genes that encoded the bacterial enzyme DNA gyrase, indicating this was the compound's target.

Gyrase is a bacterial topoisomerase: an enzyme that breaks and rejoins DNA to remove knots and entanglements and therefore is essential for bacterial growth. While gyrase itself does not occur in humans, human mitochondria have a similar enzyme called topoisomerase II, which fluoroquinolone antibiotics can inhibit, leading to potential adverse effects. However, the effectiveness of fluoroquinolones is severely compromised by growing bacterial resistance.

The John Innes team used cryo-EM microscopy to confirm that LEI-800 was indeed binding to E. coli gyrase and inhibiting it in an unprecedented way by preventing the enzyme from cutting DNA.

The search for new antibiotics is a global health emergency with new antibiotics urgently needed to keep pace with drug-resistant gramnegative bacteria. This study paves the way for the development of an

CHEMWATCH

# Bulletin Board

Gossip

JUN. 21, 2024

entirely novel class of molecules targeting gram negative bacteria that have become resistant to existing drugs.

"It's exciting that we can find an entirely new type of antibiotic in this way," says one of the authors of the study, Dr. Dmitry Ghilarov from the John Innes Centre.

"Repurposing an existing library of successful compounds derived for other uses is a valuable approach because it takes away all the costs associated with a synthesis of a new library.

"The unique binding pocket of the compound (the way in which it interacts with the target enzyme) means that the compound could offer an extra line of attack if used in tandem with existing antibiotics which are partially effective."

The approach outlined in this study promises more discoveries in the future, says Dr. Ghilarov. He adds, "It is amazing to think that we screened a small library designed to target one class of enzymes, human kinases, and found an entirely novel topoisomerase inhibitor.

"In terms of the chemistry available to drug discovery companies, that is a small amount—they screen millions of compounds so the potential for drug discovery using this approach is enormous."

Well-known examples of drug repurposing include the anti-inflammatory drug aspirin that at low doses acts as a selective anti-blood clot drug, or sildenafil (Viagra) the erectile dysfunction drug that was originally developed to control blood pressure.

Dr. Ghilarov says, "Biology is incredibly complex, there are thousands of different proteins in every cell presenting myriads of accessible surfaces, and it should not be surprising that a small molecule could bind to more than a single target.

"Repurposing is at the core of how humanity discovered medicines from nature: indeed, many anti-cancer drugs, such as doxorubicin or bleomycin are produced by soil bacteria Streptomyces to eliminate their bacterial competitors."

Next steps for this research are to further optimize LEI-800 and move forward towards clinical trials and commercialization.



The paper, "Discovery of isoquinoline sulfonamides as allosteric gyrase inhibitors with activity against fluoroquinolone-resistant bacteria," appears

Phys Org, 19 June 2024

in Nature Chemistry.

https://phys.org

## **Eating Small Fish May Prolong Life in Women**

2024-06-18

Japanese women who regularly eat small fish whole have lower levels of mortality than women who don't, according to a new study.

Given that small fish like juvenile anchovies and sardines are high in calcium, vitamin A and D, researchers from the Nagoya University School of Medicine posit that these nutrients may help reduce tumor development and cancer mortality.

These apparent benefits, however, were not seen as strongly in the male participants of the study.

The results were published in Public Health Nutrition.

#### Plenty more fish in the quay

"Previous studies have revealed the protective effect of fish intake on health outcomes, including mortality risks. However, few studies have focused on the effect of the intake of small fish specifically on health outcomes," said lead researcher Dr. Chinatsu Kasahara of the Nagoya University School of Medicine. "I was interested in this topic because I have had the habit of eating small fish since childhood. I now feed my children these foods."

To investigate further, Kasahara and their team accessed data from an ongoing Japanese health cohort. They identified 80,802 participants (42.77% males, 57.23% females, average age: 54.7) who had completed a dietary questionnaire.

The team then compared the health information and mortality levels of the participants between their first data entry and another entry after an average follow-up time of nine years.

Over that time, 2,482 of the participants died, 1,495 of whom from cancer, 340 from cardiovascular disease and 647 from other causes.

CHEMWATCH

# Bulletin Board

Gossip

JUN. 21, 2024

The female participants who reported consuming small fish every day, however, had significantly lower levels of all-cause and cancer mortality than other participants, even after considering the intake of larger fish.

Women who ate small fish 1-3 times a month, 1-2 times a week or 3 times or more a week had 0.68, 0.72 and 0.69 times the risk of all-cause mortality, respectively, and 0.72, 0.71 and 0.64 times the risk of cancer mortality, compared to those who rarely eat small fish.

Even after adjusting the data for lifestyle factors, body mass index scores and adherence to the general Japanese diet (a proxy score of healthy eating), the apparent benefits of small fish were still significant in the women who ate them.

This wasn't quite the case for the men in the study, though. While a similar trend was observed between small fish consumption and lower mortality, the link was deemed less statistically significant.

The reasons for this apparent gender divide remain unclear, but the researchers suggest the relatively limited number of male subjects in the study may have hampered the group's results.

In their paper, Kasahara and their colleagues also admit to another of the study's flaws: a large proportion of participants (40.8%) only answered the questionnaire on seafood consumption once. As these participants could well have changed their dietary habits over the following nine years, the assertion that their health outcomes are tied to their initial penchant for small fish may be tenuous.

Nonetheless, the researchers argue that, at least in Japan, regularly eating small fish may well reduce the risk of all-cause and cancer mortality in women.

Those curious about taking a bite of these snack-size swimmers have been encouraged to do so.

"Small fish are easy for everyone to eat, and they can be consumed whole, including the head, bones, and organs," Kasahara said. "Nutrients and physiologically active substances unique to small fish could contribute to maintaining good health. The inverse relationship between the intake of small fish and the mortality risk in women underscores the importance of these nutrient-dense foods in people's diets."

Technology Networks, 18 June 2024

https://technologynetworks.com



# Intermediate considered 'too reactive to isolate' finally tamed

2024-06-19

A chemical intermediate once considered too reactive to isolate has been stabilised in the laboratory for three days by researchers in Germany. The team's techniques enabled studies that were previously impossible due to the nitrene species' fleeting nature and could allow researchers to further harness the molecules' potential in synthetic chemistry.

The importance of nitrenes – lone nitrogen atoms bonded to single substituents – in chemical reactions has been known for over a century. For example, a nitrene made of a nitrogen atom bound to a single hydrogen atom has been identified as an intermediate in ammonia synthesis. However, the vast majority of nitrenes have lifetimes in the nanosecond range.

'In 1970 – my birth year – there was a book called Nitrenes, and in this book it's stated that this compound class is too reactive ever to be isolated,' says group leader Jens Beckmann at the University of Bremen in Germany. 'Nevertheless people have used nitrenes prepared in situ to do chemical reactions.'

Chemists such as Guy Bertrand at the University of California, San Diego have successfully stabilised similar highly reactive compounds such as carbenes, and these have proved immensely useful in organic synthesis. Nitrenes, however, have proved trickier because they naturally have spin triplet ground states. 'The two unpaired electrons are prone to all kinds of reactivity,' explains team member Emanuel Hupf.

The researchers kinetically stabilised the nitrene molecule using a rigid substituent called MSFluind. 'The gold standard for kinetic stabilisation was the terphenyl family of substituents – but they are susceptible to electrophilic substitution,' says Beckmann. 'This particular family of fluind ligands was published for the first time in 2011 by Kohei Tamao's group, but that was close to his retirement and he didn't get the chance to explore [the ligands'] reactivity for himself.' Beckmann says his postdoc Marian Olaru discovered Tamao's research in 2021 during an ultimately successful quest to stabilise the phosphenium ion. Other groups subsequently used fluind substituents to stabilise bismuthinidene and stibinidene, which both have triplet ground states.

In the new work, Beckmann's group irradiated MSFluindN3 with ultraviolet, leaving the nitrene MSFluindN. Using magnetometry, the researchers

Bulletin Board

Gossip

JUN. 21, 2024

confirmed that the species retained the spin triplet ground state. They also conducted x-ray crystallography, NMR spectroscopy and other imaging techniques for the first time on nitrenes. They now believe it should be possible to use it in the synthesis of bench-stable transition metal complexes. Beckmann notes that, since carbenes were first synthesised in the mid 1990s, the number of references in scientific journals has grown to over 2000 per year.

Bertrand, whose group previously stabilised the spin singlet state of nitrene using an electron-donating substituent, predicts the work will prove highly influential. He believes that the findings will draw significant attention to the fluind substituent's intriguing ability to stabilise spin-triplet states. 'If you talk about antimony or bismuth, only inorganic chemists are interested. But if you talk about carbon or nitrogen, inorganic, organic, physical ... everybody is interested,' he says; 'What is so special about this substituent to stabilise diradicals? I don't know. But it's very surprising.'

Chemistry World, 19 June 2024

https://chemistryworld.com

Curiosities \_\_\_\_

## **Inherited Traits Determine Your Coffee Intake** 2024-06-20

Coffee drinking is a heritable habit, and one that carries a certain amount of genetic baggage.

Caffeinated coffee is a psychoactive substance, notes Sandra Sanchez-Roige, Ph.D., an associate professor in the University of California San Diego School of Medicine Department of Psychiatry. She is one of an international group of researchers that compared coffee-consumption characteristics from a 23andMe database with an even larger set of records in the United Kingdom. She is the corresponding author of a study recently published in the journal Neuropsychopharmacology.

Hayley H. A. Thorpe, Ph.D., is the lead author on the paper. Thorpe, of the Department of Anatomy and Cell Biology, Schulich School of Medicine and Dentistry at Western University in Ontario, explained that the team collected genetic data as well as self-reported coffee-consumption numbers to assemble a genome-wide association study (GWAS). The idea was to make connections between the genes that were known to be associated with coffee consumption and the traits or conditions related to health.

"We used this data to identify regions on the genome associated with whether somebody is more or less likely to consume coffee," Thorpe explained. "And then identify the genes and biology that could underlie coffee intake."

Abraham Palmer, Ph.D., is also a lead researcher on the paper and a professor in the UC San Diego School of Medicine Department of Psychiatry. He said that most people are surprised that there is a genetic influence on coffee consumption. "We had good reason to suspect from earlier papers that there were genes that influence how much coffee someone consumes," he said. "And so, we weren't surprised to find that in both of the cohorts we examined there was statistical evidence that this is a heritable trait. In other words, the particular gene variants that you inherit from your parents influence how much coffee you're likely to consume."

Sanchez-Roige said the genetic influence on coffee consumption was the first of two questions the researchers wanted to address.

CHEMWATCH

# Bulletin Board

**Curiosities** 

JUN. 21, 2024

JUN. 21, 2024

"The second is something that coffee lovers are really keen on learning," Sanchez-Roige said. "Is drinking coffee good or bad? Is it associated with positive health outcomes or not?"

The answer is not definitive. The group's genome-wide association study of 130,153 U.S.-based 23andMe research participants was compared with a similar UK Biobank database of 334,649 Britons, revealing consistent positive genetic associations between coffee and harmful health outcomes such as obesity and substance use. A positive genetic association is a connection between a specific gene variant (the genotype) and a specific condition (the phenotype). Conversely, a negative genetic association is an apparent protective quality discouraging the development of a condition. The findings get more complicated when it comes to psychiatric conditions.

"Look at the genetics of anxiety, for instance, or bipolar and depression: In the 23andMe data set, they tend to be positively genetically correlated with coffee intake genetics," Thorpe said. "But then, in the UK Biobank, you see the opposite pattern, where they're negatively genetically correlated. This is not what we expected."

She said there were other instances in which the 23andMe set didn't align with the UK Biobank, but the greatest disagreement was in psychiatric conditions.

"It's common to combine similar datasets in this field to increase study power. This information paints a fairly clear picture that combining these two datasets was really not a wise idea. And we didn't end up doing that," Thorpe said. She explained that melding the databases might mask effects, leading researchers toward incorrect conclusions — or even cancelling each other out.

Sanchez-Roige says the researchers have some ideas about how the differences in results arose. To begin with, there was an apples-and-oranges aspect to the surveys. For instance, the 23andMe survey asked, "How many 5-ounce (cup-sized) servings of caffeinated coffee do you consume each day?" Compare it to the UK Biobank's "How many cups of coffee do you drink each day? (Include decaffeinated coffee)"

Beyond serving size and the caffeinated/decaf divide, the surveys made no accommodation for the various ways coffee is served. "We know that in the U.K., they have generally higher preference for instant coffee, whereas ground coffee is more preferred in the U.S.," Thorpe said.



"And then there's the frappuccinos," Sanchez-Roige added, citing the American trend of taking coffee loaded with sugary additives. Palmer mentioned other caffeinated drinks and especially in the context of the UK Biobank, tea, none of which were included in the GWAS, which addressed only coffee. Palmer added that the GWAS demonstrates the relationship between genotype and phenotype is more different than the relationship between coffee and tea.

"Genetics influences lots of things. For instance, it influences how tall you might be," he said. "And those kinds of things probably would play out very similarly, whether you lived in the U.S. or the U.K. But coffee is a decision that people make."

Sanchez-Roige pointed out that coffee comes in a variety of forms, from instant to frappuccino, and is consumed amid cultural norms that differ from place to place. A person with a given genotype might end up having quite a different phenotype living in the U.K. versus the U.S.

"And that's really what the data are telling us," she said. "Because unlike height, where your behavior doesn't really have much to do with it, your behavior and the choices you're making in your environment play out in various ways. So the interaction between genotype and environment complicates the picture."

The collaborators stressed the need for more investigation to unravel the relationships between genetics and the environment, focusing not only on coffee/caffeine intake but also other substance-use issues.

Technology Networks, 20 June 2024

https://technologynetworks.com

# Tough new pineapple leather is 60X stronger than other materials

2024-06-17

In a breakthrough for bio-based materials, scientists have made leather from the fibers of discarded pineapple leaves that's comparable to the real thing and also outperforms other existing plant products. The strong and sustainable material, which comprehensively outperformed mushroombased leather, has great potential to be produced at much larger scale for everything from clothing to bags and shoes.

Using natural rubber for adhesion, researchers from Thailand's Mahidol University created this 100% bio-based pineapple leaf fiber (PALF) leather

CHEMWATCH

# Bulletin Board

**Curiosities** 

JUN. 21, 2024

JUN. 21, 2024

through a simple process that does away with chemical treatment or additional plastics, which they say is a "significant" step forward.

"This research showcases a sustainable and economically viable alternative to traditional leather, with the potential to revolutionize the leather industry and contribute to a more environmentally friendly future," the team noted.

While animal leather alternatives are not new, they have so far come with significant challenges. 'Vegan leather,' which relies heavily on plastics in production, may be better for animals but not necessarily the planet, and has been shown to have a much shorter lifespan. There have been major steps forward in using other natural fibers, such as those found in fungi, but their mechanical properties (toughness, tear resistance) have been an ongoing issue.

So what makes pineapple a more likely source for a leather that's produced sustainably and holds its own when it comes to wear and tear? It all comes down to the extraction and preparation of the tiny fibers. The leaves – a plentiful byproduct – were cleaned and chopped into 6-mm-wide pieces. These were then ground into a thick green paste and dried, then sieved to separate non-fibrous material from the pineapple leaf fibers (PALF). The researchers then prepared both untreated PALF (UPALF) and fibers that were mixed with sodium hydroxide and washed (TPALF), to create different leather properties, and spread out on a silkscreen, similar to paper-making processes. Finally, a thin coat of natural latex was applied to the unwoven, flattened fiber sheets, which were then exposed to 70 °C (158 °F) for 24 hours and later compressed.

The researchers landed on a treatment that, when analyzed using a scanning electron microscope, had a structure that performed best in tensile and tear strength tests and optimal hardness. These leather sheets were also treated with a variety of natural stains, from carrot to coffee, to demonstrate how a variety of tones could be achieved without needing any of the toxic chemicals used in commercial tanning.

While the PALF leather had lower tensile strength and tear resistance to what is expected of animal leathers, they were comparable when the researchers performed their own tests, suggesting natural variability in traditional materials. PALF, however, was especially impressive when measured up against existing commercial leather alternatives, showing to have a tensile strength of 12.3 MPa, more than 60 times tougher than MuSkin (made from Phellinus ellipsoideus mushrooms) at 0.2 MPa. This



poor 'wear and tear' factor has been one of the large concerns with mushroom and some other plant-based leather alternatives.

PALF was nearly three times stronger and had a tear resistance of almost double that of existing pineapple leaf leather Pinatex.

The research team, led by Professor Taweechai Amornsakchai, plans to now work on adjusting the material's feel, to have it more closely resemble the softness typical of animal leather.

The research was published in the journal Sustainability and Amornsakchai explains the leather-making process in this 2019 video.

New Atlas, 17 June 2024

https://newatlas.com

# Spectroscopic technique that singles out water molecules lying on the surface reveals how they relax after being excited

2024-06-20

A more complete picture of how excited water molecules at an interface with air lose their energy has been uncovered by RIKEN scientists in a study published in the journal Nature Communications. This finding will be valuable for better understanding processes that occur at water surfaces.

Water is an anomaly in many ways. For example, its freezing and boiling points are much higher than might be expected, and it is less dense as a solid (ice) than as a liquid.

Almost all of water's unusual properties stem from weak bonds that are continually forming and breaking between neighboring water molecules. Known as hydrogen bonds, these bonds arise because oxygen attracts electrons more than hydrogen. The slightly negative oxygen in one molecule is thus attracted to the slightly positive hydrogens in other molecules.

But a tiny sliver of water molecules--those lying on the surface--experience hydrogen bonds differently than do other water molecules. In their case, the arm sticking up into the air doesn't form hydrogen bonds.

Until now, no one had been able to discover how the arms of these surface molecules relax after being stretched. That's because it is incredibly challenging to isolate the signal from these molecules.

CHEMWATCH

# Bulletin Board

**Curiosities** 

JUN. 21, 2024

JUN. 21, 2024

"We have a good knowledge of how water molecules in the body of the liquid behave, but our understanding about water molecules at the interface lags far behind," says Tahei Tahara of the RIKEN Molecular Spectroscopy Laboratory.

Over the past decade, a team led by Tahara has been trying to rectify this situation by developing highly sophisticated spectroscopy techniques to probe the interactions of water molecules at surfaces.

The team has now developed a technique based on infrared spectroscopy that is sensitive enough to detect how the oxygen-hydrogen bonds of surface water molecules relax.

Using the technique, the team found that oxygen–hydrogen bonds sticking up into the air first rotate without losing energy. They then relax in a similar way to molecules in the body of the liquid that form a hydrogen-bond network.

"In this sense, there is no big difference between molecules at the interface and inside the liquid after interaction with neighbors—they both share the same relaxation process," says Tahara. "These findings paint a comprehensive picture of how stretching of oxygen—hydrogen bonds relaxes at the surface of water."

Tahara and his team now intend to use their spectroscopic technique to look at chemical reactions that occur at the interface of water.

Phys Org, 20 June 2024

https://phys.org

## Much of the Nord Stream gas remained in the sea

2024-06-19

Much of the methane released into the southern Baltic Sea from the Nord Stream gas pipeline has remained in the water. This is shown by measurements taken by researchers from the University of Gothenburg.

At the end of September 2022, the Nord Stream gas pipeline on the bottom of the Baltic Sea exploded east of Bornholm and one of the largest unnatural methane gas emissions ever was a fact.

The methane gas from the pipeline created large bubbles at the water surface and measurements showed elevated levels of methane in the atmosphere.

## Expedition within a week

But much of the methane never reached the surface and dissolved in the water instead.

This is according to a scientific study published in Scientific Reports.

"Thanks to fortunate circumstances, we were able to organise an expedition to the area of the leak in less than a week. Based on what we measured, we estimate that between 10,000 and 50,000 tonnes of methane remained in the sea in dissolved form," says Katarina Abrahamsson, professor of marine chemistry at the University of Gothenburg.

The methane was spread over large areas and has dissolved in the water, where some is taken care of by bacteria.

Methane is also normally present in the water, formed during the decomposition of organic material in the bottom sediments.

### **Different isotopes**

"In our study, we have been able to distinguish the methane coming from the Nord Stream leak from that naturally present in the water, thanks to the fact that the methane from the gas pipeline has a different isotopic composition than that which seeps up from the bottom sediments. This is a strength of our study," says Katarina Abrahamsson.

The water in the sea normally lies in different layers due to differences in temperature and salinity.

Despite the fact that the methane leaked out of the gas pipeline at great speed and in large quantities, the researchers could not observe any major mixing in the water masses.

The stratification that normally occurs at the end of September was stable.

The levels of the leaked methane therefore varied greatly in the water.

The researchers assume that the methane was diluted in a larger body of water later in the autumn when the water was remixed due to falling water temperature.

#### **Unclear biological impact**

It is too early to say what impact the increased methane levels will have on biological life in the southern Baltic Sea.

CHEMWATCH

# Bulletin Board

**Curiosities** 

JUN. 21, 2024

JUN. 21, 2024

"The expedition also included researchers who took plankton samples in the affected area, the analyses of which are not yet complete," says Katarina Abrahamsson.

Three months after the first expedition, a return visit was made to the area and new measurements were taken. Preliminary results show that bacterial activity has been high during these three months. The researchers do not yet know how the phytoplankton and zooplankton have been affected by this.

Science Daily, 19 June 2024

https://sciencedaily.com

# **Drugs Commonly Used To Treat Enlarged Prostate May Also Decrease Dementia Risk**

2024-06-20

A new study suggests that certain drugs commonly used to treat enlarged prostate may also decrease the risk for dementia with Lewy bodies (DLB). This observational finding may seem surprising, but it mirrors previous work by the University of Iowa Health Care team that links the drugs to a protective effect in another neurodegenerative condition—Parkinson's disease.

The UI researchers think that a specific side effect of the drugs targets a biological flaw shared by DLB and Parkinson's disease, as well as other neurodegenerative diseases, raising the possibility that they may have broad potential for treating a wide range of neurodegenerative conditions.

"Diseases like dementia with Lewy bodies, or Parkinson's disease, or Alzheimer's disease are debilitating, and we don't really have any good treatments that can modify the disease progression. We can treat symptoms, but we can't actually slow the disease," explains lead study author Jacob Simmering, PhD, UI assistant professor of internal medicine. "One of the most exciting things about this study is that we find that same neuroprotective effect that we saw in Parkinson's disease. If there is a broadly protective mechanism, these medications could potentially be used to manage or prevent other neurodegenerative diseases."

The new findings published online on June 19, 2024, in Neurology, the medical journal of the American Academy of Neurology.

Large observational study links prostate drugs to lower risk of dementia with Lewy bodies

# Bulletin Board Curiosities CHEMWATCH Bulletin Board JUN. 21, 2024

DLB is a neurodegenerative disease that causes substantial and rapid cognitive decline and dementia. While less common than Parkinson's disease, DLB affects about one in 1,000 people per year, and accounts for 3 to 7% of all dementia cases. Because aging is a key risk factor for DLB, it is likely to become more common as our population gets older.

For the new study, the UI researchers used a large database of patient information to identify more than 643,000 men with no history of DLB who were newly starting one of six drugs used to treat benign prostatic hyperplasia (enlarged prostate).

Three of the drugs, terazosin, doxazosin, and alfuzosin (Tz/Dz/Az), have an unexpected side effect; they can boost energy production in brain cells. Preclinical studies suggest that this ability may help slow or prevent neurodegenerative diseases like PD and DLB.

The other drugs, tamsulosin and two 5-alpha-reductase inhibitors (5ARIs) called finasteride and dutasteride, do not enhance energy production in the brain and therefore provide a good comparison to test the effect of the Tz/Dz/Az drugs.

The team then followed the data on these men from when they started taking the medication until they left the database or developed dementia with Lewy bodies, whichever happened first. On average, the men were followed for about three years.

Because all the participants were selected to start a drug that treats the same condition, the researchers reasoned that the men were likely similar to each other at the outset of the treatment. The researchers also matched the men using propensity scores for characteristics like age, the year they started the medication, and other illnesses they had before starting the treatment, to further reduce the differences between the groups.

"We found that men who took Tz/Az/Dz drugs were less likely to develop a diagnosis of dementia with Lewy bodies," Simmering says. "Overall, men taking terazosin-type medications had about a 40% lower risk of developing a DLB diagnosis compared to men taking tamsulosin, and about a 37% reduction in risk compared to men taking five alpha reductase inhibitors."

Meanwhile, there was no statistically significant difference in risk between men taking tamsulosin and alpha reductase inhibitors.

**Approved drugs show potential** 

CHEMWATCH

# Bulletin Board

**Curiosities** 

JUN. 21, 2024

This was an observational study, and therefore the results show only an association between taking the Tz/Dz/Az drugs and a reduced risk of developing DLB rather than a causal relationship. In addition, the study only included men because the drugs are prescribed for prostate problems, which means that the researchers don't know if the findings would apply to women. However, Simmering and his colleagues are excited by the potential of these drugs, which are already FDA approved, inexpensive, and have been used safely for decades.

"If terazosin and these similar medications can help slow this progression—if not outright preventing the disease—this would be important to preserving cognitive function and quality of life in people with DLB," Simmering says.

Technology Networks, 20 June 2024

https://technologynetworks.com

# Great British Bake Off finalist discusses the parallels between chemistry and baking

2024-06-20

Last year on a Friday evening, chemical biology researcher Josh Smalley was in the lab when he received a call inviting him to appear on the 14th and latest season of "The Great British Bake Off." Starting as one of a group of 12 amateur bakers, Smalley made it all the way to the final round, where the top three contestants compete for the winning spot.

In an essay published in the journal Cell Chemical Biology on June 20, Smalley describes the overlap between chemistry and baking and how his training in one has improved his performance in the other, and vice versa.

"Baking and science have always been my two great passions," says Smalley. "I find immense joy in combining my culinary creations with an insight into the science behind them just as much as I love to translate my methodical approach and precision from a chemistry research lab to the kitchen."

Just a few months before Smalley received the call to be on the show, he finished his Ph.D. at the University of Leicester developing proteolysis targeting chimeras (PROTACs) for the selective degradation of histone deacetylase enzymes. Now post-"Bake Off," he's a postdoctoral research associate there where he develops peptidomimetic sulfinamide foldamers.

# Bulletin Board Curiosities

Smalley says that his training in the lab is what helped him handle the pressure of baking in the tent. He was determined to showcase his interests in his bakes, like in his chemistry-themed chocolate celebration box.

"Some of my proudest moments from the whole experience were when an issue occurred during a bake and I was able to find a way to overcome it without getting flustered or allowing it to compromise my performance," he says.

Smalley also speaks of the transferable skills between the two areas. "I have come to learn over the years in both scenarios how things like temperatures and clean glassware are essential for perfect results and that the order of addition can have big implications on the product," he says.

Now that he is progressing in his career as a baker, he sees himself specializing just like he has as a researcher. "I have evolved from a baker that tried their hand at everything to honing my skills and finding my own unique style in the decoration, presentation, and storytelling of my bakes," he says.

"Moving forward, I am looking to continue in academia as a chemical biology researcher but divide my time between research and a publicfacing role, promoting science through the art of baking and hopefully inspiring the next generation of scientists."

Phys Org, 2024-06-20

https://phys.org

## The US abortion drugs regulation challenge has stalled, but it will return

2024-06-19

Having failed in the US Supreme Court, anti-abortion activists are trying other ways to prevent access to approved drugs

I last wrote here in April 2023 about the US legal wrangling over the abortion drug mifepristone. To recap, anti-abortion groups are claiming that the US Food and Drug Administration (FDA) overstepped its authority in regulating the drug. It is available through mail-order prescription, even in states that are trying to restrict all methods of abortion, but an 1873 law (still on the books) bans using the mail for such material. The US Postal Service argues that this law was meant to prevent illegal activity (as it was

CHEMWATCH

# Bulletin Board

**Curiosities** 

JUN. 21, 2024

JUN. 21, 2024

at the time), but that mifepristone is now an approved drug, so the statute does not apply.

This case was argued before the US Supreme Court earlier this year, and legal observers noted that the reaction of the justices (and the questions asked) made it look very unlikely for the plaintiffs to prevail. In fact, the entire case was just thrown out, based on the question of legal standing: to proceed, the anti-abortion physicians bringing the suit needed to show that they (or any physicians at all) stood in imminent danger of harm due to the FDA's regulatory decisions. The court found they did not, especially considering the wide scope of conscience-based exemptions from having to perform abortion procedures in general. Almost no time was spent on the legality of the FDA's regulations themselves.

#### More cases to come

This issue is not going to go away, though. Although these plaintiffs didn't have legal standing, Attorneys General in the most anti-abortion states will undoubtedly round up people who are more likely to pass that test, and file another suit that will could make its way up to the Supreme Court for another round. And there are other challenges underway. Just recently, the state of Louisiana moved to classify mifepristone (and misoprostol, the usual accompaniment) as a 'dangerous controlled substances' (the same classification used for addictive drugs like opioids).

On the face of it, the penalties attached to that legislation would only apply to someone who was in possession of these drugs without a prescription, which doesn't seem like it would slow things down much. But anti-abortion groups hope that this designation (and the accompanying paperwork and security requirements) will make pharmacies more reluctant to stock and dispense the drugs, making them harder to obtain in Louisiana one way or another. Several other conservative states have considered such legislation, and they'll watch to see how the Louisiana law fares. There will surely be counter-lawsuits saying that the state legislature has overstepped its authority, and that could set up the sort of limits-of-the-FDA case that anti-abortion groups were hoping that the recent unsuccessful case would turn into.

This all starts fitting into a framework where some US conservatives seem to want the law to work in two different ways for different people. For one group (the conservatives themselves), the law would protect them from the actions and demands of others, but would not restrict their own choices. But for everyone else, the law would be there to bind but not to protect. In other words, a 'Heads we win; Tails, you lose' coin-flip game. The

# Bulletin Board Curiosities

Louisiana legislature – along with many of its citizens – do not want any federal agency (such as the FDA) to be able to tell them that they have to allow things that they themselves do not approve of. But they would be fine with a federal government that could somehow rule for the entire country that abortion was now illegal by every means, for every citizen, with no legal recourse.

That is obviously no way to run a coherent legal system. Abortion, though, is one of those issues that brings out the worst in its most passionate advocates – any weapon to hand, so long as the end result is the one you wanted. But the Supreme Court's instant focus on legal standing in the most recent case showed a real reluctance to take on any fundamental reworking of the FDA's regulatory powers – even with a group of justices more likely than any in decades to take on such a project. We'll see if they have any more enthusiasm when the issue comes around again. I would like to say 'if', but there seem to be a lot of people determined to make that happen, by any means necessary.

Chemistry World, 19 June 2024

https://chemistryworld.com

# Researchers Invent 100% Biodegradable "Barley Plastic"

2024-06-19

A biofriendly new material made from barley starch blended with fibre from sugarbeet waste sees the light of day at the University of Copenhagen – a strong material that turns into compost should it end up in nature. In the long term, the researchers hope that their invention can help put the brakes on plastic pollution while reducing the climate footprint of plastic production.

Enormous islands of it float in our oceans and microscopic particles of it are in our bodies. The durability, malleability and low cost of plastics has made them ubiquitous, from packaging to clothing to aircraft parts. But plastics have a downside. Plastics contaminate nature, are tough to recycle and their production emits more CO2 than all air traffic combined.

Now, researchers at the University of Copenhagen's Department of Plant and Environmental Sciences have invented a new material made from modified starch that can completely decompose in nature – and do so within only two months. The material is made using natural plant material

CHEMWATCH

# Bulletin Board

**Curiosities** 

JUN. 21, 2024

JUN. 21, 2024

from crops and could be used for food packaging, among many other things.

"We have an enormous problem with our plastic waste that recycling seems incapable of solving. Therefore, we've developed a new type of bioplastic that is stronger and can better withstand water than current bioplastics. At the same time, our material is one hundred percent biodegradable and can be converted into compost by microorganisms if it ends up somewhere other than a bin," says Professor Andreas Blennow of the Department of Plant and Environmental Sciences.

Only about nine percent of plastic is recycled globally, with the rest being either incinerated or winding up in nature or dumped into enormous plastic landfills.

Bioplastics already exist, but the name is misleading says Professor Blennow. While today's bioplastics are made of bio-derived materials, only a limited part of them is actually degradable, and only under special conditions in industrial composting plants.

"I don't find the name suitable because the most common types of bioplastics don't break down that easily if tossed into nature. The process can take many years and some of it continues to pollute as microplastic. Specialized facilities are needed to break down bioplastics. And even then, a very limited part of them can be recycled, with the rest ending up as waste," says the researcher.

#### Starch from barley and sugar industry waste

The new material is a so-called biocomposite and composed of several different substances that decompose naturally. Its main ingredients, amylose and cellulose, are common across the plant kingdom. Amylose is extracted from many crops including corn, potatoes, wheat and barley.

Together with researchers from Aarhus University, the research team founded a spinoff company in which they developed a barley variety that produces pure amylose in its kernels. This new variety is important because pure amylose is far less likely to turn into a paste when it interacts with water compared to regular starch. Cellulose is a carbohydrate found in all plants and we know it from cotton and linen fibers, as well as from wood and paper products. The cellulose used by the researchers is a so-called nanocellulose made from local sugar industry waste. And these nanocellulose fibers, which are one thousand times smaller than the fibers

Copyright Chemwatch 2024 © Copyright Chemwatch 2024 © Copyright Chemwatch 2024 ©



of linen and cotton, are what contribute to the material's mechanical

"Amylose and cellulose form long, strong molecular chains. Combining them has allowed us to create a durable, flexible material that has the potential to be used for shopping bags and the packaging of goods that we now wrap in plastic," says Andreas Blennow.

The new biomaterial is produced by either dissolving the raw materials in water and mixing them together or by heating them under pressure. By doing so, small 'pellets' or chips are created that can then be processed and compressed into a desired form.

Thus far, the researchers have only produced prototypes in the laboratory. But according to Professor Blennow, getting production started in Denmark and many other places in the world would be relatively easy.

"The entire production chain of amylose-rich starch already exists. Indeed, millions of tons of pure potato and corn starch are produced every year and used by the food industry and elsewhere. Therefore, easy access to the majority of our ingredients is guaranteed for the large-scale production of this material," he says.

### **Could reduce plastic problem**

strength.

Andreas Blennow and his fellow researchers are now processing a patent application that, once it has been approved, could pave the way for production of the new biocomposite material. Because, despite the huge sums of money being devoted to sorting and recycling our plastic, the researcher does not believe that it will really be a success. Doing so should be seen as a transitional technology until we bid fossil-based plastics a final farewell.

"Recycling plastic efficiently is anything but straightforward. Different things in plastics must be separated from each other and there are major differences between plastic types, meaning that the process must be done in a safe way so that no contaminants end up in the recycled plastic. At the same time, countries and consumers must sort their plastic. This is a massive task that I don't see us succeeding at. Instead, we should rethink things in terms of utilizing new materials that perform like plastic, but don't pollute the planet," says Blennow.

The researcher is already collaborating with two Danish packaging companies to develop prototypes for food packaging, among other things. He envisions many other uses for the material as well, such as for

CHEMWATCH

# Bulletin Board

**Curiosities** 

JUN. 21, 2024

JUN. 21, 2024

the interior trims of cars by the automotive industry. Though it is difficult to say when this biofriendly barley-based plastic will reach the shelves, the researcher predicts that the new material may become a reality in the foreseeable future.

"It's quite close to the point where we can really start producing prototypes in collaboration with our research team and companies. I think it's realistic that different prototypes in soft and hard packaging, such as trays, bottles and bags, will be developed within one to five years," concludes Andreas Blennow.

Technology Networks, 19 June 2024

https://technologynetworks.com

# Researchers create new class of materials called 'glassy gels'

2024-06-19

Researchers have created a new class of materials called "glassy gels" that are very hard and difficult to break despite containing more than 50% liquid. Coupled with the fact that glassy gels are simple to produce, the material holds promise for a variety of applications.

A paper describing this work, titled "Glassy Gels Toughened by Solvent," appears in the journal Nature.

Gels and glassy polymers are classes of materials that have historically been viewed as distinct from one another. Glassy polymers are hard, stiff and often brittle. They're used to make things like water bottles or airplane windows. Gels—such as contact lenses—contain liquid and are soft and stretchy.

"We've created a class of materials that we've termed glassy gels, which are as hard as glassy polymers, but—if you apply enough force—can stretch up to five times their original length, rather than breaking," says Michael Dickey, corresponding author of a paper on the work and the Camille and Henry Dreyfus Professor of Chemical and Biomolecular Engineering at North Carolina State University. "What's more, once the material has been stretched, you can get it to return to its original shape by applying heat. In addition, the surface of the glassy gels is highly adhesive, which is unusual for hard materials."

"A key thing that distinguishes glassy gels is that they are more than 50% liquid, which makes them more efficient conductors of electricity than

# Bulletin Board Curiosities

common plastics that have comparable physical characteristics," says Meixiang Wang, co-lead author of the paper and a postdoctoral researcher

at NC State. "Considering the number of unique properties they possess,

we're optimistic that these materials will be useful."

Glassy gels, as the name suggests, are effectively a material that combines some of the most attractive properties of both glassy polymers and gels. To make them, the researchers start with the liquid precursors of glassy polymers and mix them with an ionic liquid. This combined liquid is poured into a mold and exposed to ultraviolet light, which "cures" the material. The mold is then removed, leaving behind the glassy gel.

"The ionic liquid is a solvent, like water, but is made entirely of ions," says Dickey. "Normally, when you add a solvent to a polymer, the solvent pushes apart the polymer chains, making the polymer soft and stretchable. That's why a wet contact lens is pliable, and a dry contact lens isn't. In glassy gels, the solvent pushes the molecular chains in the polymer apart, which allows it to be stretchable like a gel.

"However, the ions in the solvent are strongly attracted to the polymer, which prevents the polymer chains from moving. The inability of chains to move is what makes it glassy. The end result is that the material is hard due to the attractive forces, but is still capable of stretching due to the extra spacing."

The researchers found that glassy gels could be made with a variety of different polymers and ionic liquids, though not all classes of polymers can be used to create glassy gels.

"Polymers that are charged or polar hold promise for glassy gels, because they're attracted to the ionic liquid," Dickey says.

In testing, the researchers found that the glassy gels don't evaporate or dry out, even though they consist of 50–60% liquid.

"Maybe the most intriguing characteristic of the glassy gels is how adhesive they are," says Dickey. "Because while we understand what makes them hard and stretchable, we can only speculate about what makes them so sticky."

The researchers also think glassy gels hold promise for practical applications because they're easy to make.

"Creating glassy gels is a simple process that can be done by curing it in any type of mold or by 3D printing it," says Dickey. "Most plastics with

CHEMWATCH

# Bulletin Board

**Curiosities** 

JUN. 21, 2024

JUN. 21, 2024

similar mechanical properties require manufacturers to create polymer as a feedstock and then transport that polymer to another facility where the polymer is melted and formed into the end product.

"We're excited to see how glassy gels can be used and are open to working with collaborators on identifying applications for these materials."

Co-lead author of the paper is Xun Xiao of the University of North Carolina at Chapel Hill. The paper was co-authored by Salma Siddika, a Ph.D. student at NC State; Mohammad Shamsi, a former Ph.D. student at NC State; Ethan Frey, a former undergrad at NC state; Brendan O'Connor, a professor of mechanical and aerospace engineering at NC State; Wubin Bai, a professor of applied physical sciences at UNC; and Wen Qian, a research associate professor of mechanical and materials engineering at the University of Nebraska-Lincoln.

Phys Org, 19 June 2024

https://phys.org

# **Cutting Costs and Increasing Efficiency: New Catalyst Revolutionizes Hydrogen Production**

2024-06-20

A successful demonstration could enhance the production of hydrogen from water.

Hydrogen (H2) holds great potential as a fuel to reduce greenhouse gases, particularly when produced by using renewable energy to split water molecules (H2O). However, despite the apparent simplicity of breaking water into hydrogen and oxygen, the underlying chemistry is quite complex.

Two separate simultaneous electrochemical reactions each require catalysts, chemical "deal makers" that help break and remake chemical bonds. Now, scientists at the U.S. Department of Energy's (DOE) Brookhaven National Laboratory and Columbia University say they've developed a new efficient catalyst for the more challenging part: the oxygen evolution reaction.

As described in a paper just published in the Journal of the American Chemical Society, the catalyst was designed "from the bottom up" based on theoretical calculations seeking to minimize the amount of iridium, an expensive metal used as a catalytic material, and to maximize the catalyst's stability in acidic conditions. When the team created models of the catalyst

Copyright Chemwatch 2024 © Copyright Chemwatch 2024 © Copyright Chemwatch 2024 © September 2024 © Copyright Chemwatch 2024 © Copyright Chemwatch 2024 © September 2024 © Septemb

# Bulletin Board Curiosities

and tested them in the lab, the results validated the predictions. Then, the scientists made a powder form of the catalyst, like those used in industrial applications, and showed it can efficiently produce hydrogen in a water-splitting electrolyzer.

"In this real-world test, our catalyst is about four times better than the state-of-the-art commercially available iridium catalyst," said Jingguang Chen, a chemical engineer at Columbia University with a joint appointment in the Chemistry Division at Brookhaven Lab who led the research. In other words, the new catalyst requires four times less iridium to produce hydrogen at the same rate as the commercial variety — or produces hydrogen four times faster for the same amount of iridium.

Brookhaven Lab theoretical chemist Ping Liu, who led the calculations that underpin the catalyst's design, said, "This study demonstrates how you can go from a theory-driven understanding of what's happening at the atomic level to designing a catalyst for a practical use. Our work gives us a better understanding of how this catalyst works and gets us closer to the real-world application."

The remaining challenge is to scale up production.

"We are only making milligrams of catalyst per batch," Chen said. "If you want to make megatons of green hydrogen, you'd need kilograms or tons of catalyst. We can't make this at that large scale yet."

#### **Reducing iridium**

Iridium is the catalyst of choice for the oxygen evolution reaction, which takes place at the anode of an electrolyzer. It provides the electrically charged active sites that separate tightly bound hydrogen ions (H+) from oxygen (O). In addition to freeing the H+ ions — which contribute to the harshly acidic reaction conditions — the reaction produces oxygen gas (O2) and electrons. Those electrons are needed for the second, less challenging "hydrogen evolution" reaction: the pairing up of hydrogen ions to form hydrogen gas at the electrolyzer's cathode.

"Iridium is currently one of the only stable elements for the oxygen evolution reaction in acid," Chen said. That's "unfortunate," he noted, because "iridium is even more rare, and more expensive, than platinum."

Hence, the motivation for reducing the amount of iridium.

CHEMWATCH

# Bulletin Board

**Curiosities** 

JUN. 21, 2024

JUN. 21, 2024

"In industrial catalysts made of nanoscale particles, only atoms on the surface participate in the reaction," Chen said. "That means most of the iridium on the inside of the particle is wasted."

Maybe instead of using a particle that is all iridium, a catalyst could be made of a less-expensive material with iridium only on the surface, the team reasoned.

With funding from a DOE initiative to advance clean-energy technologies, they had been exploring the use of earth-abundant elements such as titanium. They found that combining titanium with nitrogen provided enough stability for these "titanium nitrides" to survive acidic reaction conditions. Perhaps titanium nitride could serve as the core of iridium-coated catalytic particles.

But how much iridium should be layered on top? This is where the theoretical calculations come in.

### Calculating an ideal structure

"We used 'density functional theory' calculations to model how different overlayers of iridium on titanium nitride would affect the stability and activity of the catalyst under acidic oxygen evolution reaction conditions," said Liu. She and her team used computing resources at Brookhaven Lab's Center for Functional Nanomaterials (CFN) and at the National Energy Research Scientific Computing Center (NERSC) at DOE's Lawrence Berkeley National Laboratory to run the simulations.

The calculations predicted that one layer of iridium would not be sufficient to drive the oxygen evolution reaction but that two or three layers would improve both performance and catalytic stability.

"These were sort of pre-screening experiments," Liu said. "Then, we turned these screening results over to the experimental team to make real catalysts and evaluate their catalytic activity."

### Validating the predictions

First, the team created thin films in which they could create carefully controlled layers that closely resembled the surfaces used in the theoretical modeling calculations. They also created powdered samples composed of small nanoscale particles, the form the catalyst would take in industrial applications. Then, they studied the thin films — including the interfaces between the layers — and the nanoparticles using a variety of techniques.



These included transmission electron microscopy at CFN and X-ray spectroscopy studies at the Quick X-ray Absorption and Scattering (QAS) beamline of the National Synchrotron Light Source II (NSLS-II), a source of bright X-rays for deciphering samples' chemical and physical properties.

"Our hypothesis was that if the iridium bonds to the titanium nitride, this bonding would stabilize the iridium and improve the reaction," Chen said.

The characterization studies bore out the predictions.

"The synchrotron studies revealed the oxidation states and local coordination environment of the iridium and titanium atoms under reaction conditions," Chen said. "They confirmed that the iridium and titanium are interacting strongly."

"Mapping the elements of the nanoparticles at CFN confirmed the particle sizes and compositions, including the presence of iridium oxides on the surface over titanium nitride supports," he added.

Liu emphasized that the characterization studies informed the scientists' understanding of the catalyst.

"We found that the interaction between iridium and titanium is not only helpful to the stability of the catalyst but also in fine-tuning its activity," she said. "The charges change the chemistry in a way that improves the reaction."

Specifically, charges transferred from titanium to the iridium surface alter the electronic structure of the iridium active sites to optimize the binding of reaction intermediates, she explained.

"Going from one to three layers of iridium, you increase the charge transfer from the nitride to the top iridium significantly," Liu noted. But the difference between two and three layers was not very large. Two layers might be enough to allow high stability, activity, and low cost.

To make this catalyst ready for real-world use, the scientists pointed out that, in addition to tackling the challenge of scaling up production, there could also be improvements to optimize the consistency of the powders.

"When we make thin films, we can control the layers, but with powder synthesis, we don't have that kind of control," Chen said. "Our powder particles don't have a continuous iridium shell around them. But this study provides guidelines industrial chemists could use to make true core-shell structures with a uniform thin layer of iridium," he said.

Bulletin Board
Curiosities

CHEMWATCH

Bulletin Board

JUN. 21, 2024

Such catalysts could help lower the cost of water splitting and bring scientists closer to producing large quantities of green hydrogen.

SciTechDaily, 20 June 2024

https://scitechdaily.com

Copyright Chemwatch 2024 © Copyright Chemwatch 2024 © Copyright Chemwatch 2024 ©

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

#### CHEMICAL EFFECTS

<u>Distribution, sources and ecological risks of PAHs and n-alkanes in water and sediments of typically polluted estuaries: Insights from the Xiaoqing River</u>

Toxic elements identified in breast milk of mothers residing in water contaminated region of Sindh and their impact on infants' growth patterns: A case-control study

#### **ENVIRONMENTAL RESEARCH**

The environment as the first victim: The impacts of the war on the preservation areas in Ukraine

Ecotoxicological risk of asphalt pavements to aquatic animals associated with pollutant leaching

<u>Preparation of porous biochar from fusarium wilt-infected banana straw</u> <u>for remediation of cadmium pollution in water bodies</u>

### PHARMACEUTICAL/TOXICOLOGY

Exploring the impact of pharmacist-supported medication reviews in dementia care: experiences of general practitioners and nurses

The Potential Impact of Oral Nicotine Pouches on Public Health: A Scoping Review

#### **OCCUPATIONAL**

<u>Evaluation of Heavy Metal and Specific Trace Elements Levels Among Fast-Food Workers and Their Susceptibility to Atherosclerosis</u>

Bioaerosol Exposures and Respiratory Diseases in Cannabis Workers

Occasional and constant exposure to dietary ethanol shortens the lifespan of worker honey bees