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American Institute of Chemical Engineers, Cleveland Section NEWSLETTER

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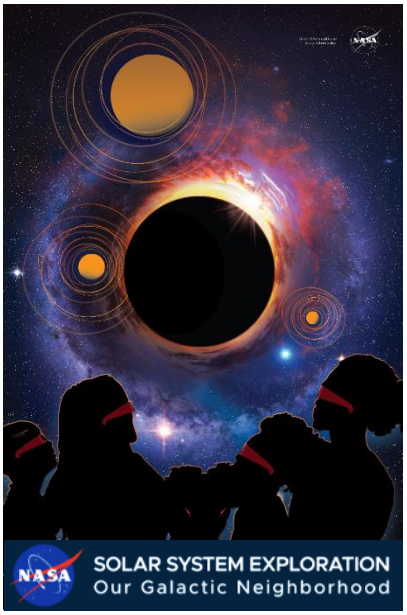


Thursday, April 4, 2024, 5:00 PM

AIChE Membership is Not Required to attend any meetings

"NEOSEF Awards Banquet & NASA Presentation on our Solar System"

The Snow Road Branch of the CCPL, Snow Road, Parma; Meeting Room
2121 Snow Road, Parma, OH 44134;

Rosanne Brunello-McCay, NASA Solar System Ambassador in Cleveland
Email address: CONTACT ROSANNE or https://solarsystem.nasa.gov/ambassadors/2621

Abstract: Let us travel through space and time with a local business owner, STEM career advocate, and NASA JPL Solar System Ambassador, who will explain why life is not a space race but a deep motivational journey! In addition, we will receive outstanding project research presentations from some of our 2024 NEOSEF Awardees! **For Viewing Enjoyment:** 1962 Kennedy Moon Speech: https://www.youtube.com/watch?v=QXqlziZV63k , 1969 NASA Armstrong & Aldrin Moon Landing: https://www.youtube.com/watch?v=S9HdPi9Ikhk , Rocky River Metroparks Solar System Walk: https://fitelix.wordpress.com/2010/05/29/the-solar-system-walk

Biography: Rosanne Brunello-McCay is an innovative, enthusiastic and ambitious business owner dealing with aerospace manufacturers. She is an advocate of stem careers. She is certified as a manufacturing engineer, educated in marketing, management, and human resources. She earned her MBA during the COVID years. As her 40-year-old business winds down and she is ready to retire, she is substitute teaching K-12, so she can continue her quest of preparing students for the future. She is a natural leader, mentor, and aerospace enthusiast. She's a NASA Solar System Ambassador from Cleveland, Ohio.

NEOSEF 2024 Awards from CLE AIChE:

The Northeastern Ohio Science and Engineering Fair
NEOSEF

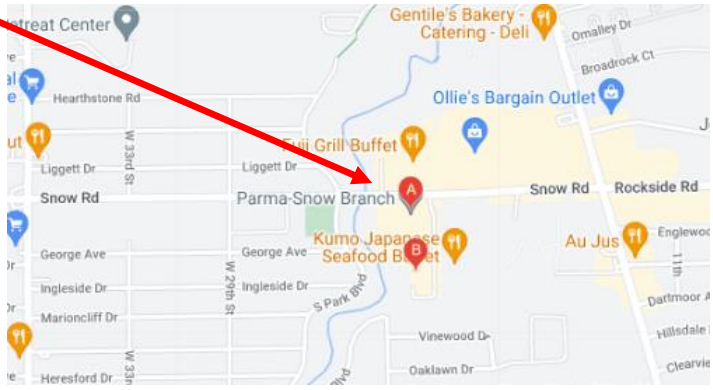
1 **Elise Moran,** *"Biohazard",* ENV 7-8, Garfield Middle School
2 **Alishba Siddiqi,** *"Is it time to say goodbye to plasic?"***,** ENV 7-8, Lake Ridge Academy
3 **Luke Wilkinson,** *"Bioplastics: Are they as effective as we thought?",* ENV 7-8, University School
4 **Tatyana Sowerby,** *"Accounting for Climate Change in projections of Soil Organic Carbon sequestration from agriculture in Northeast Ohio",* ENV 11-12, Mentor High
5 **Eashan Kosaraju,** *"SmartFarm: A comprehensive AI-powered One-Stop Crop Tool",* ENG 9-10, Solon High
6 **Amaan Siddiqi,** *"Hybrid Na-CO2 Solar Fuel Cell System",* ENG 9-10, Lake Ridge Academy
7 **John Anand,** *"Scents and Sensibility: Investigating the Influence of Visual Cues on Olfactory Perception on humans and AI using an electronic nose",* ENG 11-12, Home School

For those attending this event, a Professional Development Hour Certificate (1 PDH) will be sent to you in the following days by Joe Yurko.

Meeting Location: ***The Parma Snow Road CCPL*** *(see map below)*

2121 Snow Road
Parma, OH 44134
216-661-4240

5:00 – 6:30 pm: Social Gathering & NASA Talk
6:30 – 7:30 pm: Dinner
7:30 – 8:30 pm: Presentations with Q & A



Dinner: : Professionals: $10 each
Students: $5 each, NEOSEF Students free
Please pay CASH or Check. Thank you!
Email Joe Yurko RSVP by April 1

Dinner Menu:

1 Beef Stew, Bean Salad, Dinner Rolls
2 Chicken Stew, Bean Salad, Dinner Rolls
3 Dessert Walnut Patika with caramel sauce

RSVP Required by Monday 01Apr2024 with Joseph Yurko and AIChE at: yurkojoe5@gmail.com

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MARCH 11, 2024 CLE AICHE MEETING:

"Process Safety and Occupational Safety – Heinrich's Triangle"

WITH MARIANNE C. CORRAO, CO-FOUNDER/EXECUTIVE VP, NEXUS ENGINEERING GROUP, CLEVELAND, OHIO

MARIANNE C. CORRAO, EVENING SPEAKER, RECEIVING CLE AICHE STEERING COMMITTEE LETTER OF APPRECIATION

P.J. PECK WEARING 3-D VISION MAKING FINGER DOUBLE CLICKS TO ADVANCE THROUGH THE 3-D SOFTWARE DEMONSTRATION FOLLOWING INSTRUCTIONS BY JOE SANTOSIDES, NEXUS ENGINEER.

Enhancing Engineering Workflows with VR/AR/MR/XR Headsets at Nexus Engineering Group

Introduction

In the ever-evolving landscape of engineering and construction, embracing cutting-edge technologies is essential. Nexus Engineering Group, a forward-thinking firm based in Cleveland, Ohio, has taken a significant leap by integrating virtual and augmented reality (VR/AR) headsets into their operations. These headsets enable engineers, designers, and field personnel to visualize complex 3D models, assess constructability, and streamline collaboration.

The Role of Virtual Reality, Augmented Reality, Mixed Reality and Spatial Computing

Nexus Engineering Group employs software such as BIM Holoview to transform CAD Models into immersive 3D experiences. With extended reality or spatial computing headsets like the **Apple Vision Pro**, **Meta Quest 3** and **Microsoft Hololens 2**, engineers and owners can walk through virtual sites, inspect intricate details, and identify potential clashes before construction begins. This process significantly reduces errors and accelerates decision-making.

- 3D Model Reviews – With these headsets, the team can review the design model in a 3D collaborative environment where they can interact with the digital environment. The review can be conducted in the same office, as well as, concurrently at other locations where other reviewers can join in viewing the same model.
- Field Constructability Reviews – The technology allows the user to overlay a digital 1:1 scale model onto physical spaces. On-site personnel can visualize equipment placement, verify clearances, and assess safety considerations.

Benefits and Impact

- **Efficiency**: VR/AR/XR headsets expedite design validation, minimizing rework during construction. Engineers can spot clashes, evaluate spatial constraints, and optimize layouts seamlessly.
- **Collaboration**: Nexus Engineering Group fosters collaboration across teams. Whether it's a remote design review or an on-site walkthrough, these headsets facilitate communication and enhance understanding.
- **Safety**: By identifying constructability issues early, safety risks are mitigated. Field personnel can visualize potential hazards and plan accordingly.

Conclusion

Nexus Engineering Group's adoption of VR/AR/XR headsets exemplifies their commitment to innovation and excellence. As the industrial metaverse continues to evolve, these tools empower engineers to bridge the gap between digital models and physical reality. We look forward to witnessing more groundbreaking applications as Nexus Engineering Group pioneers the future of engineering.

About Nexus Engineering Group

Nexus Engineering Group is a full-service, independent engineering firm headquartered in Cleveland, Ohio with offices in Toledo, Ohio, Midland, Michigan, and Oak Brook, Illinois. Nexus is focused on supporting clients' specific project goals from concept to startup. Since 2005, clients have recognized Nexus as the engineering services firm of choice in the refining, petroleum midstream, chemical, manufacturing and utilities industries.

With more than 225 professionals on staff, Nexus is made up of experienced process, instrumentation and controls, structural engineering, electrical, mechanical engineering, and piping professionals with decades of hands-on conceptual and detailed system design, construction, and project management experience.

Nexus delivers project designs that reduce overall risks resulting in safer work environments. By utilizing state-of-the-art software and innovative design tools, Nexus consistently meets client project and investment requirements. Get to know us and you will agree that Nexus is not your typical engineering firm – "Engineering Relationships."

For more information, visit www.nexusegroup.com

MARCH 12, 2024: CLE AICHE JUDGING NEOSEF PROJECTS AT CSU

NORTHEAST OHIO SCIENCE AND ENGINEERING FAIR **(NEOSEF)**
Student Environmental and Engineering Projects grades 7 to 12

CLE AICHE JUDGES: JOSEPH SPAGNUOLO, BRUNO MANCINI, MICHAEL GALGOCZY, AND JOSEPH YURKO

(L-R) BRUNO MANCINI, JOSEPH SPAGNUOLO, MICHAEL GALGOCZY, AND JOSEPH YURKO: AICHE JUDGES

JUDGES (400 SITTING IN THE BLEACHERS) APPLAUD AS NEOSEF STUDENTS (ABOUT 300) ENTER THE CSU FIELDHOUSE ON THE SECOND FLOOR

JUDGES AND NEOSEF STUDENTS ON THE FIRST FLOOR AT THE CSU FIELDHOUSE

NEOSEF CHAIRPERSON WELCOME STUDENTS AND JUDGES IN THE CSU FIELDHOUSE

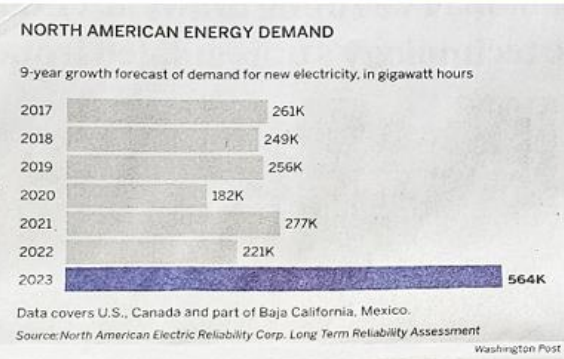
PLAIN DEALER NEWSPAPER, CLEVELAND, OHIO

The following article was reprinted from the Cleveland Plain Dealer Newspaper from the Sunday, March 10, 2024 “IN DEPTH” section A17.

ENERGY

Amid skyrocketing demand, America is running out of power

Artificial intelligence, data centers and the boom in clean-tech manufacturing are pushing aging power grids to the brink. Utilities can't keep up.



Evan Halper *Washington Post*

Vast swaths of the United States are at risk of running short of power as electricity-hungry data centers and clean-technology factories proliferate around the country, leaving utilities and regulators grasping for credible plans to expand the nation's creaking power grid.

In Georgia, demand for industrial power is surging to record highs, with the projection of electricity use for the next decade now 17 times what it was only recently. Arizona Public Service, the largest utility in that state, is also struggling to keep up, projecting it will be out of transmission capacity before the end of the decade absent major upgrades.

Virginia needs the equivalent of several large nuclear power plants to serve all the new data centers planned and under construction. Texas, where electricity shortages are already routine on hot summer days, faces the same dilemma.

The soaring demand is touching off a scramble to try to squeeze more juice out of an aging power grid while pushing commercial customers to go to extraordinary lengths to lock down energy sources, such as building their own power plants.

"When you look at the numbers, it is staggering," said Jason Shaw, chairman of the Georgia Public Service Commission, which regulates electricity. "It makes you scratch your head and wonder how we ended up in this situation. How were the projections that far off? This has created a challenge like we have never seen before."

BIG TECH, BIG USAGE

A major factor behind the skyrocketing demand is the rapid innovation in artificial intelligence, which is driving the construction of large warehouses of computing infrastructure that require exponentially more power than traditional data centers. AI is also part of a huge scale-up of cloud computing. Tech firms like Amazon, Apple, Google, Meta and Microsoft are scouring the nation for sites for new data centers, and many lesser-known firms are also on the hunt.

The proliferation of crypto-mining, in which currencies like bitcoin are transacted and minted, is also driving data center growth. It is all putting new pressures on an overtaxed grid - the network of transmission lines and power stations that move electricity around the country. Bottlenecks are mounting, leaving both new generators of energy, particularly clean energy, and large consumers facing growing wait times for hookups.

The situation is sparking battles across the nation over who will pay for new power supplies, with regulators worrying that residential ratepayers could be stuck with the bill for costly upgrades. It also threatens to stifle the transition to cleaner energy, as utility executives lobby to delay the retirement of fossil fuel plants and bring more online. The power crunch imperils their ability to supply the energy that will be needed to charge the millions of electric cars and household appliances required to meet climate goals.

The nation's 2,700 data centers sapped more than 4% of the country's total electricity in 2022, according to the International Energy Agency. Its projections show that by 2026, they will consume 6%. Industry forecasts show the centers eating up a larger share of U.S. electricity in the years that follow, as demand from residential and smaller commercial facilities stays relatively flat thanks to steadily increasing efficiencies in appliances and heating and cooling systems.

Data center operators are clamoring to hook up to regional electricity grids at the same time the Biden administration's industrial policy is luring companies to build factories in the United States at a pace not seen in decades. That includes manufacturers of "clean tech," such as solar panels and electric car batteries, which are being enticed by lucrative federal incentives.

Companies announced plans to build or expand more than 155 factories in this country during the first half of the Biden administration, according to the Electric Power Research Institute, an industry think tank. Not since the early 1990s has factory-building accounted for such a large share of U.S. construction spending, according to the group.

Utility projections for the amount of power they will need over the next five years have nearly doubled and are expected to grow, according to a review of regulatory filings by the research firm Grid Strategies.

CHASING POWER

In the past, companies tried to site their data centers in areas with major internet infrastructure, a large pool of tech talent, and attractive government incentives. But these locations are getting tapped out.

Communities that had little connection to the computing industry now find themselves in the middle of a land rush, with data center developers flooding their markets with requests for grid hookups. Officials in Columbus, Ohio; Altoona, Iowa; and Fort Wayne, Ind. are being aggressively courted by data center developers. But power supply in some of these second-choice markets is already running low, pushing developers ever farther out, in some cases into cornfields, according to JLL, a commercial real estate firm that serves the tech industry.

Grid Strategies warns in its report that "there are real risks some regions may miss out on economic development opportunities because the grid can't keep up."

"Across the board, we are seeing power companies say, 'We don't know if we can handle this; we have to audit our system; we've never dealt with this kind of influx before,'" said Andy Cvengros, managing director of data center markets at JLL. "Everyone is now chasing power. They are willing to look everywhere for it."

"We saw a quadrupling of land values in some parts of Columbus, and a tripling in areas of Chicago," he said. "It's not about the land. It is about access to power." Some developers, he said, have had to sell the property they bought at inflated prices at a loss, after utilities became overwhelmed by the rush for grid hookups.

RETHINKING INCENTIVES

It is all happening at the same time the energy transition is steering large numbers of Americans to rely on the power grid to fuel vehicles, heat pumps, induction stoves and all manner of other household appliances that previously ran on fossil fuels. A huge amount of clean energy is also needed to create the green hydrogen championed by the White House, as developers rush to build plants that can produce the powerful zero-emissions fuel, lured by generous federal subsidies.

Planners are increasingly concerned that the grid won't be green enough or powerful enough to meet these demands.

Already, soaring power consumption is delaying coal plant closures in Kansas, Nebraska, Wisconsin and South Carolina.

In Georgia, the state's major power company, Georgia Power, stunned regulators when it revealed recently how wildly off its projections were, pointing to data centers as the main culprit.

The demand has Georgia officials rethinking the state's policy of offering incentives to lure computing operations, which generate few jobs but can boost community budgets through the hefty property taxes they pay. The top leaders of Georgia's House and Senate, both Republicans, are championing a pause in data center incentives.

Georgia regulators, meanwhile, are exploring how to protect ratepayers while ensuring there is enough power to meet the needs of the state's most-prized new tenants: clean-technology companies. Factories supplying the electric vehicle and green-energy markets have been rushing to locate in Georgia in large part on promises of cheap, reliable electricity.

When the data center industry began looking for new hubs, "Atlanta was like, 'Bring it on,'" said Pat Lynch, who leads the Data Center Solutions team at real estate giant CBRE. "Now Georgia Power is warning of limitations. ... Utility shortages in the face of these data center demands are happening in almost every market."

A similar dynamic is playing out in a very different region: the Pacific Northwest. In Oregon, Portland General Electric recently doubled its forecast for new electricity demand over the next five years, citing data centers and "rapid industrial growth" as the drivers.

That power crunch threw a wrench into the plans of Michael Halaburda and Arman Khalili, longtime data center developers whose latest project involves converting a mothballed tile factory in the Portland area. The two were under the impression only a couple of months ago that they would have no problem getting the electricity they needed to run the place. Then the power company alerted them that it would need to do a "line and load study" to assess whether it could supply the facility with 60 megawatts of electricity — roughly the amount needed to power 45,000 homes.

GOING OFF THE GRID

The Portland project Halaburda and Khalili are developing will now be powered in large part by off-the-grid, high-tech fuel cells that convert natural gas into low-emissions electricity. The technology will be supplemented by whatever power can be secured from the grid. The partners decided that on their next project, in south Texas, they're not going to take their chances with the grid at all. Instead, they will drill thousands of feet into the ground to draw geothermal energy.

Halaburda sees the growth as good for the country and the economy. "But no one took into consideration where this is all going," he said. "In the next couple of years, unless there is a real focus on expanding the grid and making it more robust, we are going to see opportunities fall by the wayside because we can't get power to where it is needed."

Companies are increasingly turning to such off-the-grid experiments as their frustration with the logjam in the nation's traditional electricity network mounts. Microsoft and Google are among the firms hoping that energy-intensive industrial operations can ultimately be powered by small nuclear plants on-site, with Microsoft even putting AI to work trying to streamline the burdensome process of getting plants approved.

The Biden administration has made easing the grid bottleneck a priority, but it is a politically fraught process, and federal powers are limited. Building the transmission lines and transfer stations needed involves huge land acquisitions, environmental reviews and negotiations to determine who should pay what costs.

The process runs through state regulatory agencies, and fights between states over who gets stuck with the bill and where power lines should go routinely sink and delay proposed projects. The amount of new transmission line installed in the U.S. has dropped sharply since 2013, when 4,000 miles were added. Now, the nation struggles to bring online even 1,000 new miles a year.

Chemical Engineering Progress, CEP Magazine, American Institute of Chemical Engineers (AIChE), March 2024, Page 28

The Dogma of Process Safety

BY: SEAN J. DEE, P.E., CHRISTOPHER S. BUEHLER, P.E., RUSSELL A. OGLE, NICHOLAS REDING, NAVID ZANGANEH
https://www.aiche.org/resources/publications/cep/2024/march/dogma-process-safety

When an incident occurs, a process safety management (PSM) program is often scrutinized. PSM program failures can have significant contractual and legal implications.

Proponents of process safety may at times be mischaracterized as dogmatic, or having a point of view that is purported as authoritative without an adequate basis. A key question underlying this criticism raised by process safety skeptics is whether process safety incidents are truly preventable. This article aims to address this key philosophical (and contractual) question regarding whether catastrophic events are foreseeable and within the control of a facility's operations — two key elements of a force majeure claim (the so-called "Act of God"). The article will further discuss how the elements in a process safety management (PSM) program can help facilities identify, evaluate, and control process hazards and their associated risks, and whether shortcomings in a PSM program can impact the foreseeability and controllability of process hazards, which may be relevant in the evaluation of force majeure events.

Dogma and process safety

Dogma, as defined by Merriam-Webster's dictionary, is a point of view or tenet put forth as authoritative, without adequate grounds *(1)*. It is a concept that is frequently encountered in discussions involving specific subjects — particularly within the scope of politics and religion. However, in the parlance of process safety, it is possible for skeptics to view its proponents as being dogmatic. These criticisms focus on the fact that while progress has been made in the adoption of process safety principles, serious catastrophic incidents continue to occur globally. This issue is particularly relevant in the U.S. today as regulators consider potential changes to, and expansion of, the U.S. Occupational Safety and Health Administration's (OSHA) PSM Standard *(2)*. Resistance to these changes typically references the significant resources necessary for the implementation of a PSM program without demonstrated effectiveness of risk mitigation in a particular application *(3)*. As a result, advocates that argue for further expansion and adoption of process safety principles may encounter criticism that they argue from an authoritative point of view without adequate supporting bases (*i.e.,* dogma)…

Chemical & Engineering News, C&EN Magazine, American Chemical Society (ACS),
March 11-18, 2024, Page 43

Leadership: The heart of the American Chemical Society and the future of chemistry

By: **Wayne E. Jones Jr., chair, ACS Board of Directors**
https://pubs.acs.org/doi/10.1021/cen-10208-comment

Over the past 150 years, the American Chemical Society has grown from 35 chemists in New York to a thriving global membership community of over 200,000 individuals. We strive to improve all people's lives through the transforming power of chemistry. As the newly elected chair of the ACS Board of Directors, I have been reflecting on the key factors resulting in our longevity and how we can ensure a vibrant, successful future for ACS over the coming centuries.

I truly believe we are here today because of ACS's long-standing commitment to chemistry and to the development of our members as leaders. Throughout its history, ACS has dedicated significant resources to fostering leadership throughout the global chemistry enterprise, and I am happy to report that this commitment remains strong. Beginning with our founding, we recognized that leadership starts locally through opportunities to serve at the local section level. This recognition has expanded to the many diverse technical division disciplinary areas to which chemistry contributes. However, the world evolves, and ACS must do the same to ensure that we remain relevant and valuable to our members and true to our purpose. Looking forward, we must cultivate new ways to engage and support members in their leadership journey, supporting their development and leveraging their passion to shape the future of ACS...

Chemical & Engineering News, C&EN Magazine, American Chemical Society (ACS),
February 12-19, 2024, Page 19

Recovering hydrogen from ammonia

Ammonia technology licensor KBR has brought a cracking technology to market

By: **Alex Tullo**
https://pubs.acs.org/doi/10.1021/cen-10205-feature2

Making ammonia from nitrogen and hydrogen via the Haber-Bosch process has been critical to fertilizing the world's crops for more than a century, but there's been little need to run the reaction in the opposite direction. That's about to change.

Interest in using low-carbon ammonia as a fuel is taking off, and companies, often encouraged by government incentives, plan to spend billions of dollars building ammonia plants for this market. Some plants will make it from blue hydrogen, whose production involves reforming natural gas and capturing and storing by-product carbon dioxide. Other plants will make it from green hydrogen, which is created by electrolyzing water with renewable electricity.

Unlike hydrogen, ammonia can be easily shipped around the world. Upon delivery to the customer, it will be burned directly in ship engines or in power plants designed for coal. Or it will be cracked to get the hydrogen back for running fuel cells or power plants designed for natural gas.
The engineering firm KBR is one of a handful of companies developing technology for cracking ammonia. To say KBR has experience with the molecule is an understatement. About half the world's ammonia plants today license KBR's production technology.

"Until recently, ammonia has been a nitrogen carrier for the fertilizer market, which is feeding the world," says Elena Stylianou, global head of KBR's ammonia-cracking technology business. "That has been an amazing

market, and it has been really good to KBR. But what we've been seeing in the last 2 or 3 years is this huge interest in ammonia as a hydrogen carrier…"

Chemical & Engineering News, C&EN Magazine, American Chemical Society (ACS), February 12-19, 2024, Page 20

Making propylene directly from ethanol

By: **Katsumori Matsuoka, special to C&EN**
https://pubs.acs.org/doi/full/10.1021/cen-10205-feature3

Propylene is one of the most essential petrochemical feedstocks, used to make high-volume chemicals such as acrylonitrile, propylene oxide, and polypropylene. The three-carbon monomer is produced mostly through naphtha cracking at petrochemical plants and fluid catalytic cracking in petroleum refineries. In both cases, fossil fuels are the main raw material.

Sumitomo Chemical is developing a new technology to produce propylene directly from ethanol. Ethanol is now made mainly from crops such as sugarcane and corn, but Sumitomo points to methods emerging to make the alcohol from waste plastics, household waste, or carbon dioxide. Making propylene from such ethanol would fit with the Japanese firm's goal to be carbon neutral by 2050.

With carbon neutrality in mind, Sumitomo installed a pilot facility at its Chiba, Japan, site in 2022 that produces ethylene, a two-carbon chemical, from ethanol using technology from the French engineering firm Axens. Now Sumitomo is developing its own technology to produce propylene from the alcohol.

The roots of the technology go back to 2008, when Sumitomo participated in a project funded by Japan's New Energy and Industrial Technology Development Organization to foster use of biobased raw materials. Sumitomo's focus was on catalysts that can drive the ethanol-to-propylene (ETP) conversion. During the 5-year project, company researchers discovered a metal catalyst that aided the conversion, and they verified the approach at the bench scale.

This project ended in 2013, and Sumitomo halted its R&D. But almost 10 years later, heeding its new mandate to decarbonize, the firm has resumed work. One sweetener to restart was that the program was selected in 2022 to receive funding from the $13.8 billion Green Innovation Fund established by Japan's Ministry of Economy, Trade, and Industry. The fund will subsidize two-thirds of the firm's R&D for the project and one-half its cost of building a pilot facility…

Chemical & Engineering News, C&EN Magazine, American Chemical Society (ACS),
February 12-19, 2024, Page 21

Clean H_2 with nanotubes on the side

By: **Craig Bettenhausen**
https://pubs.acs.org/doi/10.1021/cen-10205-feature4

Hydrogen is back in style. Devices that produce and use H_2 were at the center of presentations on transportation and infrastructure from Bosch, Hyundai, Panasonic, Nikola, and others at CES 2024, the recent consumer electronics show in Las Vegas. And the climate mitigation plans of many manufacturers, especially those in the chemical industry, depend on H_2.

Most H_2today is made from fossil fuels using steam-methane reforming (SMR), an energy-intensive process that gives off about 9 metric tons (t) of carbon dioxide for every 1 t of H_2 it yields, according to the International Energy Agency. The CO_2 can be captured, but the process is expensive. Water electrolysis is a quickly growing alternative, but it's only as green as the electricity that runs it.

Pyrolysis offers a way to make H_2 while sidestepping the hassles of a CO_2 by-product. Several companies offer oxygen-free thermal reactors that decompose methane and other hydrocarbons into H_2 gas and solid carbon, usually in the form of carbon black, coke, or soot.

The chemical maker Huntsman adds a twist with a system based on floating-catalyst chemical vapor deposition that yields its carbon in the form of multiwalled carbon nanotubes. Operators feed sulfur and ferrocene into a reaction chamber, where they combine to form a catalyst. The reactor also decomposes methane into H_2 gas and carbon, which grows on the catalyst particles in long nanotubes that fall to the bottom of the reactor.

Huntsman acquired the system in 2018 when it bought Nanocomp Technologies and now is expanding production of the nanotubes from a 1 t per year plant in Merrimack, New Hampshire, to a 30 t facility starting up any day now in San Antonio.

Carbon nanotubes—graphene sheets rolled up into cylinders at the molecular scale—are a much more valuable form of carbon than carbon black, coke, or soot. Nanotubes have high electrical and thermal conductivity and a tensile strength greater than steel, all at a fraction of steel's weight…

Chemical & Engineering News, C&EN Magazine, American Chemical Society (ACS),
February 12-19, 2024, Page 29

The elements of a green catalyst

Making homogeneous catalysis greener is about more than just swapping out precious metals for earth-abundant ones

By: **Brianna Barbu**
https://pubs.acs.org/doi/10.1021/cen-10205-cover

Chemists agree that a sustainable future requires reducing reliance on precious metals such as palladium and rhodium. Many of them hold up earth-abundant first-row transition metals as green alternatives to the precious

metals used to catalyze cross couplings and other important organic reactions needed to synthesize drug molecules. First-row metals are less costly and less carbon intensive to refine, and they can do a lot of useful chemistry. But making catalytic reactions more sustainable requires thinking about more than just swapping out precious-metal catalysts for earth-abundant ones.

On a summer day about 20 years ago, Paul Chirik returned to his laboratory after a conference with a question on his mind: Why do chemists use expensive rhodium to do hydrogenation reactions? Why don't they use something more available, such as iron?
Chemists are rightfully proud of the transition-metal catalysts they developed to enable certain organic transformations. For example, rhodium catalyzes asymmetric hydrogenation, ruthenium catalyzes olefin metathesis, and palladium typically catalyzes a whole suite of carbon-carbon and carbon-heteroatom cross-coupling reactions. Each of these reactions is a Nobel Prize–winning accomplishment, but they all use some of the least available elements on earth.

"Why the heck do chemists use these things in the first place? The answer is they work," says Chirik, a professor at Princeton University. Since the cross-coupling boom of the 1970s, precious-metal catalysts have transformed the landscape of organic synthesis, medicinal chemistry, and drug discovery.

But the metals carry both a high price tag and a high carbon footprint. According to a 2014 study, the amount of carbon dioxide released from mining and refining 1 kg of palladium metal is about 3,880 kg (*PLOS One*, DOI: 10.1371/journal.pone.0101298). And that kilogram cost over $30,000 at the beginning of February 2024, according to Business Insider. Meanwhile, just one row up on the periodic table, nickel costs less than $16 per kilogram, and producing it releases just 6.5 kg of CO_2.

Chirik realized that his question was an interesting line of scientific inquiry and, potentially, valuable for industry chemists looking to make their syntheses greener and more cost effective. He has spent much of the past 2 decades working on coaxing earth-abundant metals such as cobalt, iron, and nickel to do reactions that have been dominated by precious metals. And he's far from the only person doing so.

Entire symposia at scientific conferences are now devoted to reactions with earth-abundant metals. And pharmaceutical companies including Bristol Myers Squibb (BMS), Merck & Co., Pfizer, and AbbVie have research initiatives dedicated to earth-abundant catalysis. These efforts have paid off: there are a growing number of reactions in which first-row transition metals perform on par with, or in some cases better than, precious ones.

But while chemists say they would like to use less precious metal and more earth-abundant elements for cost and sustainability reasons, switching metals is not automatically the greenest choice. "It's not always going to be beneficial or always going to be the solution," says Dan Lehnherr, a chemist at Merck.

Many variables affect sustainability. And the overall greenest way to synthesize a molecule requires a holistic view, says Fabrice Gallou, a scientific director at Novartis. "We want to tell people to go through the process of analyzing the fate of everything before concluding" what the most sustainable option is…

Chemical Engineering Progress, CEP Magazine, American Institute of Chemical Engineers (AIChE), March 2024, Page 19

Decarbonizing the Basic Chemicals Industry Using Sustainable Finance

By: **MARIAN RODRIGUEZ, ELIAS MARTINEZ**
https://www.aiche.org/resources/publications/cep/2024/march/decarbonizing-basic-chemicals-industry-using-sustainable-finance

Large investment into sustainable technologies is required to decarbonize the chemical industry. Climate-aligned finance will be a key driver for implementing decarbonization measures.

The chemical industry is as diverse as the materials and processes it involves. However, society depends heavily on a few molecules that enable most chemical value chains and provide the necessities for our daily life, from water, food, and pharmaceuticals to computers, cars, and buildings. These essential molecules are commonly referred to as basic chemicals; they include ammonia, ethylene, propylene, methanol, and aromatics — benzene, toluene, and xylene (BTX). The production of these basic chemicals dominates the chemical industry by production volume, investment, energy consumption, and carbon emissions (Figure 1) *(1)*. The basic chemicals category accounts for around 60% of the chemical industry's energy consumption *(2)* and 75% of direct and energy-related greenhouse gas (GHG) emissions *(3)*.

The main reason for the high GHG intensity of chemical production is that it relies on the use of fossil resources such as coal, crude oil, and natural gas not only as a fuel but also as a feedstock. In addition to combustion, emissions are released from a variety of chemical reactions involved in the process technologies. Due to the large volumes of these basic chemicals produced annually, the use of fossil fuels as a raw material and energy source, and the direct process-generated emissions, the chemical industry is considered a hard-to-abate sector. However, future investment in the sector needs to be directed toward decarbonization to achieve net-zero targets and cap the global average temperature rise at 1.5°C. In response to the demands for a lower carbon future for the chemical industry, several chemical companies have announced their targets for reducing GHG emissions, whether it be maintaining certain reference emission levels or aiming for carbon neutrality (*i.e.,* net zero) by 2050.

This article introduces the Basic Chemicals Criteria. The Climate Bonds Initiative developed this first-of-its-kind criteria to be the standard for climate-aligned bonds invested in decarbonization measures and projects in the basic chemicals industry. As part of the criteria development process, experts and professionals from academia and research organizations convened to advise on low-carbon requirements for green bonds in the basic chemicals industry. Included in this conversation was an industry working group with representatives from industry associations and investors, who offered feedback on the applicability of the criteria. After an extensive approval process, the final version of the criteria was launched in April 2022. A full digital version of the criteria is available at www.climatebonds.net/standard/basic-chemicals(4)...

Swiss biotech restores motor function in mice with Parkinson's

By: **Rowan Walrath**
https://pubs.acs.org/doi/10.1021/cen-10207-buscon2

A Swiss biotech has restored motor function in mice with Parkinson's disease, paving the way for human trials later this year.

In a presentation at the WORLD Symposium conference, Gain Therapeutics described a small molecule that enhances the activity of the lysosomal enzyme glucocerebrosidase, better known as GCase. The Gain team believes that by bolstering the enzyme's activity, the compound, GT-02287, would boost the lysosome's ability to clear waste. That would in turn improve mitochondrial function and decrease the incidence of cell death in people with Parkinson's linked to mutations in *GBA1*, the gene that encodes for GCase.

So far, that approach has worked—in rodent models. Gain's preclinical study showed that over 3 weeks, mice who'd been injected with α-synuclein-preformed fibrils and GCase-inhibited rat neurons to mimic *GBA1* Parkinson's regained motor function after taking GT-02287.

The mice also had less of the biomarker neurofilament light chain (Nfl) in their bloodstreams. That suggests that GT-02287 is protecting neurons, according to Gain CEO Matthias Alder, since Nfl falls off the cells when they die and enters the blood.
"We're as close as you can get to a gene therapy with a small molecule," Alder says. "We're fixing the protein expressed with a defective gene."

Gain has tested GT-02287 in human volunteers without Parkinson's. Alder says data out of that trial have shown the molecule to be safe…

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Competition to destroy ‘forever chemicals’ heats up

Cleantech start-ups vie for a piece of the PFAS destruction market

By: **Britt E. Erickson**
https://pubs.acs.org/doi/10.1021/cen-10207-cover

Scientists once wrongly assumed that the carbon-fluorine bond was almost impossible to break. And that meant there was no practical way to completely destroy per- and polyfluoroalkyl substances (PFAS).

“They were truly thought to be ‘forever chemicals,’ ” says Julie Bliss Mullen, who began investigating technologies for removing PFAS from drinking water as an undergraduate in 2010. At the time, “destruction was not really on the table,” she recalls.

But Mullen was obsessed with breaking the carbon-fluorine bond. PFAS can be removed from water, but they just get transferred to another medium and eventually make their way back into the environment, she says. To stop that cycle, you have to destroy the molecules by breaking the “unbreakable” bond.

Around 2014, as a PhD student at the University of Massachusetts Amherst, Mullen got her hands on some electrodes and, as she puts it, “started playing around with electrochemical oxidation in the lab.” The process creates hydroxyl radicals and, unlike other advanced oxidation techniques, facilitates the direct transfer of electrons. “Those electrons will almost immediately break the carbon-fluorine bond if we’re able to get PFAS onto the anode surface,” she says.

Mullen won’t say how she attracts PFAS to the anode surface. But in 2017, she and the university filed for a patent and spun out a company, Aclarity, to commercialize the technology. Mullen never did finish her PhD. Today, as cofounder and CEO of the Massachusetts-based firm, she’s seeing big interest in the technology from landfill operators and wastewater treatment plants.

Aclarity is not the only company vying for a piece of the PFAS destruction market. Dozens of start-ups are working on technologies for destroying the chemicals, which have been linked to cancer and adverse effects on the liver and immune system. Some companies are already operating at full scale; others are not far behind. And it turns out that electrochemical oxidation is just one of many ways to break the carbon-fluorine bond.

Companies are developing an array of approaches, including supercritical water oxidation, hydrothermal alkaline treatment, plasma destruction, ultraviolet light combined with photocatalysts, and sonolysis. They all claim to break down most PFAS into less harmful chemicals, such as carbon dioxide, fluoride ions, and water. But complete destruction of all PFAS, including short-chain PFAS and precursors, is a stretch for some techniques…

Chemical Engineering Progress, CEP Magazine, American Institute of Chemical Engineers (AIChE), March 2024, Page 34

Using Hydrogen to Decarbonize Industrial Fired Heaters

By: **JAMES TURNER, TONY CHAN, STEPHEN RABB, P.E**
https://www.aiche.org/resources/publications/cep/2024/march/using-hydrogen-decarbonize-industrial-fired-heaters

Switching from fuel gas to a low-carbon hydrogen fuel is a promising option for decarbonizing industrial facilities.

With the urgent need to improve sustainability, organizations in the chemical process industries (CPI) are exploring ways to decarbonize their processes and reduce greenhouse gas (GHG) emissions. For an industrial facility, GHG emissions are typically classified into three categories:

- Scope 1 emissions are those that occur directly from the facility, such as emissions that occur during the operation of equipment and processes.
- Scope 2 emissions are those that occur due to the purchase of energy, such as electricity generated by fuel firing or purchased steam from an outside supplier.
- Scope 3 emissions are those that occur either upstream or downstream in the value chain, including emissions that occur during the production of a feedstock or hydrogen that is purchased. For a refinery that makes fuels (*e.g.,* jet fuel or diesel), Scope 3 emissions account for those fuels being used in transportation vehicles and the combustion products released to the atmosphere.

The Scope 1 emissions are the emissions that the facility owner has the most control over, although they can often exert influence over Scope 2 and Scope 3 emissions based on business decisions and other commercial agreements. For most industrial facilities, the vast majority of Scope 1 GHG emissions are carbon dioxide (CO_2) emissions from the combustion of hydrocarbon fuel in steam boilers and process heaters.

An industrial facility looking to reduce Scope 1 and Scope 2 CO_2 emissions should consider five primary techniques:

1. increase energy efficiency
2. use electrification to shift fired heater/steam boiler energy needs to low-carbon electrical power
3. use a renewable fuel (*e.g.,* bio-gas) in fired equipment
4. use carbon capture on the fluegas from the fired equipment
5. convert the heater to essentially 100% hydrogen fuel.

Techniques 1 and 2 can provide incremental benefits but rarely offer substantial reductions. Technique 3 is often limited by the availability of renewable fuels to replace a facility's current fuel source. Techniques 4 and 5 are the most common ways for the majority of facilities to achieve significant reductions in their CO_2 emissions.

Technique 4 (carbon capture) requires the facility to have a suitable disposition for the recovered CO_2 (*i.e.,* capturing the CO_2 and either storing or consuming it in another process). Also, many facilities have several heaters spread out over many units, and plot space may be very limited, making this option challenging and very expensive.

This article expands on Technique 5 (converting heaters to 100% hydrogen fuel). Hydrogen is often categorized into colors based on its production technique. The two primary ways to produce low-carbon hydrogen are to make green hydrogen via electrolysis of water, using low-carbon electricity, or to make blue hydrogen via steam methane reforming (SMR) or autothermal reforming (ATR) and capture the CO_2 produced…

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Capturing carbon in New York City

By: **Craig Bettenhausen**
https://pubs.acs.org/doi/10.1021/cen-10208-feature1

Down in the subbasement of a luxury apartment building in Manhattan, New York residents gave up five precious parking spaces to make room for a new idea: equipment that will strip carbon dioxide out of the flue gas from the building's twin 350-horsepower boilers, which crank out about 3.4 MW of power each.

Instead of exhausting the hot, wet products of methane combustion from the roof, Paramount Tower will drop treated water into the sewer, vent a room-temperature mix of oxygen and nitrogen at street level, and send CO 2 away as liquid in a refrigerated truck.

The building's carbon capture equipment is from the start-up CarbonQuest, which is also building a network of customers who want CO2 . The first buyer is Glenwood Mason Supply, a concrete-block maker across the East River in Brooklyn. Carbon capture is one of several ways that buildings in New York City are complying with Local Law 97, an aggressive climate change regulation that puts caps on greenhouse gas emissions from new and existing structures larger than 25,000 ft^2 (2,322 m^2).

Though CO_2 is a liability for large landlords in New York City—as well as almost everyone else—it's also an opportunity for companies aiming to commercialize technologies that use CO_2. Incentives, demand for low-carbon spaces, and a strong local talent pool are making the city into a hub for cleantech businesses, including those focused on carbon capture and utilization. The city is not likely a place where technologies for making chemicals and materials from CO_2 will be deployed at scale, but it could be a fertile breeding ground for climate-tech start-ups…

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Effective Procedures and Process Safety

By: **ROB FISHER**
https://www.aiche.org/resources/publications/cep/2024/march/effective-procedures-and-process-safety

Clearly written and intuitive procedures are a crucial component of safe operations. Avoid vague terms and systemic error drivers in procedures to improve field performance and process safety.

Many organizations that deal with process safety struggle to develop effective procedures. Effective procedures require time and effort to understand the error drivers that put personnel at risk. As an operator's vulnerability to error increases, so does the likelihood of a process safety event. When procedure writers, reviewers, and approvers are unaware of critical process attributes, the person using procedures often gets blamed when problems occur.

I am a consultant who has deployed the concepts of human error reduction, human and organizational performance (HOP), procedure and written guidance excellence, and effective incident analysis and learning in over 400 organizations, 25 countries, and 14 languages. I want to convey what I've learned over 30 years of assisting companies that rely on process safety to reduce their risk and improve performance. This article discusses the role of effective procedures in process safety and shares best practices from industry deployments of the concepts and tools related to field error reduction. These include a discussion of the systemic drivers of procedural deviations, the top five most common error drivers in written guidance, and some key principles to enable process safety. This will allow organizations to understand the next logical steps in improving their procedures…

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Visiting East Palestine 1 year later

12 months after a freight train derailed and dumped toxic chemicals in an Ohio town, locals worry about lingering pollutants and adverse health effects

By: **Priyanka Runwal**
https://pubs.acs.org/doi/10.1021/cen-10206-cover

If you drive through East Palestine, things seem normal. But look more closely, and reminders of a grim day in the town's history still linger. On Feb. 3, 2023, a freight train carrying hazardous chemicals derailed as it passed through the town, upending the lives of many residents. Although no one was killed or injured, concerns about environmental contamination and health risks remain. The US Environmental Protection Agency maintains that the air, drinking water, and soil are safe, and rail operator Norfolk Southern continues to clean up the mess. Several community members have grown distrustful of the EPA and the railroad company; others just want to put the accident behind them.

Krissy Hylton grew up with the rumbling of freight trains and the blaring of their horns. As a child, she loved laying pennies on the tracks before trains passed and collecting the flattened coins. Her home in East Palestine, Ohio—a small town near the Pennsylvania border—is about three blocks from train tracks owned by Norfolk Southern. "Now I hate hearing that train," she says.

Last year on Feb. 3, a train transporting frozen vegetables, semolina flour, malt liquor, lube oil, and industrial chemicals derailed from those same tracks, upending the 49-year-old's life and that of many other residents of East Palestine and nearby towns. According to a preliminary report released by the National Transportation Safety Board (NTSB), a wheel bearing overheated and caused the derailment. A video shows sparks and flames around the 23rd railcar that started a fire. Thirty-eight cars veered off the track. Eleven of them were carrying hazardous materials that spilled and fueled the large fire.

Especially worrisome were five tank cars containing vinyl chloride, a highly flammable carcinogen used to make the plastic polyvinyl chloride (PVC). Authorities intentionally released and burned the liquefied vinyl chloride on Feb. 6 to prevent a potential explosion.

A towering cloud of smoke wafted above the town and stretched into Pennsylvania. More than 2,000 people living near the derailment evacuated their homes. Hylton watched the thick black plumes from Patterson, Pennsylvania—a township about 20 minutes' drive from East Palestine—and wondered when she and her family would be able to return to their home. "I thought we were going to be gone for just another day or two," she says.

But to this day, her family and dozens of others remain displaced…

Chemical & Engineering News, C&EN Magazine, American Chemical Society (ACS),
February 26, 2024, Page 6

Lasers make hydrogen from ammonia and water

By: Mark Peplow, special to C&EN
https://pubs.acs.org/doi/10.1021/cen-10206-scicon1

Laser pulses that can shred ammonia molecules dissolved in water may offer a way to generate hydrogen gas without using heat, pressure, or catalysts (*J. Am. Chem. Soc.* 2024, DOI: 10.1021/jacs.3c13459). The proof-of-principle work by researchers at Sun Yat-sen University demonstrates an unusual way to exploit ammonia as a carrier for green hydrogen, an idea that is quickly gaining traction in many industries.

"Green" hydrogen is produced by electrolyzing water with renewable electricity, and it can be used to decarbonize various industrial processes, to power fuel cells in vehicles, and even as a means to store excess renewable energy.

Many companies are turning to ammonia as an easier way to ship hydrogen. Ammonia is much easier to liquefy, and it is richly packed with hydrogen atoms, which can be liberated by ammonia decomposition reactions.

Unfortunately, the most common ammonia decomposition method involves thermal crackers that operate at over 850 °C using nickel on aluminum oxide as the catalyst. Alternative methods, including electrochemistry or photochemistry, typically require expensive precious-metal catalysts (*Ind. Eng. Chem. Res.* 2021, DOI: 10.1021/acs.iecr.1c00843).

The Sun Yat-sen researchers have now taken a completely different approach to recovering hydrogen from ammonia. They use laser pulses to cause brief yet intense heating within an ammonia-water solution held inside a purpose-built reactor. The laser delivers 10 pulses per second to a 1-mm-wide spot within the liquid. Each pulse lasts just 10 nanoseconds and delivers enough energy to instantaneously raise the temperature of the target spot tens of thousands of degrees, turning the molecules there into a bubble of plasma. This plasma consists of a soup of radicals, including $^{\bullet}H$, $^{\bullet}OH$, and $^{\bullet}NH_2$, which quickly react to form hydrogen, nitrogen, and other gases…

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Plug Power starts producing H_2 in Georgia

By: **Craig Bettenhausen**
https://pubs.acs.org/doi/full/10.1021/cen-10208-buscon9

Plug Power has begun production of hydrogen at its 40 MW electrolysis plant in Woodbine, Georgia. The facility, billed as the largest electrolytic liquid H 2 facility in the US, has a capacity of 15 metric tons per day. It will buy renewable energy credits from the local electrical grid, according to the Atlanta Journal-Constitution . Plug is distributing the resulting hydrogen to its network of forklift and automotive fueling stations…

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Accelerating discovery with Azure Quantum Elements

By: Michael Eisenstein, *C&EN BrandLab*
https://cen.acs.org/sponsored-content/accelerating-discovery-with-azure-quantum-elements.html

In simulating properties of molecules and materials, computational chemistry has the potential to accelerate scientific discovery for a wide variety of applications by reducing the need for costly and drawn-out experiments. But current computational methods are inadequate for exploring the vast and complex space of possible materials—thus limiting their effectiveness and performance.

Azure Quantum Elements, a Microsoft platform built with artificial intelligence (AI) and cloud-powered high-performance computing (HPC), offers scientists an opportunity to examine immense regions of the chemical universe at unprecedented speeds. In one recent demonstration, Microsoft researchers used Azure Quantum Elements to rapidly search tens of millions of possible materials for use as a battery electrolyte—the conductive medium that facilitates the transit of ions between electrodes. After narrowing this virtual field in just a week, they turned to a major US National Laboratory to select and test the most promising candidates. They even identified one particularly interesting material that could reduce dependency on lithium, whose increasing scarcity is a critical concern for future energy-storage applications.

This entire process took just nine months, including creating a proof-of-concept battery with the newly synthesized candidate. Even though the team is still characterizing and optimizing these candidate materials, this project demonstrates how the quick analytical capabilities of Azure Quantum Elements can help chemists and materials scientists get projects off the ground faster than ever and focus on the creative work of developing innovative and functional tools and products.

STREAMLINING DISCOVERY

When Microsoft announced Azure Quantum Elements in June 2023, CEO Satya Nadella declared that the goal was to “compress the next 250 years of chemistry and materials science progress into the next 25.”

This is no simple feat, says Nathan Baker, product leader of Azure Quantum Elements at Microsoft and a former chemist. “Computational chemistry is hard,” he explains. “It’s hard because it needs high-end computing, and that high-end computing is hard to procure, it’s hard to scale up, and it’s hard to maintain.” The goal of Azure Quantum Elements is to make these capabilities more broadly available and usable for researchers who may not be deeply familiar with cutting-edge computing.

The Azure Quantum Elements team achieved this goal with a multipronged approach. The first component is cloud-based HPC, which provides the flexible and scalable processing power that scientists need to analyze materials and chemical reactions at ever-larger scales. These HPC capabilities are wedded to a sophisticated toolbox of AI models, which have been trained on a dataset of millions of materials simulations and massive amounts of published scientific data from chemical literature.

AI-assisted analysis can eliminate certain time-consuming calculations by using this training material to generate data-informed predictions about critical properties of a particular substance or chemical formulation—for example, parameters that influence electrochemical behavior. Of course, there are still

many things that AI cannot predict and are better resolved with computer simulations grounded in real-world physical and statistical principles. “I believe firmly that there’s never going to be a replacement for simulation, because simulation doesn’t just give you an answer. It gives you insight, and that insight drives the design,” Baker says. But even in this context, AI can help derive physical models that lead simulations that are more efficient and accurate. By combining AI and HPC, the Microsoft team estimates that researchers can speed up key aspects of their analytical workflows by up to 500,000-fold compared with conventional computational methods.

Azure Quantum Elements also supports a wide variety of popular computational chemistry tools. Connecting all these processes can be technically daunting for researchers focused on laboratory work rather than on computational methods. To further simplify these processes, Microsoft also released Copilot in Azure Quantum Elements, an AI-powered interface that relies on the same large language model framework underlying systems like ChatGPT. Users can input queries to the platform in plain English—or whatever the scientist’s language of choice may be—on a particular chemistry problem and receive an equally clear response from the algorithm. Copilot can also cue up the algorithmic tools required to perform the analysis. “That really removes barriers for people,” Baker says.

TURBOCHARGING BATTERY DEVELOPMENT

The battery electrolyte development effort began as a proving ground to demonstrate the efficiency and utility of Azure Quantum Elements to the chemists and materials scientists on the Azure Quantum team. Materials development involves much winnowing down of candidate materials to home in on the most promising. By starting with a bigger pool in the early stages, scientists can potentially stack the odds in favor of success. Azure Quantum Elements’ analytical capabilities allowed Microsoft researchers to begin at a truly massive scale, with a starter set of 32.6 million possible materials.

One material proposed by Azure Quantum Elements offered such an opportunity, achieving good conductance while using about 70% less lithium than existing electrolytes.

The first round of AI-assisted screening narrowed that number to half a million potential electrolytes. Most of these were culled during an assessment of properties related to the material’s ability to facilitate the movement of ions, such as redox potential and band gap. Filtering 32.6 million starting points down to 800 semifinalists took just 80 h of computing. This represents a dramatic time savings relative to conventional computational methods, with which “screening that many materials would have taken two decades,” Baker says. The options were then narrowed to 150 via physics-based simulations that analyzed each material’s molecular-scale properties and behavior.

At this point, Microsoft reached out to a major US National Lab team to get its perspective on the fruits of Azure Quantum Elements’ labors. The team saw opportunities for further refinement and suggested additional screening parameters, including eliminating materials that are excessively chemically reactive or that incorporate conductive but costly elements such as platinum or gold. After applying these parameters and further considering the list of finalists, the team converged on four materials that appeared to be sufficiently cost effective, conductive, and stable for use as a battery electrolyte.

Most modern lithium-ion batteries rely on electrolytes based on lithium salts. The flow of lithium ions between the battery’s electrodes results in the generation of current, whereas applying a charge to the battery reverses that ionic flow, which regenerates the battery’s current-generating capacity. Lithium is extremely lightweight and electrochemically active, making it a valuable material for batteries. Unfortunately, the demand for lithium currently outstrips production capacity, and lithium is generally extracted via environmentally damaging mining processes. As a result, there is considerable interest in reducing lithium dependence.

One material proposed by Azure Quantum Elements offered such an opportunity, achieving good conductance while using about 70% less lithium than existing electrolytes. Remarkably, this feature was not even among the parameters applied during screening. The lithium ions are substituted with positively charged sodium or potassium, both of which are abundant and far easier to obtain than lithium. After synthesizing this material and experimentally validating the properties predicted by Azure Quantum Elements, the US National Lab team assembled a simple proof-of-concept battery using this electrolyte and showed that it could generate a stable charge at both room temperature and under high heat.

SPURRING CHEMICAL CREATIVITY

This isn't the end of the story. Although the low-lithium electrolyte exhibited reasonable conductance, it was not able to outperform other state-of-the-art materials. Further testing and optimization of this material will thus be necessary, and several other candidates identified by Azure Quantum Elements have yet to be assessed by the US National Lab.

"We got a hit, and now we need to optimize that lead," says Baker, who draws parallels to the process that the pharmaceutical industry uses to turn vast chemical libraries into safe and effective drug candidates. He also sees lessons that could lead to greater efficiency in future projects of this nature, including earlier use of more aggressive filtering measures based on desirable material parameters to narrow the field sooner.

Nevertheless, the results of this project highlight opportunities for researchers in a wide range of industries to dramatically accelerate their early-stage R&D efforts. Microsoft has already attracted many commercial partners, including chemical industry leaders like Johnson Matthey and AkzoNobel, to explore Azure Quantum Elements' capabilities. Baker is particularly excited about the potential to use this platform to model chemical reactions and design catalysts that efficiently execute those reactions—an important capability in manufacturing, energy generation, environmental remediation, and other applications.

The Azure Quantum Elements platform is designed to interface seamlessly with emerging quantum computing capabilities. These computing technologies are still under development and are primarily being used in an exploratory fashion. But Baker predicts that as quantum computing matures, it will enable researchers to confidently assess the ground-truth accuracy of their models and thereby develop even more computationally efficient and successful processes for materials discovery.

Azure Quantum Elements already has the potential to be a game changer. "Scientific discovery is too slow—the Edisonian approach doesn't scale the way we need it to scale," Baker says. As more and more researchers use the platform, he is eager to see how they leverage the power of AI and HPC in their work. "Watching this get out into industry and have an impact is thrilling," he says. "Just seeing the creativity of customers with the platform is really exciting."

CLE AIChE: Cleveland Chapter

Fall 2023 – Spring 2024 Program Planning

(as of Mar2024)

Month	Topic, Speaker	Location	AIChE Officer Responsible
September 8, 2023 (Friday 6 PM)	Oktoberfest Social Event	German Central Farm, Parma	Joe Yurko, $7/guest admission + $ food & beverage? https://germancentralfoundation.com/oktoberfest
October 11, 2023 (Wednesday 6 PM)	Brewery Tasting Tour	Market Garden Brewery, OH City	Mike Galgoczy, $20/guest with 20 guests. Dinner: 7 PM Market Garden Brewpub & Restaurant.
October 30, 2023 (Wednesday 5:30PM)	ASM Joint Meeting: H2 effect on heating metals, Justin Dzik, PE	FIVES North American Combustion, Inc.,	Joe Spagnuolo & Joe Yurko: $30 Non-members, $15 Retirees, $5 Students. German Dinner, Presentation, and Tour facility. https://www.fivesgroup.com/energy-combustion
November 14, 2023 (Tuesday 6 PM)	History of ACS 7-National Chemical Landmarks Sites in Cleveland, Helen Mayer Spkr	The Sanctuary, Rockside Road Independence, 44131	Joe Yurko, Dinner menu ordering for professional members, Students cost: $5 http://places.singleplatform.com/shulas-steak-house-8/menu#menu_5599999
December 7, 2023 (Thursday 6 PM)	Nuclear Power an Introduction, Speaking: Andrew Ohrablo	The Sanctuary, Rockside Road Independence, 44131	Joe Yurko, Dinner menu ordering for professional members, Students cost: $5 http://places.singleplatform.com/shulas-steak-house-8/menu#menu_5599999
January 29, 2024 (Monday 6 PM)	Chemical Process Safety Analysis, Speaking: Gurmukh Bhatia, CPSA	CCPL Independence 6361 Selig Drive Independence, 44131	Joe Yurko, Dinner for professional member's cost: $10, Students cost: $5 CCPL Independence Branch: 216-447-0160, Menu: vote on recipe
February 15, 2024 (Thursday 6 PM)	Appalachian Regional Clean H2 Hub ARCH2 DOE Award, Andrew Thomas, JD, CSU	The Sanctuary, Rockside Road Independence, 44131	Joe Yurko, Dinner menu ordering for professional members, Students cost: $5 http://places.singleplatform.com/shulas-steak-house-8/menu#menu_5599999
March 11, 2024	Safety Engineering in Oil Refining processes; Marianne Corrao Speaking	The Sanctuary, Rockside Road Independence, 44131	Mike Galgoczy, Dinner menu ordering for professional members, Students cost: $5 http://places.singleplatform.com/shulas-steak-house-8/menu#menu_5599999
March 13, 20 & 27 Wednesday 6-8 pm *CANCELLED*	Chemical Process Safety Analysis Seminars; Gurmukh Bhatia, CPSA	Cleveland Analytical LLC 15666 Snow Road Brook Park, OH	Joe Yurko, Dinner cost is included in the seminar expense. Seminar expense: TBA at a later time. Certificates will be awarded for each class as well as a final certificate.
April 4, 2024 Thursday 5-8 pm	NEOSEF Awards Banquet Rosanne Brunello-McCay NASA Solar System Ambas.	CCPL Parma Snow Road Branch 2121 Snow Road	Joe Spagnuolo, Moderator NEOSEF Students, CCPL Snow Road Branch, Parma 44134, $10 members, $5 students, NEOSEF students free. Dinner: Beef Stew & Chicken Stew
May	Cleveland Cliffs Steel Mill Tour, TBA	CCPL Independence 6361 Selig Drive Independence, 44131	Bruno Mancini. Joe Yurko, Dinner for professional member's cost: $10, Students cost: $5 CCPL Independence Branch: 216-447-0160, Menu: vote on recipe.

In person events -- Remote meetings if non-contact required / COMPLETED MEETING / PLANNED MEETING / PROPOSED MEETING