ENERCE NOVATON Summer 2022



PennState College of Earth and Mineral Sciences Earth and Mineral Sciences Energy Institute

Letter from the (interim) Mixector



Welcome to the summer 2022 edition of the EMS Energy Institute (EI) Newsletter. This edition highlights faculty research in several topical areas, introduces new faculty, and highlights the honors received by our students, faculty, and staff.

It is hard to believe that a year has already passed since publishing our last newsletter. It

is also hard to believe that I have served almost two years as EI's interim director. I have been assured that the hiring of a new director is imminent. While it has been a privilege serving as the interim director, some aspects of the institute have been put on hold while we have been waiting for a new director. Specifically, we have been waiting to prepare our five-year strategic plan so the new director can put their 'fingerprint' on it.

The research, education, and outreach efforts of the institute continue to focus on energy and energy-related environmental effects and involve researchers in the College of Earth and Mineral Sciences and the College of Engineering, along with collaborators worldwide. Current research projects cover the production and use of energy along with carbon dioxide capture, storage, and utilization, and the recovery of critical materials from various feedstock streams.

The faculty and staff of the institute have been very busy over the last year while still dealing with the COVID-19 pandemic. Research labs reopened and all research was ongoing by last summer. Staff had the option to work remotely until August 2021 at which time they could work either in a hybrid mode (some days remotely, other days in the office) or full time in the office. These options were offered through the 2022 spring semester.

Despite the pandemic and difficulties that some encountered working remotely, the institute experienced a very successful year. In the 2021-22 fiscal year, the institute's staff assisted faculty in preparing 125 proposals, which resulted in thirty-three projects being funded for a total of approximately \$8.1 million in research funding. From July 2021, through February 2022, seventy-seven proposals were prepared with thirty-six projects funded for a total of approximately \$10.2 million in research funding. Two staff members, Kelly Rhoades and Heather Harpster, are mostly responsible for assisting the faculty in proposal preparation. They were assisted by a third staff member, Christy English (until August 2021 when she accepted another position within the University) and then Stephanie Emigh, with post-award activities. I am extremely proud of what these staff members accomplished with pre-award and post-award activities while the institute was short one front office staff member. They are now getting additional support from Paige McCarthy who started at the institute in March.

I want to take this opportunity to thank all EI faculty members, research staff, students, and visiting scholars whose ideas and hard work have advanced energy science and engineering research. I also want to thank all our staff members whose hard work supports our faculty-driven research efforts. I am very proud of how the staff have handled the pandemic and continued to work efficiently, accurately, and productively. And I want to thank all those who assisted me in keeping the operation of the institute running smoothly while we await a new director.

Bruce G. Miller Interim Director and Research Professor, EMS Energy Institute



Energy Innovation is an annual publication from the EMS Energy Institute in the College of Earth and Mineral Sciences. The EMS Energy Institute is a leading research and development organization focused on energy science and engineering.

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EMS Energy Institute

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Upcycling plastic waste into graphite, used in electric vehicles and renewable energy storage, could positively contribute to the global economy, preserving resources, saving energy, and reducing carbon dioxide emissions, according to Penn State researchers.

Plastics are an incredibly important element in U.S. consumerism due to their versatile and highly durable nature. They are used in everything from product packaging to construction to electronics and machinery. However, with growing demand comes the dark side of plastic consumption—millions of tons of non-recyclable plastic waste.

According to McKinsey & Company, approximately thirty-seven million tons of plastic are used every year. Packaging and food service plastics represent about sixteen million tons of that total, and these are typically "single-use" plastics that are used and then discarded. In fact, Americans consume roughly one hundred pounds of packaging and food-service plastics per person, per year.

"We literally have mountains of plastic waste, millions of tons every year, and most of it is still going into the landfill," said Randy Vander Wal, professor of energy and mineral engineering, materials science and engineering, and mechanical engineering at Penn State. "But what if we have the opportunity to take a waste product that has no destiny per se and turn that into graphite?" The main types of plastic resin found in single-use packaging and food service applications are polyethylene terephthalate (PET), used in soft drink bottles; high-density polyethylene (HDPE), used in milk jugs; low-density polyethylene (LDPE), used in plastic bags, containers, films, and wraps; and polypropylene (PP), used in yogurt containers and bottle caps. Together, these plastic types make up approximately 85 percent of single-use volume, according to the EPA, and only about 12 percent of this material is recycled and 16 percent is burnt with municipal trash. The majority—more than 70 percent, or eleven million tons—is sent to landfills where it can take hundreds of years to break down.

Juxtaposed with an abundance of plastic waste is a forthcoming shortage in quality graphite.

"When everyone thinks of lithium-ion batteries, they think of lithium, which is a critical mineral, but quality carbon in the form of graphite is also needed in lithium-ion batteries," Vander Wal said. "And there will be a huge shortfall in the graphite needed for batteries."

Credit: Adobe Stock

In addition to lithium-ion batteries, certain industrial practices require graphite as well. For instance, in electrodes in aluminum refining and for electric arc furnaces used in steel manufacturing, among others.

"Every electric vehicle, like the Tesla Model 3, requires at least seventy kilograms of carbon," Vander Wal said. "For every one million electric vehicles, a 10 percent increase of the current graphite market is projected."

Currently, petroleum-derived cokes (a byproduct of the oil refining process), coal tar pitches (remnants from the distillation of coal tar), and mined graphite are the main sources for graphitic carbons used in energy storage methods such as lithium-ion batteries. Petroleum derived cokes and coal tar pitches are nonrenewable resources and demand a lot of energy to produce. In addition, their production produces high emission levels of volatile organic compounds. Meanwhile, natural graphite is a limited resource, and the mining process is environmentally destructive.

Under a seed grant from the Materials Research Institute, Vander Wal and his team will take single-use plastic waste and turn it into high quality graphite. To do this, they will use graphene oxide to provide the oxygen required for stabilization and an aromatic framework to guide the reconstruction of single-use plastics into a graphitic material. Compared to traditional catalysts, no purification or catalyst removal is required as the graphene oxide additive will have the same composition as the final graphite. Since low-density LDPE and PET plastics melt, they facilitate uniform mixing with the graphene oxide. During the heat treatment processing, the graphene's chemical structure is imparted onto the surrounding plastic as it decomposes.

Furthermore, this graphitization heat treatment can be performed at varied scales and does not require significant infrastructure.

The researchers believe this work could create a new path for graphite manufacturing through the energy savings of a lower temperature process and the environmental benefits due to reduced carbon dioxide emissions. In addition, upcycling waste plastic into high-value graphitic carbons will lead to improved recycling economics, increased recycling infrastructure investment, and recycling workforce growth, while reducing greenhouse gas emissions. This becomes even more important as clean energy technology drives the demand for carbon as a material. In fact, lithium-ion battery production is expected to more than double by 2025, according to the Northern Graphite Corporation.

"We're looking at a way to intersect a waste product with little commercial value and turn it into a commercial product with value but also facilitate the clean energy transition," Vander Wal said.

Other researchers on this project include Ekaterina Bazilevskaya, staff scientist at the Penn State Materials Characterization Lab; Adri van Duin, professor of mechanical engineering at Penn State; Ramakrishnan Rajagopalan, associate professor of engineering at Penn State Dubois; and Carlos Leon y Leon, senior materials scientist at Morgan Advance Materials.

The Pennsylvania Recycling Markets Center Corporation (RMC) is also contributing to this research, courtesy of Robert J. Bylone Jr., president and CEO. The RMC is an independent, Pennsylvania nonprofit corporation with a mission to reduce or eliminate barriers that lead to new expanded use of Pennsylvania's recycled materials. The RMC has an affiliation with Penn State and is headquartered at Penn State Harrisburg with an office in Pittsburgh.



Randy Vander Wal, Penn State



Robert J. Bylone Jr., RMC

Eco-friendly carbon-dioxide conversion process may revolutionize existing method

By Jennifer Matthews

A new, environmentally friendly, single-step process has been developed to convert carbon dioxide into higher hydrocarbons using plasma, according to scientists and engineers.

Converting carbon dioxide into usable liquid fuels and value-added chemicals like plastics offers not only a possible solution to reduce carbon dioxide emissions, but also the potential to alleviate dependence on fossil fuels. However, carbon dioxide conversion through catalysis—an acceleration of a chemical reaction—normally requires multiple steps and high temperature (roughly 400–750 degrees Fahrenheit) and high pressure (150 to 600 pounds per square inch), conditions that require a great deal of energy to create. Finding a better way to convert waste carbon dioxide under mild conditions remains a major challenge in catalysis.

Researchers from Penn State, the Chinese University of Hong Kong, and Sichuan University may have found a solution. The team has developed a one-step, plasma-enabled catalytic process to convert carbon dioxide into higher hydrocarbons. Unlike traditional processes, this method of hydrogenation is operated at low temperature (75 degrees Fahrenheit) and pressure (15 pounds per square inch) using a dielectric barrier discharge packed-bed plasma reactor.

The key component to make this new process work is the addition of non-thermal plasma, which provides a distinctive medium for performing catalytic conversion at low temperatures due to its non-equilibrium characteristics, the scientists said.

"There are a lot of high energy electrons within the plasma phase," said Xiaoxing Wang, associate research professor at the Penn State EMS Energy Institute. "These electrons can activate both carbon dioxide and hydrogen molecules in the gas phase through excitation and dissociation without the need of surface adsorption and activation as required for traditional thermal catalysis, so the reaction can be operated at low temperature."



Researchers have found a way to convert carbon dioxide into liquid fuels and value-added chemicals using plasma, which allows the process to be both lower temperature and lower pressure compared to traditional methods. Credit: Adobe Stock



A 3D rendering of a ball of energy and plasma in the core of a reactor. Credit: Adobe Stock

Plasma itself can enable carbon dioxide hydrogenation into carbon monoxide at room temperature. Though various catalysts have previously been studied for plasma-catalytic carbon dioxide hydrogenation, these experiments have only yielded carbon monoxide and methane, with only one report showing a higher hydrocarbons selectivity of roughly 14 percent. This new study is the first time this process has yielded a higher hydrocarbons selectivity of 46 percent at a carbon dioxide conversion rate of 74 percent.

This work, recently published in Green Chemistry, shows the substantial impact of the catalyst-bed configuration on plasmacatalytic carbon dioxide hydrogenation to higher hydrocarbons in one step at low temperature and atmospheric pressure, the scientists said.

Currently, the researchers are using a conventional aluminum oxidesupported Fisher-Tropsch catalyst for the process. They believe the method could be improved further and are developing an even more effective catalyst, through exploration into how plasma contributes to the carbon dioxide conversion and hydrocarbon formation in the plasma-enabled two-catalyst-bed process.

"Carbon dioxide conversion is facing the challenge of climate change," Wang said. "We need to do something to reduce carbon dioxide emissions. If we can convert carbon dioxide back into fuels, we close the carbon loop and make the whole process much more sustainable and greener. This work provides a new strategy in developing new processes for carbon dioxide hydrogenation at low temperature and pressure."

Penn State researchers involved in this study were Sven G. Bilén, professor of engineering design, electrical engineering, and aerospace engineering; Sean D. Knecht, assistant teaching professor of engineering design; Jiajie Wang, visiting graduate student; and Mohammad S. AlQahtani, graduate student.

Other researchers included Chunshan Song, distinguished professor emeritus at Penn State and dean of faculty of science at the Chinese University of Hong Kong; Wei Lun, professor of chemistry at the Chinese University of Hong Kong; and Wei Chu, professor of chemical engineering, Sichuan University.

A Penn State EMS Energy Institute seed grant provided funding for this research.

Penn State awarded \$3.4 million contract to target plastic waste By Courter Robinson

Penn State was awarded a \$3.4 million contract from the REMADE Institute, a public-private partnership established by the United States Department of Energy, to fund research targeting the inefficient methods currently used to process and upcycle mixed plastic waste. The project is one of twenty-two projects recently funded by REMADE. The project received \$1.7 million in federal funds with an additional \$1.7 million in cost-share by the project partners.

A global analysis of all mass-produced plastics found that a total of 8.3 billion metric tons of virgin plastics is estimated to be generated worldwide to date. As of 2015, 79 percent of plastic waste, which contains numerous hazardous chemicals, has been left to accumulate in landfills or natural environments with approximately 12 percent incinerated and only 9 percent recycled.



A global analysis of all mass-produced plastics found that a total of 8.3 billion metric tons of virgin plastics is estimated to be generated worldwide to date. Credit: PIXABAY.

Upcycling is a process of recycling where the resulting product is of a higher value than the original item that was discarded. The research team led by Hilal Ezgi Toraman, assistant professor of energy engineering and chemical engineering, is developing a flexible, two-stage chemical recycling process that decomposes multiple types of plastic and then converts to valuable chemicals that can be used to create new products.

Through the project, "Chemical Recycling of Mixed PET/Polyolefin Streams Through Sequential Pyrolysis and Catalytic Upgrading," the interdisciplinary team will simultaneously assess the financial and environmentally viability of bringing the proposed process from the lab to the industrial scale based on integrated technoeconomic analysis and life cycle assessment tools.

"Current commercial processes either operate below the necessary scale or are only applicable for single plastic types, not mixed plastics," said Toraman, who also holds the College of Earth and Mineral Sciences' Virginia S. and Philip L. Walker Jr. Faculty Fellowship. "When you consider the sheer amount of plastic, the development of a process that minimizes the steps needed for commercial implementation by accepting mixed, dynamic plastic inputs—there is immense potential to significantly affect the U.S. economy and environment."

The first step to developing the new upcycling process hinges on a better mechanistic understanding of how dynamic plastic waste mixtures decompose and interact in chemical recycling processes. Built on Toraman's past work, decomposition of plastic waste will be instigated via high temperatures in micro-pyrolysis setups. The study focuses on two of the most common plastics, polypropylene (PP) and polyethylene terephthalate (PET) which are found in multilayered packaging, carpeting residue, and films.

In the proposed two stage process, the second step is to convert the PET, PP mixture pyrolysis products using low-cost, stable catalysts to valuable chemicals such as benzene, toluene, xylene, and olefins.

Toraman noted several plastic upcycling approaches for mixed plastics failed due to the inability to handle the compositional complexity. However, the team's modular approach will aim to provide the necessary flexibility to succeed and can even be optimized through kinetic reaction models and simulations.

"This two-stage process has the potential to revolutionize plastic recycling," Toraman said. "System designs can then be tailored to a broad range of plastic waste streams, and predictive design decisions can be implemented to reduce energy demand and greenhouse gas emissions." REMADE awarded a total of approximately \$32.6 million dollars in new technology research to 22 projects, from its fourth requestfor-proposal solicitation aimed at accelerating the nation's transition from the current linear "make-consume-discard" economy to a more sustainable, circular economy focused on reuse, recycle, upcycle.

"Our mission is to reduce energy consumption and decrease emissions, while increasing the United States' manufacturing competitiveness," said Nabil Nasr, REMADE's chief executive officer.

Toraman hopes this research overcomes the critical barrier of labor-intensive sorting and handling practices and forwards the John and Willie Leone Family Department of Energy and Mineral Engineering's mission of environmental responsibility in the recovery, processing, and utilization of earth resources.

REMADE was established by the U.S. Department of Energy in 2017 with member organizations from industry, academia, national laboratories, trade associations, and non-profit entities to accelerate the U.S.'s transition to a circular economy.

Other members of the team include Penn State professors: Konstantinos Alexopoulos, assistant professor of chemical engineering; Michael Janik, associate department dean and professor of chemical engineering; Prasenjit Mitra, professor of information sciences and technology; Robert Rioux, Friedrich G. Helfferich Professor of Chemical Engineering; and Rui Shi, assistant professor of chemical engineering. From Northwestern University, Linda Broadbelt, associate dean and professor of chemical and biological engineering is also a team member.

Additional contributors to this project include Siemans Process Systems Enterprises and Shaw Industries Group Inc.

Grant to reduce, eliminate toxicity of coal mine dust



Barbara Arnold, professor of practice in mining engineering and principal investigator. Credit: Penn State, Creative Commons

Increases in lung diseases have been related to respirable coal mine dust. Penn State has been awarded \$327,849 from the National Institute for Occupational Safety and Health (NIOSH) to fund research targeting ways to reduce or eliminate the toxicity of respirable coal mine dust.

Recent reports from NIOSH, which has tracked the burden of black lung disease in underground coal miners since 1970, show a steady increase in respiratory disease for miners who have worked for at least twenty-five years underground. NIOSH estimates 10 percent of miners are affected, with one in five coal miners from Central Appalachia showing evidence of the disease—the highest level recorded in twenty-five years.

Barbara Arnold, professor of practice in mining engineering and principal investigator on the project, said the goal of the team's research is to conduct foundational research to reduce the trend. "My dad was a coal miner," Arnold said. "He never developed any lung-related health issues, but black lung is a very debilitating, incurable disease and to see this increase is concerning. Our aim with this project is to see if we can do something to all of those respirable dust particles to essentially turn off the toxicity so it's safe even if they are inhaled."

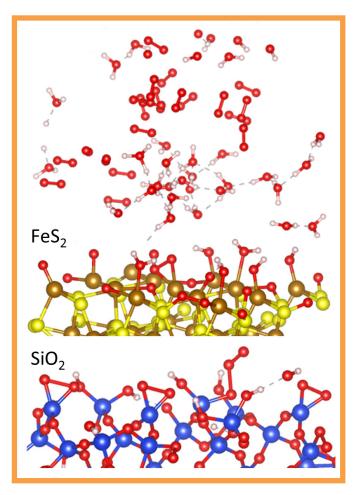
According to Arnold, finding and understanding what to turn off has been a challenge for researchers as respirable coal mine dust is a complex mixture of ultrafine particles. The complexity increases as each particle may have a different chemical composition, size, shape, and age. The type of mine can also change the particulate properties. Despite the dynamic variables, previous research hints at a potential culprit for toxicity: hydroxyl radicals, charged molecules that when attached to lung tissue may be the first step towards developing respiratory disease.

"A lot of folks have been doing research focused on coal mine dust, both globally and in the Mining Engineering program at Penn State with its history of the Respirable Dust Center," Arnold said. "But I looked at it from a mineral processing perspective, not a mining perspective, and I thought we need to really look at the surface chemistry of the materials at play."

This project will investigate the use of chemical additives to reduce or eliminate dust toxicity.

"One application might be something like flypaper," Arnold said. "Can the dust be trapped with a nonhazardous chemical that will turn off the toxicity so miners can work safely and turn around this alarming rise in respiratory disease?"

The team will investigate coal mining related respirable dust including ultrafine particles of coal, coal-related quartz, coalrelated pyrite, and diesel particulate matter, individually and in blends. The goal is to provide insight into the chemicals required for each different material, which could lead to possible additive combinations to be used for different coal components.



Water and oxygen interacting with quartz and pyrite surfaces.

"We plan on testing the coal-related pyrite as well, because there is some evidence that the iron in pyrite can cause issues in toxicity," Arnold said.

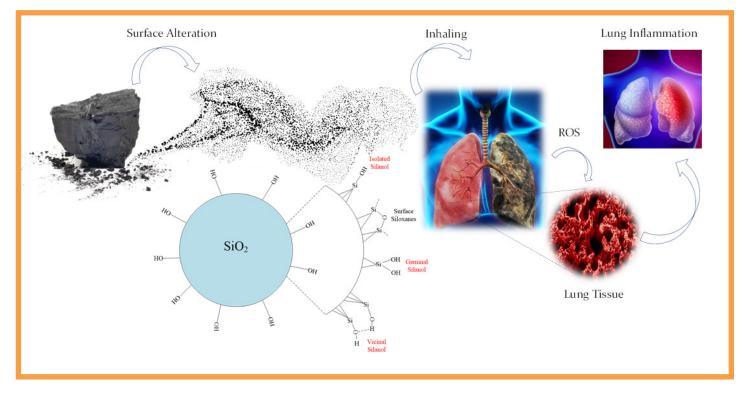
In addition, fresh particles and aged particles will be tested to determine if particle surface chemistry changes with aging and oxidation.

Tests will also be conducted with simulated lung fluid to determine if particle toxicity is enhanced in that medium and, therefore, in the lung. During the project, researchers will collaborate with industry representatives regarding applications of any promising chemical additives for future study or implementation.

Arnold hopes the expanded focus on pyrites and crystalline silica from quartz will build the groundwork for wider applications such as metal and non-metal mining, and even to construction where crystalline silica dust is generated when working with brick or concrete.

"Quartz is ubiquitous; it is in everything," Arnold said. "If we can figure out what we can do with quartz that gives us a chance at understanding what to do with coal, and we can really improve the lives of so many beyond just miners."

Mohammad Rezaee, the Centennial Career Development Professor in Mining Engineering and assistant professor of mining engineering, and Sekhar Bhattacharyya, chair of the Mining Engineering program and associate teaching professor, both in the John and Willie Leone Family Department of Energy and Mineral Engineering, are co-principal investigators on the project.



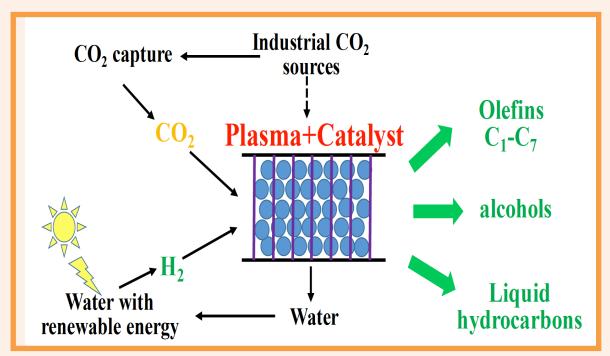
Ultrafine dust from components like quartz SiO, can react with the lung tissue causing inflammation and disease.

EMS Energy Institute Seed grants

In Spring 2019, the EMS Energy Institute announced a new call for seed grant proposals to encourage exploratory and collaborative research with new ideas that will likely advance energy science and technology significantly and potentially lead to new externally funded research projects. The following three areas were considered:

- Energy production and upstream research, including conventional and unconventional resources, and enhanced recovery of conventional and unconventional resources
- Energy utilization and downstream research, including conversion and upgrading of energy involving new concepts and novel processes, renewable energy utilization, and carbon dioxide management, including carbon capture, utilization, and storage.
- · Energy systems, materials, and energy techno-economics

Nine proposals were submitted and were evaluated by a panel of senior faculty members according to the following criteria: concept and rationale; objectives, approach, and expected results; and team qualifications and collaboration. The EMS Energy Institute selected four proposals for seed grants in May 2019 for one year of funding with the possibility of renewal for a second year depending on the results and planned future work. However, due to the COVID-19 pandemic, all seed grants were granted an additional year. Each of the following seed grants received \$15,000 from the EMS Energy Institute.



Schematic diagram of the proposed CO2 capture & conversion process.

Energy utilization and downstream research

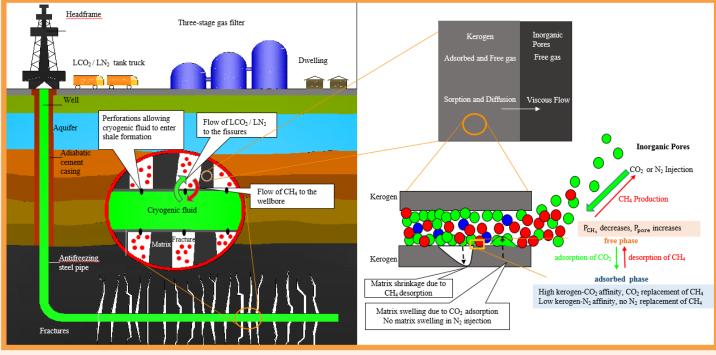
Title: Low-Temperature Plasma-Assisted Catalytic Conversion of Carbon Dioxide to Value-added Chemicals and Fuels

PI and Co-PI: Xiaoxing Wang (EMS Energy Institute) and Sean D. Knecht (College of Engineering)

Overview: To mitigate climate change, the reduction of anthropogenic carbon dioxide (CO₂) emissions is of paramount

importance. Catalytic conversion of CO₂ to value-added chemicals and fuels is potentially an attractive and sustainable solution for mitigating CO₂ emissions. The researchers sought to develop a new and more efficient process for catalytic CO₂ conversion with hydrogen to chemicals and fuels with the assistance of lowtemperature plasma. Through the research, the team gained deep insight on the physical and chemical aspects of CO₂ and hydrogen dissociation/reactions in a dielectric barrier discharge plasma reactor; studied and identified the key parameters for plasmaassisted CO₂ hydrogenation to improve the knowledge base in

Research



Enhanced gas recovery using cryogenic stimulation

the plasma-catalysis scientific community; identified and clarified the synergistic effects of coupling non-thermal plasma with catalysis; and developed a catalyst that works effectively for the plasma- assisted CO_2 conversion process. The work facilitates the development of new technology for catalytic CO_2 conversion in a more energy-efficient manner.

Results: The results of this work demonstrated the significant impact of the catalyst-bed configuration on plasma-catalytic CO₂ hydrogenation to higher hydrocarbons in one-step operated at low temperature and atmospheric pressure. With proper catalystbed configuration, high C2+ hydrocarbons selectivity of 46 percent at CO₂ conversion of over 70 percent is achieved. C₂+ hydrocarbons are likely formed through the plasma-driven gasphase methane conversion. Thus, the key in optimizing the catalystbed configuration is the balance between methane formation and plasma reactions for carbon-chain-growth from methane. It should also be pointed out that the catalyst used in this work is a conventional alumina-supported cobalt catalyst for Fischer-Tropsch synthesis. With further optimization of cobalt catalyst and/ or development of more effective catalysts, the plasma-promoted catalytic CO₂ hydrogenation to higher hydrocarbons could be more promising. The present work may broaden the utilization of the plasma-catalyst synergy for effective CO₂ conversion to higher hydrocarbons.

Energy production and upstream research

Title: Exploring Nonaqueous Cryogenic Stimulation and Its Application in Gas Shale Reservoir to Maximize Gas Production and Minimize the Environmental Footprint

PI and Co-PI: Shimin Liu (College of Earth and Mineral Sciences and the EMS Energy Institute) and Ming Xiao (College of Engineering)

Overview: The shale gas revolution has dramatically changed the energy landscape of North America. Despite this enormous success, significant technological challenges remain. To improve the gas production from underperforming wells, the researchers explored, investigated, and tested an innovative cryogenic stimulation technology on shale and quantified its effectiveness on gas production enhancement. The fluid dynamics behaviors of gas within shale are key for success of this early and exploratory technology. The study presented an atomic-to-pore scale fluid dynamic study of shale gas reservoirs under nonaqueous cryogenic liquid nitrogen and liquid carbon dioxide treatments through a combination of experimental and numerical simulation approaches. With a multiscale approach, combining experimental and numerical strategies, the fundamental mechanism of multiscale fluid-shale interactions under cryogenic treatment were uncovered and its impact on the long-term shale gas production was quantified.

Results: The repetitive applications of cryogenic treatment reduced macropore volume and increased mesopore volume. For the tested sample, the diffusion coefficient of the coal sample that underwent three cycles of freezing and thawing was lower than that of the coal sample that underwent a single cycle of freezing and thawing.

Research

The outcome of this study provides a scientific justification for the post-cryogenic fracturing effect on diffusion improvement and gas production enhancement, especially for high "sorption time" coalbed methane (CBM) reservoirs. In other core experiments for a gas-filled specimen, both the normal and shear fracture stiffness decrease monotonically with freezing time as more cracks are created in the coal bulk. For a water-filled specimen, ice formation due to cryogenic treatment leads to grouting of the coal bulk. Accordingly, the fracture stiffness of wet coal increases initially and then decreases with freezing time. A coal bed with higher water saturation is preferable when applying cryogenic fracturing because fluid- filled cracks can endure larger cryogenic forces before complete failure, and the contained water aggravates coal breaking as ice pressure builds up from the volumetric expansion of the water-ice phase transition and applies additional splitting forces on pre-existing or induced fractures and cleats. The researchers also confirmed the stiffness ratio is sensitive to fluid content. The measured stiffness ratio is 0.7-0.9 for dry coal but less than 0.3 for saturated coal.

Title: Mapping Reservoir Rock Composition of Conventional and Unconventional Deposits with Intelligent Imaging

PI and Co-PI: Zuleima Karpyn (College of Earth and Mineral Sciences and the EMS Energy Institute) and Sharon Huang (College of Information Sciences and Technology, and Huck Institutes of the Life Sciences)

Overview: The proposed project aimed to advance hydrocarbon production from conventional and unconventional reservoirs by developing novel machine learning and image analysis tools to enable automated, three-dimensional mapping of mineral constituents in reservoir rocks using high-fidelity X-ray microtomography imaging. Results from this work will support improved representation and modeling of rock-fluid interactions affecting the mobility and trapping of oil, brine, and gas in complex geologic systems. This proposal also intended to stimulate new synergies between research groups in the College of Earth and Mineral Sciences and the College of Information Sciences and Technology and build research capacity at Penn State in the area of image data science, which can be transferable to many fields interested in constructing material compositional maps.

Results: Pore-scale X-ray CT data of synthetic porous cores representing reservoir rock pore topology and two-phase fluid occupancy was developed.

Energy systems and materials

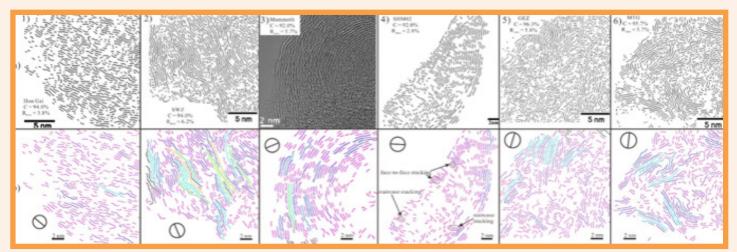
Title: Graphene Production from Attrition Milling of Anthracite Coal at the Bench Scale

PI and Co-PI: Jonathan P. Mathews (College of Earth and Mineral Sciences and the EMS Energy Institute) and James H. Adair (College of Earth and Mineral Sciences and the EMS Energy Institute)

Overview: Anthracite micronization followed by a controlled hydrometallurgical processing (acid treatment and controlled attrition milling approach) was proposed to generate graphene at the bench scale using a scalable approach. Through careful selection of the anthracite and by controlling the milling process, it was expected that the graphene oxide produced could be engineered to meet graphene size needs. The abundant graphene components in anthracite also make this an inexpensive graphene source that has the potential to overcome the high cost that limits current use.

Results: During this investigation, anthracite coal was acid-treated and micronized in a multi-step process. The rheology of the reduced-sized liquid was followed as a function of milled and unmilled materials. This resulted in the proof-of-concept even with the limited data, however graphene was not generated due to restrictions/limitations/timing imposed by the COVID-19 pandemic.

Chunshan Song, former director of the EMS Energy Institute, retired in 2020 and a new director will begin in 2022. Future seed grant opportunities will be determined at that time.



1a) Lattice fringes and raw HRTEM micrographs of anthracites with carbon content (wt.%, daf) and mean maximum reflectance (Rmax). b) False colored HRTEM fringes (colored by fringe length) showing the mean fringe orientation (the diameter angle in the circle), Lattice fringes and raw HRTEM micrographs are reprinted with permission of copyright holder. IMAGE: Yuzhen Han

End of Year Awards

End of Year Awards

Wilson Banquet and Awards Presentation

The College of Earth and Mineral Sciences' annual celebration of accomplishments was hosted virtually on April 24, 2022. The following EI students, affiliates, and researchers were honored.



Gladys Snyder Junior Faculty Grant

The Gladys Snyder Junior Faculty Grants are given to young faculty for the development of new courses or the improvement of current offerings; for travel to professional meetings special course and seminars; to broaden the studies of junior faculty members; and/ or to recognize significant contributions of faculty in their first five years in research efforts.



Barbara Arnold, Professor of Practice in Mining Engineering

"3-D Printing in Energy and Mineral Related Laboratory and Engineering Courses"

Faculty Advising Award



Jonathan Mathews, Professor of Energy and Mineral Engineering

George H. Deíke, Jr. Research Grant

The George H. Deike, Jr. Research Grant promotes innovative research of high scholarly merit. The award recipient receives \$50,000 from the George H. Deike, Jr. Research Endowment Fund and a recognition memento.



Joel Landry, Assistant Professor of Environmental and Energy Economics

"Assessing the Efficiency and Equity Impacts of the Electric Vehicle Transition Under Alternative Policy Pathways"

Promotion and Tenure



Hamid Emami-Meybodi, Associate Professor, Energy and Mineral Engineering

John T. Ryan, Jr. Faculty Fellow

This award is designed to assist faculty in continuing and furthering their contributions in teaching, research, and public service.



Chiara Lo Prete, Associate Professor of Energy Economics



Sara Andreoli, EMS Energy Institute



Howard B. Palmer Faculty Mentoring Award



Luis Ayala, William A. Fustos Family Professor of Petroleum and Natural Gas Engineering in the College of Earth and Mineral Sciences, was the recipient of the 2022 Howard B. Palmer Faculty Mentoring Award. The award honors and recognizes outstanding achievement by a faculty member with at least five years of service who effectively guides junior faculty. Howard Palmer was the senior associate dean of The Graduate School from 1984 to 1991.

Institutes of Energy and the Environment Seed Grants

annanannannannannannan The following EME Energy Institute researchers were 2020-21 Institutes of Energy and the Environment (IEE) seed grant recipients in the Integrated Energy Systems category:

Integrated Energy Systems



Randy Vander Wal, professor of energy and mineral engineering, for the project "Lignin Derived Graphite for Renewable Energy Storage and Transportation Electrification."



Hannah Wiseman, professor of law and Wilson Faculty Fellow in the College of Earth and Mineral Sciences and Andrew Kleit, professor of energy and environmental economics, for the project "Expanding the Policy Foundation for Electricity Prosumers: Lessons from New York and California."

2021 Department of Energy and Mineral Engineering student awards



The 2021 John and Willie Leone Family Department of Energy and Mineral Engineering awards banquet recognized students and faculty in the department. The banquet is held in conjunction with the G. Albert Shoemaker Lecture. EMS Energy Institute students who received awards are listed below.



Nathan Gendrue Ph.D. student

Outstanding Graduate Teaching Assistants



Jiayi Yu Ph.D. student



Yiming Zhang Ph.D. student

Charles B. Darrow Awards



Shubhadeep Banik Ph.D. student



Sandra Ike Ph.D. student

<u>Graduate Merit Award</u> <u>in Mining and Mineral</u> Process Engineering



Mark Hovingh Graduate student

People

New Faculty & Stall

The EMS Energy Institute welcomes the following new members who have joined the Institute since our last publication. Detailed profiles can be found at **energy.psu.edu**.



Ozge Deniz Bozkurt Postdoctoral Scholar

Bozkurt has bachelor of science degrees in chemical engineering and molecular biology and genetics from Istanbul Technical University. She has a master of science degree in life science and technology from Delft Technical University and completed her master's thesis on the kinetics of anaerobic digestion. She received her doctorate from Koc University, wherein she conducted experimental research on heterogeneous catalysis. Bozkurt worked in the oil and gas industry for almost three years as a senior R&D engineer with a specialization in renewable fuels. In March 2022, she joined the Toraman Research Group at Penn State to research catalytic and non-catalytic pyrolysis of mixed plastic waste.



Waleed Mohammed Mahmoud El Sayed Research Assistant

El Sayed is a research assistant for Meng Weng. He earned his doctorate and master of science in applied microbiology and his bachelor of science in microbiology, all from Al-Azhar University. Prior to joining Penn State, he was a researcher at the Marine Microbiology Laboratory, Marine Environment Division, at the National Institute of Oceanography and Fisheries Red Sea branch.



Stephanie Emigh Financial Coordinator

Emigh joined the Energy Institute in August 2021 as a financial coordinator. Prior to joining the institute, she worked at Penn State Mail Services as a financial assistant for fifteen years.

People

Mamoru Fujii Research Assistant

Fujii is a research assistant for Randy Vander Wal. He earned his bachelor of industrial chemistry in catalysts and ceramics from Chuo University and was a fellow of graduate school at Shonan Institute of Technology. Prior to joining Vander Wal's team, Fujii worked with Chunshan Song. Fujii's research centers on materials and development of inorganic functional material such as catalysts and ceramics but also building evaluation methods including system design. He is also a member of the American Chemical Society.

> Paige McCarthy Administrative Assistant

McCarthy joined the EMS Energy Institute in March 2022 as an administrative assistant. She received her associate of science degree from Penn State in criminal justice last year.

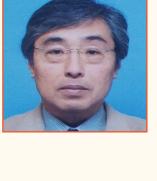
Anne Menefee Assistant Professor

Menefee is an assistant professor of energy and mineral engineering and a co-funded faculty in the Institutes of Energy and the Environment. Her research is broadly focused on decarbonizing the energy sector through subsurface systems for low-carbon energy production, energy storage to enable renewables, and carbon sequestration. She holds a doctoral degree and master of science in environmental engineering from the University of Michigan and a bachelor of science in civil engineering from the University of Virginia.

Fnu Pushap Raj Postdoctoral Scholar

Raj received his doctorate in supramolecular chemistry from the Indian Institute of Technology where he studied the development of dipodal organic receptors as fluorescence sensors for heavy metals ions, pesticides, and biomolecules. He worked as a postdoctoral fellow at Changnam National University before joining Penn State as a postdoctoral scholar in the John and Willie Leone Family Department of Energy and Mineral Engineering where he developed nanomaterials-based biosensors for enzyme and bacteria pathogen detection. His current research is focused on the design and synthesis of polymer chelators for critical minerals extractions. Raj is advised by Athanasios Karamalidis.







Recent & Upcoming Events

Celebrating Women in Energy and Water Research Lecture Series launched fall 2021



Joan B. Rose

A new seminar series was established by EME to celebrate women conducting energy and water research, to highlight their successes, to engage women students, and to provide an opportunity for faculty to establish and expand their professional network and mentoring relationships.

The first two seminars in the Celebrating Women in Energy and Water Research Lecture Series, one experimental and the other technical, were held on September 16, featuring Joan B. Rose, Homer Nowlin Chair in Water Research at Michigan State University.

The lecture series was established in 2021, with support from the Penn State Educational Equity Equal Opportunity Planning Committee. The series includes both experiential seminars aimed toward a broad, interdisciplinary audience and technical seminars dedicated to the speaker's research. Recordings of the seminars are available on EME's YouTube channel: https://www.youtube.com/channel/UCpyCPzOOjBve6q41_w9aJkw



The theme for the upcoming Energy Days 2022, which will be held May 25 and 26 at the Penn Stater Hotel and Conference Center, is Mobilizing Energy and Climate Solutions. The focus will be on what it will take to mobilize solutions that achieve net zero emissions or beyond. Within this theme, there will be four conference tracks:

- 1. Advancing Technology Research and Development
- 2. Addressing Energy Inclusion, Equity, and Justice
- 3. Catalyzing Capital Investment
- 4. Achieving Implementation

Keynote speakers, panels, breakout sessions, and a poster session will allow for deep discussion and engagement within these tracks.



The seminar series, Energy of the Future, established in 2019 by the John and Willie Leone Family Department of Energy and Mineral Engineering (EME) in the College of Earth and Mineral Sciences, aims to further the discussion on important energy topics and inspire collaboration across institutions. Recent seminars included:

- September 30: "Characterizing and Controlling the Propagation of Mechanical Discontinuity Using Unsupervised, Supervised, and Reinforcement Learning Techniques," Siddharth Misra, associate professor in the Harold Vance Department of Petroleum Engineering and the Department of Geology and Geophysics at Texas A&M University.
- October 15: "Climate and Energy Transition," David A.T. Donohue, technical specialist, businessperson, attorney, and founder and president of the IHRDC and the Arlington Group.
- October 21: "Control of Plasma Chemistry and Dynamics for Low Carbon Energy Conversion," Yiguang Ju, Robert Porter Patterson Professor at Princeton University.
- November 11: "Locally Desirable Energy Development," Hannah Wiseman, professor of law and Wilson Faculty Fellow in the College of Earth and Mineral Sciences at Penn State.
- December 2: "Battery Systems Engineering—Enabling Mobility and Grid Independence," Christopher D. Rahn, associate dean for innovation and J. Lee Everett Professor of Mechanical Engineering in the College of Engineering at Penn State. He also is the director of the Mechatronics Research Laboratory and co-director of the Battery and Energy Storage Technology Center.

Dope Labs Science Communication Week at Penn State

The topic-specific workshops were designed to introduce early career faculty, graduate students, and postdoctoral researchers to the broader science communication community and teach them to use social media, storytelling, and a web presence to network with other scientists and engage with diverse audiences. The event was run by Dope Labs Podcast creators and hosts Zakiya Whatley and Titi Shodiya and sponsored by the Earth and Environmental Systems Institute with support from the College of Earth and Mineral Sciences, the EMS Energy Institute, and the college's Department of Geosciences, Department of Materials Science and Engineering, and the John and Willie Leone Family Department of Energy and Mineral Engineering.

Dope Labs Science Communication Week took place in February via Zoom.

Honors

Penn State recognized for **green power leadership**

The U.S. Environmental Protection Agency (EPA) recently recognized Penn State in its latest "Top 30 College and University List" of the largest green power users from the Green Power Partnership. Penn State ranks No. 14 nationally and No. 2 in the Big Ten in terms of total kilowatt-hours (kWh) used of green energy. Penn State uses more than 106 million kWh of renewable energy annually, which represents more than 33 percent of its total power needs and, according to the EPA, is equivalent to the annual electricity use of nearly 10,000 average American homes. Penn State's choice to use green power helps advance the voluntary market for green power, as well as the development of those sources. The EPA defines green power as electricity produced from solar, wind, geothermal, biogas, eligible biomass, and lowimpact, small hydroelectric sources.



Credit: Patrick Mansell

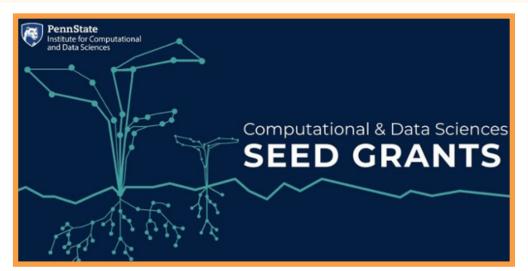
Karpyn named inaugural Donohue Family Professor

Zuleima Karpyn, associate dean for graduate education and Zresearch in the College of Earth and Mineral Sciences and professor of petroleum and natural gas engineering, was named the inaugural Donohue Family Professor. Former Penn State professor David Donohue and his son, Timothy, both alumni of the University, established the professorship with a \$1 million gift. The Donohue Family Professorship supports a faculty member whose research focuses on petroleum and natural gas engineering.



Rezaee selected for professorship designed to boost early career

Mohammad Rezaee, assistant professor of mining engineering in the John and Willie Leone Family Department of Energy and Mineral Engineering, was selected to receive the Centennial Career Development Professorship in Mining Engineering in the College of Earth and Mineral Sciences. Rezaee's research focuses on developing sustainable mining waste disposal practices from which valuables such as critical elements can be recovered for commercial use while the remaining materials are processed to generate environmentally benign materials. His work centers around the extraction of critical elements from primary and secondary sources, coal preparation, mineral processing, environmental management, and computational fluid dynamics and scale modeling.



Institute awards **computational and data** sciences seed grants

F rom making our roads safer to paving the way to exoplanet discovery, the Institute for Computational and Data Sciences (ICDS) seed grants have funded fourteen projects backed by researchers from across the disciplines and around the University. The 2021-22 ICDS seed grant program is designed to help scientists use the latest computational technology and cutting-edge data science techniques to deepen understanding and develop innovation across fields and disciplines. Of the fourteen grants, two were awarded to EI researchers, including **Yashar Mehmani**, assistant professor of energy and mineral engineering, for his work titled "Using AI to Map Infrared Spectra to Geomechanical Properties from the Micron to Meter Scale" and **Hilal Ezgi Toraman**, Virginia S. and Philip L. Walker Jr. Faculty Fellow and assistant professor of energy engineering and chemical engineering, for her work titled "Development of Data Mining Tools and an Open Source Web-Based Data Platform to Support the Sustainable Development of Plastic Recycling."



Materials Research Institute announces seed grant recipients

The Penn State Materials Research Institute (MRI) has announced the 2021 recipients of seed grants that will enable University faculty to establish new collaborations with partners outside their own units for exploration of transformative ideas for high-impact materials science and engineering. Twelve grants totaling more than \$500,000 were awarded by MRI in partnership with Penn State's Applied Research Laboratory and the Pennsylvania Recycling Markets Center. **Randy Vander Wal**, professor of energy and mineral engineering and materials science and engineering, was chosen for his project "Upcycling Plastic Waste to Graphitic Carbons."

Mining engineering faculty member named a Henry Krumb Lecturer

Mohammad Rezaee, assistant professor of mining engineering in the John and Willie Leone Family Department of Energy and Mineral Engineering, has been named a 2021-22 Henry Krumb Lecturer by the Society for Mining, Metallurgy, & Exploration (SME). The Krumb Lecture Series was established in 1966 so that SME sections could hear prominent minerals professionals speak on subjects in which they have recognized expertise. Providing professional development opportunities for the mining industry is an invaluable service provided by the Krumb Lecturer and adheres to the spirit of Henry Krumb himself.



Associate professor recognized as rising star in energy research

Shimin Liu, Joseph Kreutzberger Early Career Professor and associate professor of energy and mineral engineering, is one of twenty-nine researchers recognized as a rising star by Energy & Fuel, an international scholarly journal focused on fundamental and applied research within the energy and fuels fields. The journal cited his significant contributions in the field of energy research. Early- and midcareer researchers make up a significant portion of the research workforce and play critical roles in driving knowledge discovery and technological advances in the increasingly globalized research landscape, and Energy & Fuels established the annual recognition to celebrate the contributions of these researchers.

Sanjay Srinivasan named distinguished member by Society of Petroleum Engineers

Sanjay Srinivasan, department head of the John and Willie Leone Family Department of Energy and Mineral Engineering, has been

Credit: SPE

honored as a distinguished member by the Society of Petroleum Engineers (SPE). One of twenty-two recipients

selected for 2021, he joins 696 other members honored since the establishment of the award in 1983. The Distinguished Member award recognizes SPE members who achieve distinction deemed worthy of special recognition, who made significant contributions to the society, or who have attained eminence in the petroleum industry or the academic community.

Battery metals from mine waste: Potential economic benefits for the commonwealth

Pennsylvania has a long history of mining and metallurgical activities dating to the Industrial Revolution that helped fuel the economy of the commonwealth and the nation. Coal markets have waned recently due to the transition away from coal to other energy sources, leading to many economically distressed areas in the state. New findings by a team led by Penn State researchers suggest potential economic opportunities from the domestic production of critical minerals. The team evaluated cobalt and



Recovery of critical minerals from mine waste could provide domesticallysourced materials for the lithium-ion battery needed to run electric vehicles. Credit: PIXABAY

manganese from the byproducts of mining and metallurgy from past industrial activities. Preliminary estimates indicate that waste left by coal mining activities in Pennsylvania contain tens of thousands of metric tons of cobalt and hundreds of thousands of metric tons of manganese. In addition, more than 5,500 metric tons of manganese are being discharged through acid mine drainage, with the untreated portion reaching the commonwealth's waterways each year.



Max Lloyd, assistant research professor of geosciences at Penn State, tested samples from around the world. From the left are wood, lignite, subbituminous and bituminous coal. Credit: Patrick Mansell, Penn State / Penn State, Creative Commons

Coal creation mechanism uncovered

The mechanism behind one of the first stages of coal creation may not be what has long been thought, according to Penn State researchers who found that microbes were responsible for coal formation and production of methane. The finding has implications for methane fuel recovery from some coal fields. The researchers looked at methoxyl groups in coal samples from around the world and used stable isotopes to show that organic material eventually becomes coal through microbial action.

New, environmentally friendly method to extract and separate rare earth elements



A new method improves the extraction and separation of rare earth elements—a group of seventeen elements critical for technologies such as smartphones and electric car batteries—from unconventional

A new method improves the extraction and separation of rare earth elements from unconventional sources, including industrial waste, such as the mine tailings pictured here, and electronic waste. Credit: Barsamuphe, Wikimedia Commons

sources. New research led by scientists at Penn State and the Lawrence Livermore National Laboratory demonstrates how a protein isolated from bacteria can provide a more environmentally friendly way to extract these metals and to separate them from other metals and from each other. The method could eventually be scaled up to help develop a domestic supply of rare earth metals from industrial waste and electronics due to be recycled.



Rice University graduate student Valeriia Sobolevskaia at the on-campus well site being developed to help geoscientists continue development of fiber-optic sensors to find and evaluate small faults at underground carbon dioxide storage reservoirs. Credit: Ajo-Franklin Lab

Seismic study will help keep carbon underground

Scientists from Rice University, Penn State, and the Lawrence Berkeley National Laboratory, are developing sophisticated fiber-optic sensors and seismic sources to find and evaluate small faults deep underground at sites that store carbon dioxide to keep it out of the atmosphere. The U.S. Department of Energy awarded Rice geoscientist Jonathan Ajo-Franklin \$1.2 million to adapt his lab's distributed acoustic sensing method to monitor storage sites where reactivation of small faults could allow leakage into adjacent groundwater or the atmosphere. The project is part of \$4 million in grants announced in May 2021 to enhance the safety and security of carbon storage.



Penn State to lead **critical minerals consortium** powered by \$1.2 million from DOE

A region famous for the coal that once fueled a growing nation is now the focus of a \$1.2 million project, led by Penn State researchers, aimed at establishing domestic supplies of critical minerals needed to produce modern technology from cell phones to fighter jets.

Penn State will lead the Consortium to Assess Northern Appalachia Resource Yield to assess and catalog northern Appalachian-basin critical mineral resources and waste streams; develop strategies to recover the materials from these streams; and identify potential supply-chain or technology gaps that will need to be addressed. The project, funded by the U.S. Department of Energy, is part of a broader, national effort to produce rare-earth elements and critical minerals.

Institutes of Energy and the Environment director to step down

Tom Richard, director of the Penn State Institutes of Energy and the Environment (IEE), will step down from his position with the institutes after more than thirteen years of dedicated leadership. Richard has served as director of IEE since 2008, shortly after the IEE expanded and first adopted energy as part of the institutes' name and mission. In that time, Richard has overseen the growth of IEE from thirty-two to seventy-one co-funded faculty members with more than 500 faculty affiliates, and from less than \$10 million in active research awards to more than \$100 million. Richard will continue to serve Penn State as a professor of agricultural and biological engineering.



News



Researchers awarded grant to advance geothermal energy science

Over the last decade, geothermal energy has progressed throughout the world as an environmentally friendly, sustainable source of energy. Using the heat from the Earth's crust, geothermal power plants harvest and store energy in massive underground reservoirs carved out of stone. Once built, the reservoirs are inaccessible and monitored remotely—but they are not infallible. Earthquakes and more can fracture the subsurface rock, risking the integrity of the reservoir and endangering energy production. **Parisa Shokouhi**, associate professor of engineering science and mechanics and acoustics, is working to predict possible breaks and how to mitigate the potential fallout. Her team began its work in 2017 with a grant from the U.S. Department of Energy's Basic Energy Sciences program. The program renewed the grant for a total funding amount of nearly \$1.2 million.

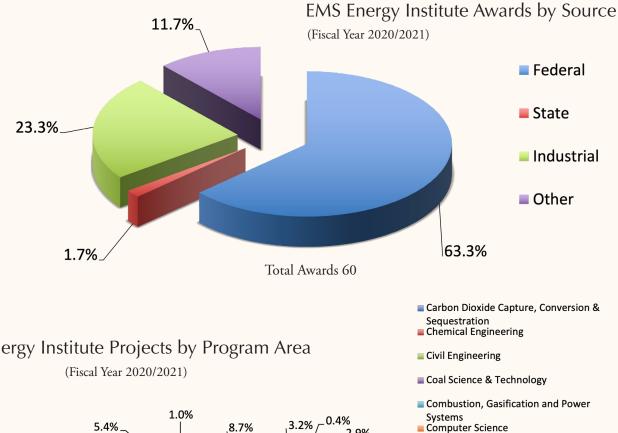


Credit: Adobe Stock

Grant to fund new processing techniques **for Gallium extraction**

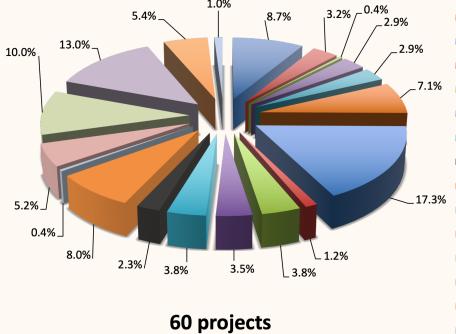
A thanasios Karamalidis, assistant professor of energy and mineral engineering, was awarded the Dean's Fund for Postdoc-Facilitated Innovation Award in the College of Earth and Mineral Sciences for his work titled "Phosphate Functionalized Cellulose Sponge for Highly Efficient Gallium Extraction and Separation from Industrial Waste." Under his broader research efforts in the space, he and his colleagues Michael Hickner, professor at Penn State, and Timothy Ramadhar, assistant professor at Howard University, collaborate in an interdisciplinary project targeting to develop new selective adsorbents for the extraction and separation of gallium (Ga) from industrial liquid wastes. Ga is a critical mineral, which is mostly used for integrated circuits and optoelectronics, such as LEDs, and in biomedical, radiopharmaceutical, and other fields. The fact that there are no gallium-focused mines in conjunction with increasing demand for the element paints a picture of a challenging problem. Karamalidis said that the outcomes of the proposed study can serve in the development of new processing techniques for Ga extraction from industrial wastes, contributing to contemporary circular economy approaches, which will also help meet the demand of Ga in the future. The developed materials and technologies could also provide new insights for extracting other critical materials including other rare earth elements.

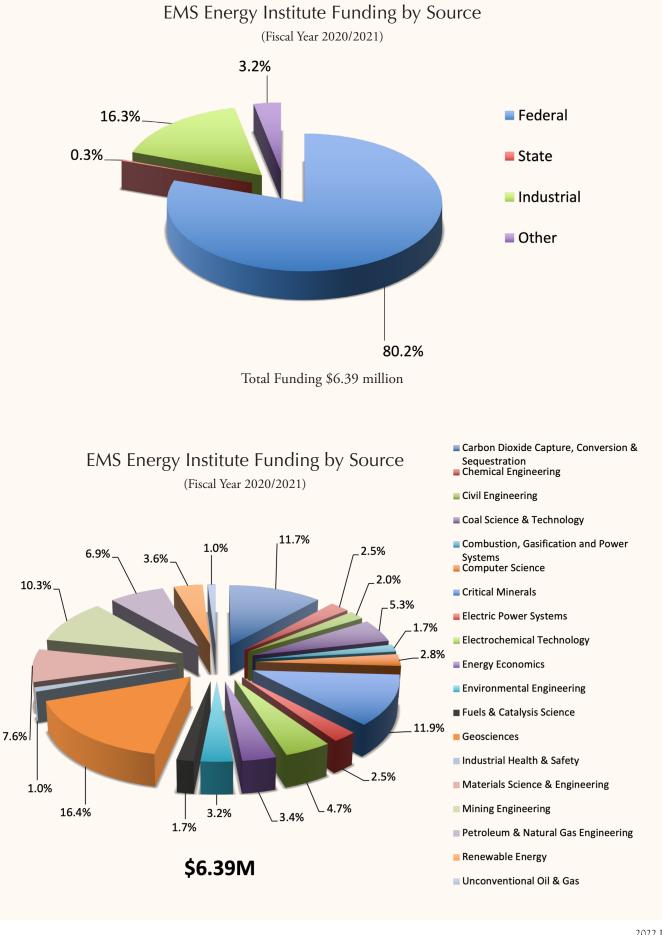
NDING Summary of projects



- Critical Minerals
- Electric Power Systems
- Electrochemical Technology
- Energy Economics
- Environmental Engineering
- Fuels & Catalysis Science
- Geosciences
- Industrial Health & Safety
- Materials Science & Engineering
- Mining Engineering
- Petroleum & Natural Gas Engineering
- Renewable Energy
- Unconventional Oil & Gas

EMS Energy Institute Projects by Program Area





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