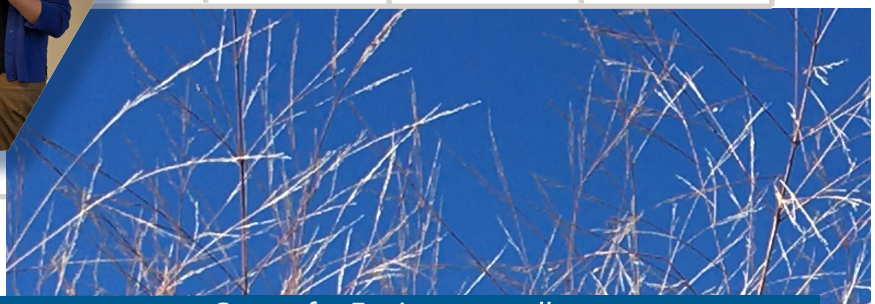
KU

CENTER FOR ENVIRONMENTALLY BENEFICIAL CATALYSIS

The University of Kansas



Center for Environmentally

CEBC

Beneficial Catalysis

Growing the Seeds of Innovation

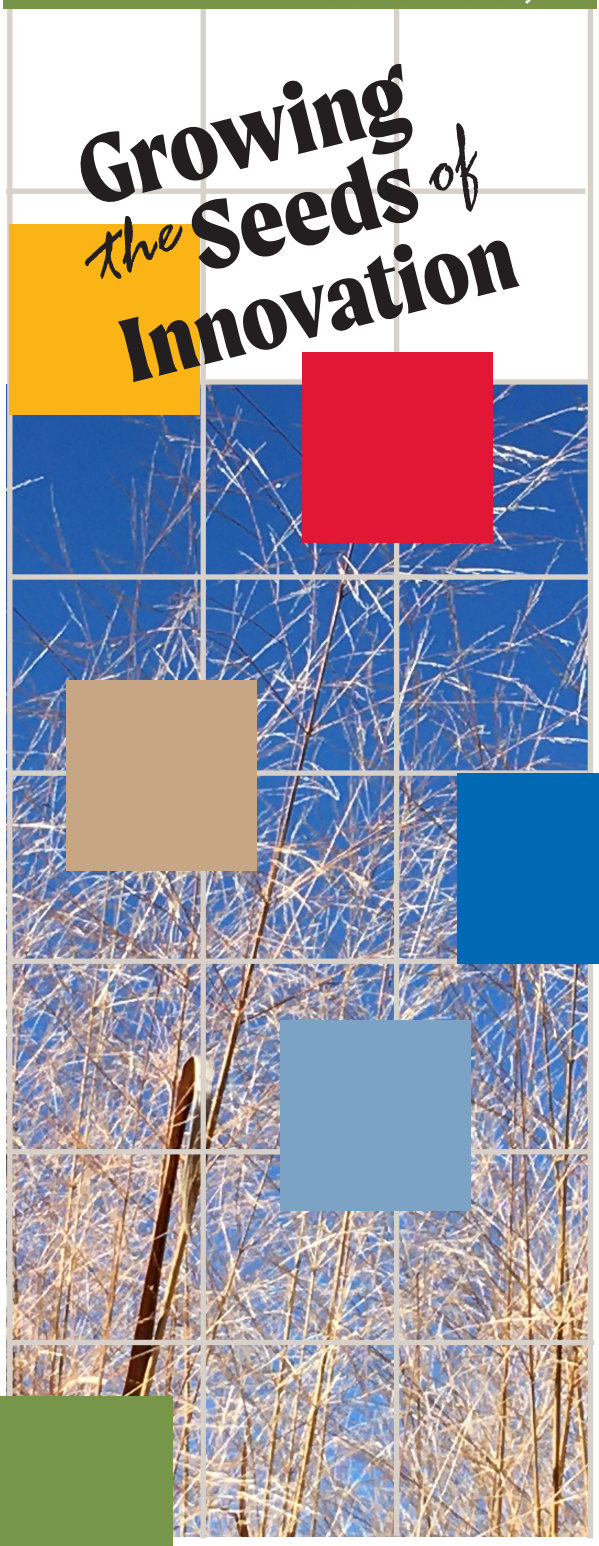
2024 Annual Report

Center for Environmentally
CEBC
Beneficial Catalysis

CENTER FOR
ENVIRONMENTALLY
BENEFICIAL CATALYSIS

The University of Kansas

Growing the Seeds of Innovation



Our mission is straightforward:

Invent cleaner, safer, energy-efficient technologies that protect the planet and human health.

Our approach is unique:

Faculty and students from multiple disciplines collaborate at the CEBC to discover technologies that minimize carbon footprint and toxicity, and are economically viable.

We actively partner with chemical companies. This industry-focused approach, uncommon in many university research programs, helps maximize the potential impact of our fundamental discoveries.

As the chemical industry's global output continues to expand, the Center's mission is more relevant than ever.

www.cebc.ku.edu

The Center for Environmentally Beneficial Catalysis
Tel: (785) 864-6050, Email: cebc@ku.edu

Contributors: Ana Chicas-Mosier, Nancy Crisp, Chris Lyon
Designer: Nancy Crisp

From Aspiration to Achievement

The CEBC has enjoyed another successful year in terms of research funding, faculty and student recruitments, and research outputs. As it enters its third decade as an erstwhile National Science Foundation (NSF) Engineering Research Center (NSF ERC), the CEBC's mission to develop resource-efficient catalytic technologies to make everyday products avoiding toxic reagents is more relevant now than ever. Technologies with such characteristics not only maximize feedstock usage toward desired products but also avoid waste generation and subsequent cleanup. Chemical companies have long embraced such traits as being keys to a successful business strategy that simultaneously promotes economic viability and environmental stewardship.

During the last two decades, CEBC researchers have been addressing sustainability grand challenges in industrial chemical processing. Examples featured in this report include sustainable plastics production and recycling, biomass valorization, circularity of critical elements and green hydrogen production. Establishing the significance of trace impurities in sustainable plastics recycling, the discovery of new synthetic routes for making renewable plastics precursors and harnessing machine learning for catalyst design are worthy products of note. These core research projects have harnessed expertise in catalysis, tunable solvents, multifunctional reactors, computational chemistry, data sciences and sustainability assessment to advance discovery and innovation. Such collaborations are initiated and sustained through major grants from federal (NSF, DOE, DARPA) and philanthropic organizations (Schmidt Sciences). CEBC member companies have taken advantage of the unique research capabilities/tools that result from the core projects to sponsor proprietary projects. This open innovation model continues to be a unique feature of CEBC's successful track record of spawning core research projects of value to industry.

To celebrate CEBC's accomplishments over the past 20 years, the 2024 Green Chemistry and Engineering Conference in Atlanta (organized by the ACS Green Chemistry Institute) hosted a stimulating session that featured distinguished scientists from academia and industry. CEBC's sustained vibrancy and successes beyond NSF ERC funding was noted as a significant accomplishment by almost every speaker. We were especially delighted that current and former editors-in-chief of Green Chemistry, ACS Sustainable Chemistry and Engineering and ACS Catalysis accepted to speak at the session.

CEBC has been a valuable resource for KU to attract outstanding faculty and student talent. Recent recruitments and accomplishments of our faculty and student researchers are highlighted in the report. We are proud to feature the placements of some of the 500+ CEBC alumni who have gone on to successful careers in industry and academia.

Science funding by federal and state legislatures is facing challenges and causing anxiety to the academic research enterprise. In addition to developing effective coping strategies, it is vitally important for stakeholders to articulate the significance of research investments to society and U.S. leadership. We must make effective use of science communication resources available through organizations such as AAAS and ACS to train faculty and students to effectively engage with local legislators and congressional delegations. The CEBC education and outreach program has been and will remain active on both of these fronts. We are providing up-to-date and transparent information to our scholars as we navigate periods of uncertainty and remain resilient as a community during difficult times.

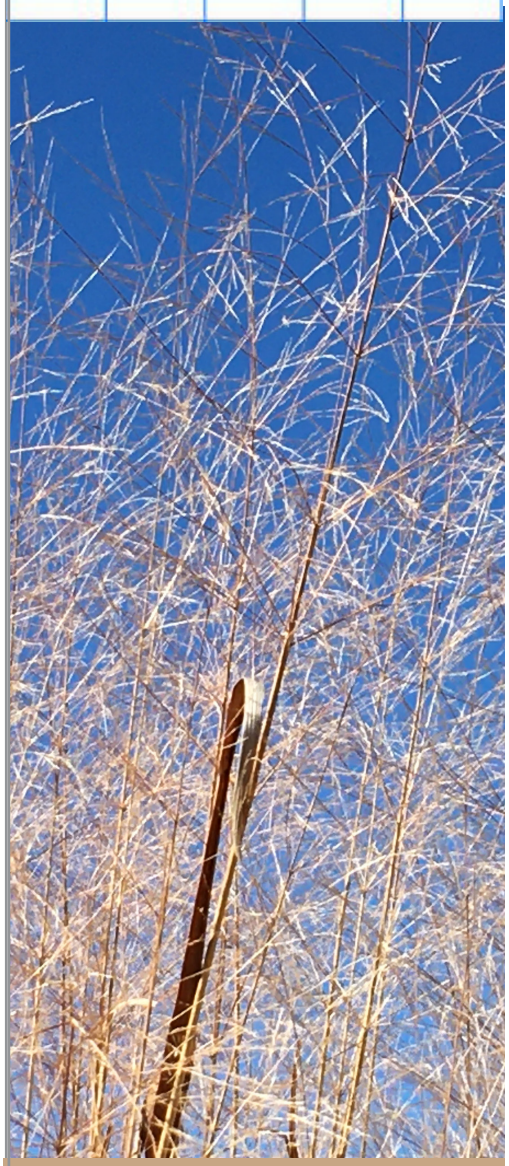
Continued stewardship and support from KU leadership at all levels will be critical to the sustained success of CEBC. I wish to thank all those, past and present, and especially the CEBC Industry and Science Advisory boards, who have contributed to keeping the CEBC's mission strong and vibrant. I am confident that the CEBC will continue to attract outstanding talent that will enable it to reach even greater heights in the coming decades.

Sincerely,

Bala Subramaniam

Dr. Bala Subramaniam
CEBC Director

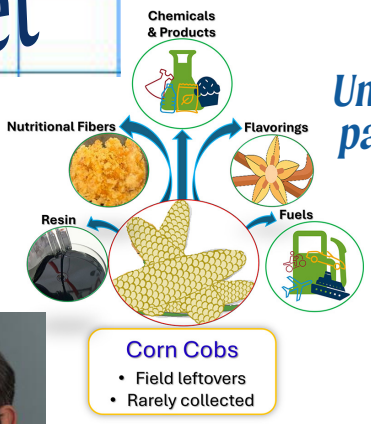
from the Director



Protecting the Planet

New grants to help CEBC find cleaner, safer solutions for existing chemicals and processes

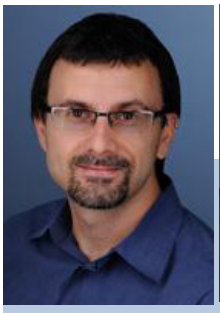
Universities, private industry and national lab partner to convert waste for sustainable uses

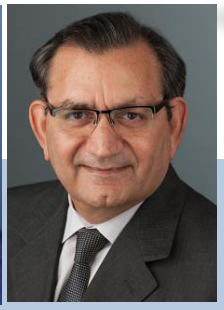


VIFF $10,000,000 2024-2029 The CEBC is collaborating on a new Schmidt Sciences Virtual Institute on Feedstocks of the Future (VIFF) and Foundation for Food & Agriculture Research (FFAR) grant to develop a process to convert agricultural and municipal waste into nutrients and feedstocks for manufacturing of everyday products.

CEBC Director Bala Subramaniam is co-PI on the project and will lead efforts to upcycle agricultural waste into feedstock pellets. Two CEBC member companies—ADM and Johnson Matthey—will provide guidance on scaling up technologies developed through this project. "Johnson Matthey is excited to continue to deepen our relationship with CEBC by supporting the Schmidt Sciences VIFF technology project initiative," said Jerry Springs, director of research & development at Johnson Matthey.

"Our team's goal is to demonstrate a technology that can transform diverse sources of chemical feedstocks, ranging from agricultural leftovers to municipal solid waste, into pellets that can be easily processed to make everyday products," said Subramaniam. "Successfully solving this challenge will revolutionize biorefineries and transform agro-based economies like Kansas and beyond into chemical manufacturing hubs that will be sustained for generations."



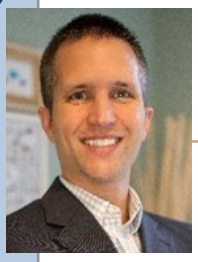


Quantum chemistry, machine learning and experimental catalysis bridge the propylene gap

NSF $602,669, 2024-2027 *CEBC Chemistry faculty member, Professor Marco Caricato (L) and CEBC Director, Professor Bala Subramaniam (R) will team up to develop a sustainable method for making propylene, a vital chemical critical to the production of polymeric materials.*

The team will determine the reaction mechanism for the metathesis of ethene and 2-butene to form propene on silica-supported W or Mo catalyst in the presence of a second metal such as Nb, and investigate the structural and electronic effects of varying the second metal. The knowledge gained will lead to the design of better-performing catalyst materials.

Potential applications include making renewable propylene from ethylene obtained from bioethanol, whose demand as a fuel is expected to decline.



CEBC and Avium to develop new technologies to increase efficiency in green hydrogen production

DOE $5,000,000 2024-2027 Dr. Kevin Leonard (L) is leading a multi-sector Department of Energy funded project to make green hydrogen a reality. In collaboration with Avium, LLC, founded by Leonard and his former PhD student Joe Barforoush, they will develop new catalysts and technologies to improve the efficiency and reliability of green hydrogen production. Green hydrogen may provide an avenue for long-term storage of sustainably sourced energy when an overabundance is created. For example, in the summer, an excess of solar power is often generated, which could be stored and used when solar energy is more scarce (i.e., winter).

Traditionally, hydrogen is made from natural gas, but worldwide hydrogen production results in hundreds of millions of tons of greenhouse gas emissions. Avium's catalysts make green hydrogen production more efficient.

According to Leonard, the benefits might well extend beyond sectors where hydrogen is already used. "People are interested in green hydrogen for traditional applications, but also for emerging ones," he said. A commodity chemical, hydrogen is used in fertilizers, cement production, metal processing and refining. Leonard sees green hydrogen as critical in creating sustainable, petroleum-free fuels. He says green hydrogen is a key part of the transition to clean energy. "Green hydrogen can help make the chemical industry more sustainable by enabling more efficient production of fuels and fertilizers," he said.

New Faculty & Staff Energize CEBC with New Areas of Research

ASTER LSAMP $3,500,000 2024-2029

Dr. Ana Chicas-Mosier
CEBC Education Director

Dr. Ana Chicas-Mosier is co-PI and Program Director for the newly awarded Aligning STEM Trainees for Enterprising Research (ASTER) Louis Stokes Alliance for Minority Participation (LSAMP). This award will support undergraduate STEM research at six regional higher education institutions including KU, University of Nebraska-Lincoln, Pittsburg State University, Johnson County Community College, Kansas City Kansas Community College, and Southeast Community College (Lincoln). Undergraduate researchers will receive professional development, multi-tier mentorship, and financial support. The CEBC is excited to be home to this important and interdisciplinary grant. ASTER students will work on a variety of research projects spanning chemistry, neuroscience, genetics, combinatorics, fluid mechanics, particle physics, construction materials and more.

Snapshot of the impact

- 20 students selected for the 2024-2025 University of Kansas cohort spanning the entire science, technology, engineering, and mathematics spectrum
- 33 students from partner institutions include 10 from area community colleges
- 16 faculty mentors have participated in mentorship training
- 75 participants joined the first alliance-wide virtual professional development and community building session

DARPA $171,969 | *NASA* $26,166

Dr. Elizabeth Corson
Fred Kurata Assistant Professor of Chemical Engineering

Defense Advanced Research Projects Agency (DARPA)

Small-Scale, Transportable Electrochemical Ammonia Synthesis System using only Local Groundwater and Electricity

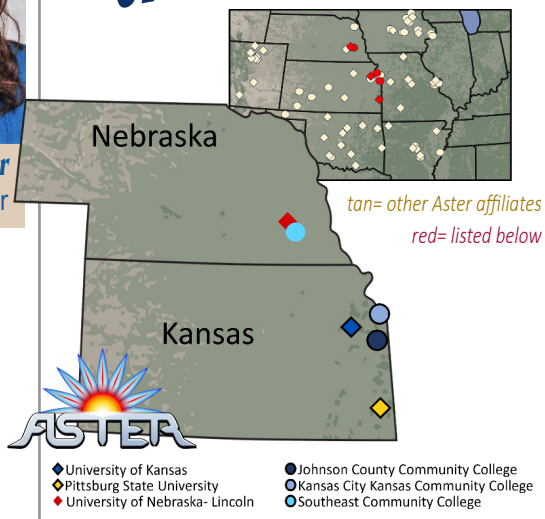
This research effort studies the application of using local groundwater and electricity to electrochemically reduce nitrate to ammonia, an energy-dense fuel. The goal is to reveal the mechanisms of catalyst deactivation caused by the most common ions found in groundwater, and explore solutions to address them through catalyst design and electrochemical operating conditions. The ion deactivation mechanisms are being studied using in situ IR and Raman spectroscopy and ex situ product analysis, supported by novel electrochemical cell design.

National Aeronautics and Space Administration (NASA)

Plasmon-Enhanced Electrochemical Carbon Dioxide Reduction

Electrochemical carbon dioxide (CO_2) reduction could mitigate climate effects caused by the burning of fossil fuels while producing valuable fuels and chemicals. Beyond our planet, the conversion of CO_2 to products enables in-situ resource utilization (ISRU) that can lift the burden of bringing supplies from Earth. The key challenges of electrochemical CO_2 conversion are low selectivity, which requires costly separation, and low efficiency, which increases the operating costs from electricity. With this grant, Dr. Corson and a graduate student will travel to the NASA Glenn Research Center to meet with NASA scientists to establish a research collaboration addressing the selectivity and efficiency of CO_2 reduction through plasmon-enhanced electrocatalysis, using light and electricity to control the reaction.

Protecting the Planet



Good Vibrations: Rapid Solar Panel Recycling

DOE $1,300,000 2023-2027 *Collaborating with the Idaho National Laboratory and First Solar Inc., P.I. Dr. Bala Subramaniam and Associate Researcher Dr. Hongda Zhu have developed a technology that uses benign solvents and acoustic vibrations to rapidly delaminate solar panels and recover the critical energy.*

Solar power is cost-competitive and avoids carbon emissions associated with conventional energy sources. By 2050, the demand for solar power is estimated to be as much as 100 Terawatts. Critical materials such as cadmium (Cd) and tellurium (Te) are essential to produce high efficiency CdTe photovoltaic panels. To economically produce such solar cells, cost effective and environmentally benign technologies to recover and recycle critical minerals are needed.

CEBC's recycling technology will promote sustainable production of solar panels by replacing sluggish conventional recycling processes that crush the solar panels into particles and use concentrated acid–oxidant mixture for recovering the elements.

Protecting the Planet

KU student's NRT research recognized at international Gordon Research Conference

Brianna Farris (second from left above), received the Best Poster Award at the Green Chemistry Gordon Research Conference in Barcelona, Spain in July 2024. Her poster, "Using Large Language Models to Gain Insights into Electrocatalysis," so impressed the reviewers that they also invited Brianna to give a flash talk on the research.

NSF-funded collaboration with University of Galway

Brianna Farris, PhD student in the Leonard laboratory, travelled to Ireland for one month to learn about Natural Language Processing at the University of Galway with Prof. Paul Buitelaar. This NRT-based collaboration brought together chemical engineering expertise from KU with computational expertise from Ireland.

The project expands on Brianna's research investigating machine learning applications as a strategy to mine knowledge gaps in catalysis. A publication is in preparation and demonstrates the inter-disciplinary and international opportunities the NRT program has created.

Multi-year NSF grants tout multiple impacts heading into their final year

NSF Research Traineeship (NRT) $3,000,000 2019-2025

The National Science Foundation Research Traineeship is in its final year with more than 50 graduate students supported through professional development, inter-disciplinary research, and innovative coursework.

Researchers have successfully used machine learning techniques to identify yet unexplored catalyst-electrolyte combinations for nitrogen reduction reactions, and demonstrated automated analysis of voltammograms that could identify kinetic rate constant and transfer coefficients in milliseconds. The integration of machine learning into catalysis can rapidly analyze and accurately generate areas for future research exploration.

Snapshot of the impact

- Engagement with graduate students from chemical engineering, chemistry, computer science, mechanical engineering, bioengineering, and environmental engineering
- New graduate certificate in Machine Learning for Scientists and Engineers
- 11 masters and doctoral degrees
- 16 peer-reviewed publications to date

Advanced Manufacturing of Renewable and Recyclable Polymers (R2P) $4,000,000 2021-2025

A multi-campus program to develop renewable and recyclable polymers is in its fourth year. Funded by the National Science Foundation, the R2P project brings together researchers from KU's CEBC, the University of Delaware's (UD) Center for Plastics Innovation, and Pittsburg State University's (PSU) National Institute for Materials Advancement. The team is working to design biobased polymer precursors that can be made into plastics and more easily recycled.

The transition from petroleum-based plastics to more sustainable alternatives is a challenging research field. Getting from the raw biomass material to an actual plastic polymer requires several steps, and each step must be optimized for the end product to compete with traditional plastics. Two recent papers by authors at KU and UD highlight some of the advances being made.

Led by UD graduate student Charles Fields and KU postdoc Preeti Jain, one paper reports an improved method to produce a plastic precursor, 4,4′-DMBP, at much faster rates and at high purity.

A second paper focuses on the techno-economic analysis required to simulate commercial scale production of BFDCA, and estimate the cost and environmental impacts of its production. This analysis requires extensive physical property data. KU graduate student Samir Castilla-Acevedo and several coworkers at KU and UD developed a physical property model that can be used to carry out these calculations.

Meanwhile, collaborators at PSU are working to incorporate these materials into polymer samples that can be evaluated for their performance, and scientists at KU and UD are testing different approaches to recycling them.

Welcome!
New CEBC faculty member

Dr. Manar Shoshani
Assistant Professor
KU Department of Chemistry

Education:
- NSERC Postdoctoral Fellowship, 2018-2021, California Institute of Technology
- PhD Chemistry, 2018, University of Windsor
- BSc. Chemistry, 2013, University of Windsor

Notable:
- NSF CAREER Awardee, 2024
- Thieme Chemistry Journal Awardee, 2024
- Dalton Transaction New Talents: The Americas, 2024
- ACS PRF Undergraduate New Investigator Award, 2023
- UT Faculty STARs Awardee, 2021, as an assistant professor in the Department of Chemistry, the University of Texas Rio Grande Valley
- Governor General Gold Medal, 2019

Research Interests: Research in the Shoshani lab is focused on the conversion of cheap and abundant precursors to value-added products including liquid fuels, functionalized heterocycles, and polymeric materials. The group's approach utilizes well-defined, homogeneous multimetallic complexes to achieve a comprehensive understanding of the reactivity pathways involved, enabling the design of cooperative catalytic strategies.

Catalyzing Discovery

CEBC Director named AAAS Fellow, also honored by Great Plains Catalysis Society (GPCS)

In early 2024, the American Association for the Advancement of Science (AAAS) announced its 2023 class of fellows. CEBC Director, Dr. Bala Subramaniam received this high scientific honor. He was recognized for "seminal contributions in sustainable catalysis and engineering research via publications of high impact, licensed technologies and professional leadership, including the founding of KU's Center for Environmentally Beneficial Catalysis."

AAAS President Willie E. May (L) presents Dr. Bala Subramaniam (R) with an AAAS Fellows Certificate

Dr. Subramaniam also was honored as the recipient of the 2024 Great Plains Catalysis Society Award. The GPCS noted Bala's discoveries in metal-incorporated mesoporous silicates with tunable acidity, and harnessing tunable media to influence rates and selectivity in multiphase catalysis.

Faculty Promotions

Dr. Alan Allgeier
Professor
Chemical Engineering

Alan Allgeier is now a full Professor in KU Chemical and Petroleum Engineering. He seeks to promote sustainable catalysis and manufacturing by understanding fundamental reactions of catalytic species and developing novel characterization methods of fluids in contact with porous media.

Dr. Kevin Leonard
Professor
Chemical Engineering

Kevin Leonard is now a full Professor in KU Chemical and Petroleum Engineering. He seeks to advance fundamental understanding to design new electro-catalytic systems to improve the efficiency of and reduce fossil carbon emissions associated with fuel and chemical production.

Dr. Justin Hutchison
Associate Professor
Civil, Environmental & Artchitectural Engineering

Justin Hutchison is now an Associate professor in KU Civil, Environmental and Architectural Engineering. His research focus is protein and enzymatic (biocatalytic) applications to treat drinking water, and to offer alternative catalytic processes that promote the use of earth-abundant metals.

Faculty Awards

***Alan Allgeier**, Prof. of Chemical Engineering, received the Miller Faculty Scholar Award and Miller Award for Service to the Profession from KU School of Engineering*

***Rachael Farber,** Asst. Prof. of Chemistry, received the November 2024 KU Dept. of Chemistry Sutton Family Research Impact Award*

***Justin Hutchison**, Assoc. Prof., Civil, Environmental & Architectural Engineering, received the KU School of Engineering Miller Award for Research*

***Ward Thompson,** Prof. of Chemistry, was named as Richard S. Givens Professor of Chemistry, and awarded the KU Department of Chemistry Sutton Family Research Impact Award in both February and April 2024*

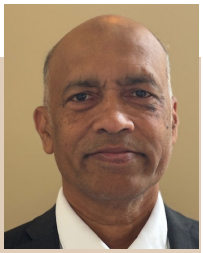
Partnering with Industry

Where in the WORLD are the CEBC alumni?

More than half of former CEBC students, postdocs and researchers are employed in the chemical industry after leaving KU. Several (in red) have returned to deliver seminars as part of ***CEBC's Industry Colloquia*** *series. A partial list of these CEBC alumni who continue to help protect the planet in their daily endeavors:*

AbbVie: ***Simon Velasquez Morales****, Nan Wang •* ***ADM,*** *Derek Butler •* ***Advanced Reactor Technology****, Sagar Sarsani (co-founder) •* ***AmSpec Group, Hong Jin*** *•* ***Aspen Tech****, Faisal Baksh •* ***Avium, LLC, Joe Barforoush*** *(co-founder) •* ***Benet Labs****, David Sconyers •* ***Braskem****, Priya Srinivasan •* ***Chemours****, Bill Gilbert •* ***Chevron Phillips Chemical,*** *Julie Leseberg, Anand Ramanathan •* ***Deloitte****, Luan Nguyen •* ***Delrin Acetal Homopolymer****, David Mennick •* ***Dow Chemical Co.,*** *Swarup Maiti •* ***Eastman Chemical,*** *Chad Johnson, Bhuma Rajagopalan •* ***Eli Lilly****, Sylvia Nwosu •* ***ENCINA****, Meng Li •* ***Evonik****, Jack Ford •* ***EVRI****, Pallavi Bobba •* ***ExxonMobil****, Madhav Ghanta, Wei Ren •* ***Hcpect****, Tie-Pan Shi •* ***Honeywell****, Venu Arunajatesan •* ***INEOS****, Chi-Cheng Ma •* ***Inpria****, Amy Jystad •* ***Intel Corp., Dylan Jantz****, Brandon Kinn, Tim McDonald, Ankit Verma, Pubudu Wimalasiri •* ***LyondellBasell, Arely Torres*** *•* ***Mars Corp.,*** *Manoj Kumar •* ***Metatechno Lanka Co. Ltd.,*** *Hiranya Mendis •* ***Michelin****, Yuanchun Li •* ***Pfizer, Kakasaheb Nandiwale*** *•* ***Phillips 66,*** *Kening Gong •* ***PPG Industries****, Pansy Patel •* ***Prairie Food,*** *Griffin Roberts (co-founder) •* ***Reliance Industries, LLC****, Amit Chaudhari •* ***Solentis****: Murilo Toledo Suekuni •* ***TCG Green Chemistry, Inc.,*** *Aravind Gangu •* ***Zoetis****, Tapan Maji*

Welcome, Affiliate Research Scientists



Dr. Anil Guram
>30 years combined, Union Carbide, Symyx Technologies, Amgen, and Art of Elements

Dr. Anil Guram joined the CEBC as an Affiliate Research Scientist to lend support in chemical catalysis research and development. Dr. Guram has extensive industrial expertise in homogeneous and heterogeneous catalysis with more than 30 years' industrial work experience at commodity and fine chemical companies including Union Carbide, Symyx Technologies, Amgen, and Art of Elements. He is an established innovator of high-throughput experimentation workflows/tools for catalysis research, and has developed numerous chemical technologies including catalysts, reactions, and processes to promote both academic and industrial chemical research. He has authored more than 75 journal and patent publications. Dr. Guram is currently engaged as a Chief Scientist at Art of Elements, LLC providing consulting and R&D services to chemical and pharmaceutical companies.

Dr. Bill Gong
BP, 26 years
Origin Materials, 7 years

Dr. William (Bill) Gong joined the CEBC as an Adjunct Researcher in August 2024. Bill has over 30 years of research and development experience from BP (26 years, Senior Research Scientist), and Origin Materials (7 years, Senior Principal Scientist). Bill's interests span catalytic oxidation (Mid-Century Catalyzed Oxidation) to chemical conversions of renewables to specialty and commodity chemicals. In the last 10 years of his career with BP, he researched in the area of carbohydrates to aromatics. Bill also has extensive experience managing several external collaborations on behalf of BP and Origin Materials. For several years, Bill also served as a CEBC Industry Advisory Board member representing Origin Materials.

2024 Industry Advisory Board at Spring Meeting

L to R; * Denotes Board Members

* Pasquale Iacono, Chevron Phillips Chemical Co.; Chengbao Ni, Chevron Phillips Chemical Co.; * Derek Butler, ADM; Erik Hagestuen, ADM; * Edmond Lam, ACS Green Chemistry Institute; Justin Kamplain, Chevron Phillips Chemical Co.; * Jerry Springs, Johnson Matthey; Anand Ramanathan, Chevron Phillips Chemical Co.; * Sree Pavani, W.R. Grace; Jessica Lamb; Chevron Phillips Chemical Co.

CEBC Welcomes New Members to Science Advisory Board

Engaging Science Advisors

Dr. Gregg Beckham

National Renewable Energy Lab

Senior Research Fellow and Group Leader

Research Interests: Biomass conversion, plastics recycling and redesign

Notable:

National Academy of Engineering, elected 2025; Plastics Recycling and Upcycling Gordon Research Conference co-chair and founder, 2023; Lignin Gordon Research Conference co-chair and founder, 2018

Education:

- Ph.D., Chemical Engineering, Massachusetts Institute of Technology
- Master's, Chemical Engineering Practice, Massachusetts Institute of Technology
- Bachelor, Chemical Engineering, Oklahoma State University

Dr. Elizabeth Biddinger

The City College of New York

Associate Professor, Chemical Engineering

Research Interests: Biomass utilization, CO_2 utilization, catalysis, chemical engineering, decarbonization, electrochemical engineering, energy storage technologies, ionic liquids

Notable:

ECS Industrial Electrochemistry & Electrochemical Engineering Division, Vice Chair 2024-2026, Secretary/Treasurer 2022-2024; ACS Sustainable Chemistry & Engineering Associate Editor, 2022-Present; Center for Decarbonizing Chemical Manufacturing Using Sustainable Electrification (DC-MUSE), Deputy Director, 2020-Present; AIChE Catalysis & Reaction Engineering Division Director, 2017-2019

Education:

- Postdoctoral Fellow, Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia, 2010-2012
- Ph.D., Chemical and Biomolecular Engineering, 2010, The Ohio State University
- B.S. Chemical Engineering, Mathematics minor, Magna Cum Laude, 2005, Ohio University

Dr. Justin Notestein

Northwestern University

Chair, Chemical and Biological Engineering
Director, Center for Catalysis and Surface Science (CCSS)

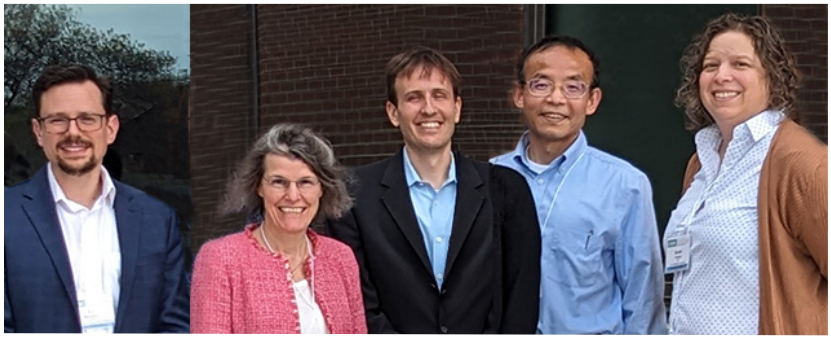
Research Interests: Catalysis science, energy, materials, and nanoscience. The Notestein research team develops novel designs and syntheses of catalysts, adsorbents, and other functional materials especially for the purposes of more sustainable routes to important chemicals and fuels.

Notable:

More than 150 papers and patents in catalysis; Five times named to teaching honor roll

Education:

- Ph.D. Chemical Engineering, University of California, Berkeley
- B.S.E Chemical Engineering (magna cum laude), Princeton University, NJ

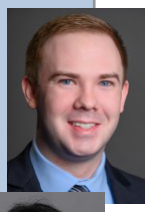


Science Advisory Board at 2024 Spring Meeting

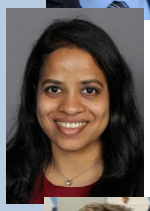
L to R: ***Ive Hermans****, University of Wisconsin-Madison,* ***Friederike Jentoft (board chair)****, University of Massachusetts Amherst,* ***Justin Notestein****, Northwestern University,* ***Hai-Ying Chen****, Oak Ridge National Laboratory,* ***Rachel Getman,*** *The Ohio State University*

Educating future leaders

Congratulations! 2024 Graduates



Samuel Brunclik, Ph.D. Chemistry
Advisor, Tim Jackson
Now a NIH IRACDA post-doctoral researcher at KU

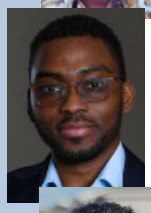


Riddhi Golwankar, Ph.D. Chemistry
Advisor, James Blakemore
Now a Postdoctoral Researcher at Los Alamos National Laboratory

Joseph Karnes, Ph.D. Chemistry
Advisor, James Blakemore

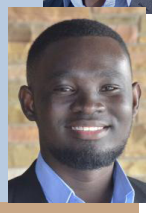
Emily Mikeska, Ph.D. Chemistry
Advisor, James Blakemore
Now a Postdoctoral Researcher at Argonne National Lab

Ngun Za Luai Mang, M.S. Environmental Engineering
Advisor, Justin Hutchison
Now a Staff Research Scientist at Desert Research Institute



Dacosta Osei, M.S. Chemical Engineering
Advisor, Ana Morais
Now an Associate Process Engineer at Conagra Brands

Felix Sotvik, M.S. Chemical Engineering
Advisor, Kevin Leonard



Nigel Twi-Yeboah, M.S. Chemical Engineering
Advisor, Alan Allgeier
Now a Project Management Consultant at Nextera Energy

Trainees Receive Awards in 2024

Conference Awards

Brianna Farris *Advisor: Kevin Leonard*
- Best Poster Award at the 2024 Green Chemistry Gordon Research Conference

Emma Russin *Advisor: Justin Hutchison*
- MOAWWA/MWEA Conference Student Poster Competition 2nd Place

Alejandra Torres Velasco *Advisor: Juan Bravo-Suárez*
- Travel Award for Attending the 18th International Congress on Catalysis, awarded by the North American Catalysis Society
- Best Poster Presentation, awarded by the Great Plains Catalysis Society, August 2024
- Presentation Award Winner, awarded at the 2nd Virtual Symposium of LatinXinChE

Departmental Recognition

Natalie Lind *Advisor: James Blakemore*
- KU Chemistry Department, H.P. Cady Award

Emily Mikeska *Advisor: James Blakemore*
- KU Chemistry Department Ernest & Marvel Griswold Award in Organic Chemistry

Alejandra Torres Velasco
Advisor: Juan Bravo-Suárez
- KU Chemical & Petroleum Engineering Department, Outstanding Graduate Teaching Assistant

Scholarships & Fellowships

Elizabeth Bartlett *Advisor: Ward Thompson*
- National Science Foundation Graduate Research Fellowship 2024 Honorable Mention
- University of Kansas Department of Chemistry Graduate 2024 Scholarship
- KU Self Fellow

Shreyaa Brahmachari *Advisor: Marco Caricato*
- KU Chemistry Department Burton & Cheryle McKenzie Scholarship
- KU Chemistry Department Wilson Summer Scholar

Sam Brunclik *Advisor: Tim Jackson*
- KU Chemistry Department Charles & Beatrice Kulier Scholarship

Fynn Cooper *Advisor: James Blakemore*
- KU Chemistry Department Cornelius McCollum Research Scholarship

Alex Ervin *Advisor: James Blakemore*
- KU Chemistry Department Burton & Cheryle McKenzie Scholarship

Natalie Lind *Advisor: James Blakemore*
- KU Self Fellow

Lindsey Penland *Advisor: Rachael Farber*
- KU Chemistry Department Elmer McCollum Research Scholarship

Emma Russin *Advisor: Justin Hutchison*
- Terry L. McKanna Scholarship
- Kansas Water Environment Association Scholarship

New Postdoctoral Researchers at CEBC

Educating future leaders

Sangeeta

Ph.D. 2023, Chemical Science IISER Mohali, Punjab India
Rajasthan University, Jaipur, India: M.Sc. 2017, Chemistry ; B.Sc. 2015, Chemistry, Zoology and Botany

Dr. Sangeeta Mahala joined the CEBC in March 2024, and is working on an ADM project to establish a cost-effective reaction protocol for the transformation of biobased polyols over a heterogeneous catalyst. Sangeeta's research focuses on the reaction mechanism, catalyst synthesis and characterization of material with various analytical techniques. Her past research includes the synthesis and characterization of metal oxide and metal organic framework catalysts to convert sugar in fructose and 5-hydroxymethylfurfural, an important pre-cursor for biobased liquid fuels. Sangeeta is also a CEBC safety committee member.

Sahil

Ph.D. 2023, Chemistry, Panjab University, Chandigarh, India
Guru Nanak Dev University Amritsar Hons. School: M.Sc. 2016 Chemistry; B.Sc. 2014, Chemistry

Dr. Sahil Kumar is focused on developing environmentally benign processes for the epoxidation of olefins using robust heterogeneous catalysts. During his Ph.D., Sahil worked extensively on the development of water-tolerant metal oxide-based solid acid catalysts for the transformation of carboxides derived from mango seed shells into high-value chemicals. This work equipped him with expertise in advanced catalyst characterization techniques, including X-ray Photoelectron Spectroscopy (XPS) and chemisorption analyses such as NH_3-TPD, CO_2-TPD, and H_2-TPR. Notably, Sahil had the opportunity to work with the University of Strathclyde, Glasgow as part of the prestigious Newton-Bhabha fellowship in 2022 for four months sponsored by The British Council, UK. There, he contributed to research on producing bio-based surfactants from cellulose and conducting theoretical studies using computational tools, advancing green chemical innovations. Outside of research, Sahil enjoys cooking new dishes, singing, and exploring adventurous activities.

Kinithi

Ph.D. 2024, Materials Science & Inorganic Chemistry, University of Louisville, Kentucky, USA
B.S. 2017, Analytical Chemistry, College of Chemical Sciences, Colombo, Sri Lanka

Dr. Kinithi Wickramaratne is a solid-state and materials chemist specializing in electrochemical energy conversion, catalysis, and energy storage. Her expertise includes the design, synthesis, and characterization of metal oxides for applications in fuel cells, electrocatalysis, and pseudocapacitive charge storage. She has extensive experience in electrochemical water splitting, CO_2 reduction, impedance spectroscopy, and analyzing capacitance contributions in energy storage materials. At the CEBC, Kinithi's research focuses on in-situ electrochemical methods to address energy and environmental challenges. She works to convert nitrate pollutants into ammonia through in-situ electrochemical reduction, offering a sustainable solution for fertilizer and fuel production. She is developing strategies for the co-reduction of CO_2 and nitrate to produce renewable urea. Her work bridges electrochemistry with sustainable energy solutions, offering more eco-friendly alternatives for various applications.

Ravi Teja

Ph.D. 2022, Chemical Engineering, Oklahoma State University, Stillwater
M.Tech. 2015, Chemical Engineering (Spl. in Process Design), University of Petroleum and Energy Studies, Dehradun, India
B.Tech. 2013, Chemical Engineering Sathyabama University, Chennai, India

Dr. Ravi Teja Addanki Tirumala specializes in high-pressure electrochemistry using CO_2 and N_2O-expanded media. Ravi has extensive experience in pilot plant operations and detailed engineering in the catalytic and polymer sectors. His expertise encompasses photocatalysis, electrochemistry, solar cells, and battery materials. He has made significant contributions, particularly during his tenure at Oklahoma State University and Pluss Advanced Technologies in Delhi. His work in photocatalytic and electrocatalytic materials have potential applications in the fertilizer, pharmaceuticals, care chemicals, and fine chemical industries. Ravi's scholarly record includes 15 peer-reviewed publications, four patents, and a role as Co-PI in research grants. An active member of the American Chemical Society, he is deeply engaged in professional development, NSF proposal reviews, and CEBC outreach initiatives.

Spreading the seeds

WinterFLY

WinterFLY 2024/2025 was the largest yet with students from three departments joining the fun! This year, students played teambuilding games, integrated their creativity with science through collage-making, learned about and practiced leadership skills, and toured the Spencer Museum of Art. WinterFLY was borne of the NRT program to bring students together across disciplines for socialization and interdisciplinary skill-building. This was the last official NRT WinterFLY but the event has consistently demonstrated the value of bringing students together as a method to improve the graduate student experience.

Attendees *(Above, left to right)*
Alexander Lara (EECS), Paul Nyankey (CPE), Darik Rosser (CPE), Abdullah Bahdad (CPE), Jared Bartlett (CPE), Josena Frame (CPE), Eli Walther (CPE), Bri Farris (CPE), Mukhtiar Ali (CPE), Kara Poge (Environmental Engineering), Shelby Atherton (CPE)

CEBC Trainees Share Their Research Experience with the Community

Carnival of Chemistry

The annual Carnival of Chemistry, hosted by the KU Department of Chemistry, welcomes more than 300 kids and their families to explore the Gray-Little building and learn about chemistry firsthand. The CEBC hosted an exploration of size, using benchtop microscopes and images of transmission electron microscopes. CEBC graduate student, Alejandra Torres Velasco, used MatLab to program a virtual experience for the kids to "see" catalysts at nanometer scale.

Postdoc Nakisha Mark helps Prof. Alan Allgeier's son use a benchtop microscope

Emporia State University

Emporia State University holds an annual Enhancing Your Future with Science and Mathematics event that hosts more than 200 girls in 6th-8th grade. The event engages them in science workshops, discussions with women scientists, and hands-on activities. CEBC Teaching and Research Postdoctoral Researcher, Nakisha Mark, talked about what it means to be a woman in chemistry, and led an experiment converting corn starch into plastics.

Middle school students at Enhancing Your Future with Science and Mathematics

Full Circle Monthly Outreach

The CEBC continued its monthly outreach event at Full Circle Afterschool Program at the Lawrence Housing Authority. Each month, we explore a new chemistry topic with a hands-on activity such as the chemistry of DNA extraction, green energy, and distillation.

Graduate student Darik Rosser helps students during a Full Circle activity

Raintree Montessori Monthly Outreach

In 2024, we added a monthly outreach activity at Raintree Montessori in Lawrence, KS. The first- through third-grade students have engaged with non-Newtonian fluids, made plastic from corn starch, and used cabbage to determine the pH of common household liquids.

Raintree elementary students make plastic from cornstarch

Faculty Invited Talks 2024

Alan Allgeier, *Professor of Chemical Engineering*

- ACS 2024 Annual Spring Meeting, New Orleans, LA, March
- Characterization of Porous Materials (CPM)-9 Conference, Delray Beach, FL, May

Juan Bravo Suárez, *Assoc. Professor of Chemical Engineering*

- Great Plains Catalysis Society 2024 Webinar Series, May

Rachael Farber, *Assistant Professor of Chemistry*

- Truman State University, Kirksville, MO
- University of South Dakota, Vermillion, SD
- University of Tulsa, Tulsa, OK
- ACS Midwest Regional Meeting, Omaha, NE, October
- Oklahoma State University, Stillwater, OK

Elizabeth Corson, *Asst. Professor of Chemical Engineering*

- Electrochemistry Gordon Research Conference, Discussion Leader, Ventura, CA, January
- DyMERS Seminar, University of Kansas, Department of Chemistry, February
- 245th Electrochemical Society Meeting, San Francisco, CA, May
- ACS San Diego Section (virtual), August
- Great Plains Catalysis Society Fall Symposium, Norman, OK, August
- University of Nevada, Reno, Department of Chemistry, Reno, NV, September
- AIChE Annual Meeting, San Diego, CA, October

Justin Hutchison, *Assoc. Professor of Civil/Enviro./Arch. Engineering*

- University of Nebraska, Environmental Engineering Seminar, Lincoln, February
- American Chemical Society Spring Conference, New Orleans, LA, March
- BioNexus, Kansas City, Kansas, April
- KU Environmental Engineering Conference, Lawrence, KS, April
- Pratt City Commission, Pratt, KS, August
- Kansas Department of Health and Environment, Lawrence, KS, August

Tim Jackson, *Department Chair & Professor of Chemistry*

- ACS 2024 Annual Spring Meeting, New Orleans, LA, March

Kevin Leonard, *Professor of Chemical Engineering*

- ACS Green Chemistry Conference, Atlanta, GA, June
- ACS Catalysis Division Summer School, August

Ward Thompson, *Professor of Chemistry*

- National Meeting of the American Chemical Society, New Orleans, LA, March
- Gordon Research Conference, "Vibrational Spectroscopy," Smithfield, RI, August
- Telluride Science Research Conferences, Telluride, CO, July and September
- Sandia National Lab Chemical Sciences, Geosciences, and Biosciences (CSGB) Seminar (virtual), September
- Statistical Thermodynamics and Molecular Simulations (STMS) Virtual Seminar Series, December

Spreading the seeds

Dr. Bala Subramaniam and Dr. Alan Allgeier

hosted a symposium at the American Chemical Society Spring Annual Meeting titled "Promoting Industrial Decarbonization and Sustainability: A Session Celebrating Twenty Years of the Center for Environmentally Beneficial Catalysis (CEBC)." The symposium highlighted the more than 20 years of innovation and discovery by the CEBC such as industrially relevant and less carbon-intensive chemical technologies, which has been guided by quantitative sustainability assessment, machine learning, and industry partnerships.

International Talks

Alan Allgeier
Professor of Chemical Engineering

- University of Lancaster, UK, Seminar, June
- 18th International Congress on Catalysis (ICC), Lyon, France, July

Tim Jackson
Department Chair & Professor of Chemistry

- International Conference on Hydrogen-Atom Transfer, Monteporzio Catone, Italy, June

Kevin Leonard
Professor of Chemical Engineering

- CDT in Sustainable Chemistry Winter Showcase, University of Nottingham, UK, Keynote Address, February
- DOE ARPA-E / European Innovation Council, September

Ward Thompson
Professor of Chemistry

- International Conference on Ionizing Processes, University of Notre Dame, August

Growing the seeds

International Conferences

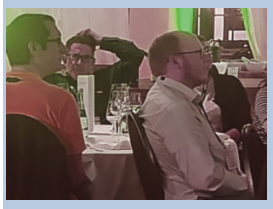
SPAIN

(L to R) Grad students ***Darik Rosser, Shelby Atherton*** *and* ***Brianna Farris*** *of Dr. Kevin Leonard's (R) lab attended the* ***Green Chemistry Gordon Research Conference*** *in Barcelona, Spain, in July. Brianna gave an invited talk and won a "Best Poster" award.*

FRANCE

Grad student **Alejandra Torres-Velasco** *of Dr. Juan Bravo-Suárez's lab, and Postdoctoral Researcher* **Nakisha Mark** *of Dr. Bala Subramaniam's lab attended the* ***18th International Congress on Catalysis*** *in Lyon, France, in July. Alejandra won a North American Catalysis Society travel award to attend.*

GERMANY



Alex Ervin *(R), a graduate student in Dr. James Blakemore's (L) lab, attended the* ***Karlsruhe Institute of Technology 2024 Workshop and Conference*** *in Karlsruhe, Germany in October. The five-day conference combined the International Workshop on Advanced Techniques in Actinide Spetroscopy (ATAS) and the AnXAS International Workshop on Speciation, Techniques, and Facilities for Radioactive Materials at Synchrotron Light Sources.*

USA

Lindsey Penland *(L), a graduate student in Dr. Rachael Farber's (R) lab, attended the* ***AVS 70th International Symposium & Exhibition*** *in Tampa, FL, in November. The week-long event included topics in machine learning, big data, and emerging artificial intelligence across the many different topical areas of AVS.*

Conferences Attended

MARCH

- **National Postdoctoral Association Annual Conference,** *Seattle, WA*
  Postdoctoral Researcher, Apoorva Ranjekar
- **American Chemical Society Spring Meeting,** *New Orleans, LA*
  Faculty: Alan Allgeier, James Blakemore, Juan Bravo Suárez, Justin Hutchison, Kevin Leonard, Bala Subramaniam; *Associate Researcher*, Hongda Zhu; *Students*: Sam Brunclik, Samir Castilla (talk), Sahan Godahewa (poster), Thanuja Jayawardena (poster), Khanh Le (poster), C.J. Ponge (talk), Nathaniel Sheehan (talk)
- **Department of Energy Conference,** *Arlington, VA*
  Associate Researcher Hongda Zhu

APRIL

- **Department of Defense DEPSCoR Meeting,** *Norman, OK*
  Associate Professor Juan Bravo Suárez

JUNE

- **Gordon Research Conference, Catalysis,** *New London, NH*
  Postdoctoral Researchers: Loveneesh Kumar (poster) and Anoop Uchagawkar
- **American Chemical Society, 28th Annual Green Chemistry & Engineering Conference** *Atlanta, GA*
  Professor Kevin Leonard
- **Department of Energy, ARPA-E Workshop,** *Washington, DC*
  Professors Alan Allgeier and Kevin Leonard
- **EPSCoR Summit,** *Washington, DC*
  Professor Kevin Leonard

JULY

- **Gordon Research Conference, Water & Aqueous Solutions,** *Holderness, NH*
  Student, Elizabeth Bartlett (poster)
- **Gordon Research Conference, Lignin,** *Boston, MA*
  Associate Researcher Sandip Singh

AUGUST

- **American Chemical Society Fall Meeting,** *Denver, CO*
  Faculty: Alan Allgeier and James Blakemore*; Postdoctoral Researcher* Preeti Jain (talk); *Students:* Sam Brunclik and Nigel Twi-Yeboah
- **Great Plains Catalysis Society Fall Symposium,** *Norman, Oklahoma*
  Faculty: Alan Allgeier, Juan Bravo Suárez (talk), Elizabeth Corson (talk) and Bala Subramaniam (plenary lecture, GPCS Award); *Associate Researchers:* Sandip Singh (talk) and Kirk Snavely; *Postdoctoral Researchers*: Preeti Jain, Loveneesh Kumar (talk), Sahil Kumar, Nakisha Mark, Priyanka Pal (talk), Apoorva Ranjekar (talk), and Kinithi Wickramaratne (talk); *Students*: (all gave talks) Hashim Alzahrani, Ben Auer, Jared Bartlett, Samir Castilla, Prathusha Kothinti, Bhagyesha Patil, Odiri Siakpebru, and Alejandra Torres-Velasco

OCTOBER

- **NRT Annual Conference,** *Washington, DC*
  Professor Kevin Leonard and *Student* Darik Rosser
- **American Institute of Chemical Engineers Annual Meeting,** *San Diego, CA*
  Professors Kevin Leonard and Bala Subramaniam*; Associate Researcher* Sandip Singh*; Postdoctoral Researchers* Preeti Jain and Anoop Uchagawkar; *Students:* Hashim Alzahrani (talk), Shelby Atherton (poster), Abdullah Bahdad (poster), Tate Bestwick (poster), Brianna Farris (poster), Prathusha Kothinti (talk), Darik Rosser, Nigel Twi-Yeboah (talk)

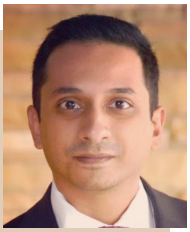
Special Recognition

Natalie Lind, *a graduate student in Dr. James Blakemore's lab, was selected as one of four recognized at the 21st Kansas Capitol Graduate Research Summit in Topeka in March.*

Alejandra Torres Velasco, *a graduate student in Dr. Juan Bravo Suárez's lab, won a monetary award for her September presentation at the* ***2nd Virtual Symposium of LatinXinChE****, sponsored by AIChE and Dow.*

Tate Bestwick, *a grduate student in Dr. Kyle Camarda's lab, attended the* ***Gaussian Process and Uncertainty Quantification Summer School*** *in Manchester, UK, in September. The four-day program presented a deep dive into practices and modelling of Gaussian Processes.*

Ben Auer, *an undergraduate in Dr. Alan Allgeier's lab, was selected for the* ***Future Leaders in Chemical Engineering Symposium at North Carolina State University.*** *The two-day October event recognized top U.S. undergraduates in chemical engineering, with 18 participants sharing their research.*



Abdullah Bahdad, *a graduate student in Dr. Kevin Leonard's lab, won second place in the* ***AIChE Student Competition in Sensors*** *at the organization's Annual Meeting in October for his work titled "360b Anodically Grown Pt(II) Oxide Micro electrode/Nanoelectrode pH Sensor."*

Where in the WORLD are the CEBC alumni?

Nearly half of former CEBC students, postdocs and researchers are employed in academia worldwide, or at U.S. national labs or government agencies. They include:

Academia: *•* ***Geoffrey Aiken****, Lancaster University (UK) •* ***Jason Bates,*** *University of Virginia •* ***Sam Brunclik****, University of Kansas •* ***Andrew Danby****, University of York (UK) •* ***April French,*** *University of Kentucky •* ***Xin Jin and Wenjuan Yan****, China University of Petroleum (PRC) •* ***Jesse Kern,*** *University of Central Oklahoma •* ***Michael Lundin****, University of Kansas •* ***Alexander Mironenko****, University of Illinois Urbana-Champaign •* ***Pablo Palafox,*** *College of St. Scholastica (MN) •* ***Zeke Piskulich****, Rutgers University (NJ) •* ***Bibhas Sarkar,*** *Birla Institute of Technology & Science, Pilani (India) •* ***Julian Silverman,*** *Fashion Institute of Technology (NYC) •* ***Ziwei Song****, Yanshan University (PRC) •* ***Kyle Stephens,*** *Paul Scherrer Institut (Switzerland) •* ***Anoop Uchagawkar****, University of Kansas •* ***Gayan Wijeratne****, University of Alabama •* ***Jian-Feng Wu****, Lanzhou University (PRC) •* ***Hongda Zhu****, University of Kansas •* ***Xiaobin Zuo****, Ottawa University (KS) •* ***Shirley Xie****, Youngstown State University (OH)*

National Labs & Government: *• Ames National Lab,* ***Yuting Li*** *• Argonne National Lab,* ***Emily Mikeska, Christian Nilles*** *• Berkeley National Lab,* ***Dupeng Liu*** *• Los Alamos National Lab,* ***Riddhi Golwankar*** *• Oak Ridge National Lab,* ***Domenick Leto, Victor Sharma*** *• Pacific Northwest National Lab,* ***Bhanupriya Boruah, Mi Yeon Byun, Honghong Shi*** *• Sandia National Lab,* ***Matthew Stalcup*** *• U.S. Department of Energy,* ***Robbie Hable, Kourosh Kian*** *• U.S. Food & Drug Administration,* ***Jing Fang***

Growing the seeds

Grad student awarded one of chemistry's highest honors

Fynn Cooper, *a graduate student in Dr. James Blakemore's lab, was named the* ***2024 SCI America Perkin Medal Scholar.*** *One of the highest honors given for outstanding work in American industrial chemistry, the medal was presented to Fynn by the Society of Chemical Industry in Philadelphia, PA, in September.*

Sandip Singh a *Topics in Catalysis* guest editor

CEBC Associate Researcher Dr. Sandip Singh recently served as one of three guest editors for a special issue of TOPICS IN CATALYSIS. Released in February 2025 by SpringerNature, the volume comprises a collection of research papers presented at the International Conference on Materials for Sustainable Energy, Environment, and Health (ICMSEEH-2023) held in October 2023 at Pandit Deendayal Energy University (PDEU), Gandhinagar, Gujarat, India.

The 18 articles selected by the editors for the special issue address pressing global challenges at the intersection of sustainable energy production, environmental protection, and improved human health.

2024 Publications

Complete list at
www.cebc.ku.edu/publications

Bahdad, A. O. O.; Leonard, K. C., Anodically Grown Pt(II) Oxide Microelectrode/Nanoelectrode pH Sensor. *J. Electrochem. Soc.* **2024**, *171* (11), 117512. doi:10.1149/1945-7111/ad8c35

Bartlett, E. R.; Borkowski, A. K.; Nilles, C. K.; Blakemore, J. D.; Thompson, W. H., Entropy drives accelerated ion diffusion upon carbon dioxide expansion of electrolytes. *J. Phys. Chem. B* **2024**, *128* (19), 4783-4791. doi:10.1021/acs.jpcb.4c00540

Castilla-Acevedo, S. F.; Szobody, T. P.; Boydston, C. M.; John, J. S.; Amaya-Roncancio, S.; Allgeier, A. M., Efficient hydrodeoxygenation of tetrahydrofuran 2,5-dicarboxylic acid to adipic acid over Pt-MOx catalysts: An experimental and computational study. *Catal. Today* **2024**, *436*, 114722. doi:10.1016/j.cattod.2024.114722

Corson, E. R.; Guo, J.; Tarpeh, W. A., ATR-SEIRAS Method to Measure Interfacial pH during Electrocatalytic Nitrate Reduction on Cu. *J. Electrochem. Soc.* **2024**, *171* (4), 046503. doi:10.1149/1945-7111/ad3a22

Golwankar, R. R.; Ervin, A. C.; Makos, M. Z.; Mikeska, E. R.; Glezakou, V.-A.; Blakemore, J. D., Synthesis, Isolation, and Study of Heterobimetallic Uranyl Crown Ether Complexes. *J. Am. Chem. Soc.* **2024**, *146* (14), 9597-9604. doi:10.1021/jacs.3c12075

Golwankar, R. R.; Makos, M. Z.; Cajiao, N.; Neidig, M. L.; Oliver, A. G.; Day, C. S.; Day, V. W.; Glezakou, V.-A.; Blakemore, J. D., Activation and Functionalization of the Uranyl Ion by Electrochemical Reduction. *Inorg. Chem.* **2024**, *63* (52), 24542-24553. doi:10.1021/acs.inorgchem.4c03349

Grotemeyer, E. N.; Aghaei, Z.; Jackson, T. A., Spectroscopic Properties and Reactivity of a MnIII-Hydroperoxo Complex that is Stable at Room Temperature. *Chem. - Eur. J.* **2024**, *30* (70), e202403051. doi:10.1002/chem.202403051

Kamkar, M.; Leonard, K. C.; Ferrer, I.; Loo, S. C. J.; Biddinger, E. J.; Brady, D.; Carrier, D. J.; Gathergood, N.; Han, H.; Hermans, I.; Hii, K. K. M.; Hwang, B. J.; Loh, W.; Meier, M. A. R.; Marr, A. C.; Newton, G. N.; Srubar, W. V., III; Yan, N.; Tam, M. K. C.; Chen, J.; Moores, A. H.; Subramaniam, B.; Licence, P.; Serrano, J. F., Artificial Intelligence (AI) for Sustainable Resource Management and Chemical Processes. *ACS Sustainable Chem. Eng.* **2024**, *12* (8), 2924-2926. doi:10.1021/acssuschemeng.4c01004

Karnes, J. P.; Kumar, A.; Hopkins Leseberg, J. A.; Day, V. W.; Blakemore, J. D., Trivalent Cations Slow Electron Transfer to Macrocyclic Heterobimetallic Complexes. *Inorg. Chem.* **2024**, *63* (19), 8710-8729. doi:10.1021/acs.inorgchem.4c00230

Karnes, J. P.; Oliver, A. G.; Day, C. S.; Day, V. W.; Blakemore, J. D., Tunability in heterobimetallic complexes featuring an acyclic "tiara" polyether motif. *ChemRxiv* **2024**, 1-61. doi:10.26434/chemrxiv-2024-p6wg1

Melfi, D. T.; Scurto, A. M., Viscosity of imidazolium ionic liquids and mixtures of ILs from entropy scaling using the PC-SAFT and ePC-SAFT equations of state. *J. Mol. Liq.* **2024**, *401*, 124500. doi:10.1016/j.molliq.2024.124500

Mikeska, E. R.; Curry, T. D.; Wilson, R. E.; Blakemore, J. D., Electroanalytical characterization of Np(VI)/Np(V) redox in a pentadentate ligand environment and stabilization of Np(V) by hydrogen bonding. *ChemRxiv* **2024**, 1-43. doi:10.26434/chemrxiv-2024-cpkqj

Mikeska, E. R.; Curry, T. D.; Wilson, R. E.; Blakemore, J. D., Electroanalytical characterization of Np(vi)/Np(v) redox in a pentadentate ligand environment and stabilization of $[NpVO_2]+$ by hydrogen bonding. *Dalton Trans.* **2024**, *53* (48), 19126-19142. doi:10.1039/d4dt02557a

Mikeska, E. R.; Lind, N. M.; Ervin, A. C.; Khalife, C.; Karnes, J. P.; Blakemore, J. D., Observations regarding the synthesis and redox chemistry of heterobimetallic uranyl complexes containing Group 10 metals. Radiochim. *Acta* **2024**, *112* (3), 149-160. doi:10.1515/ract-2023-0237

Mikeska, E. R.; Makos, M. Z.; Glezakou, V.-A.; Blakemore, J. D., Reactivity and cross-reactivity in redox activation of the uranyl ion. *ChemRxiv* **2024**, 1-50. doi:10.26434/chemrxiv-2024-nhgcl

Mikeska, E. R.; Wilson, R. E.; Blakemore, J. D., PCET-driven reactivity of neptunyl(VI) yields oxo-bridged Np(V) and Np(IV) species. *ChemRxiv* **2024**, 1-23. doi:10.26434/chemrxiv-2024-3rrhz

Mikeska, E. R.; Wilson, R. E.; Sen, A.; Autschbach, J.; Blakemore, J. D., Preparation of neptunyl and plutonyl acetates to access non-aqueous transuranium coordination chemistry. *ChemRxiv* **2024**, 1-37. doi:10.26434/chemrxiv-2024-kqthl

Neupane, P.; Bartels, D. M.; Thompson, W. H., Exploring the Unusual Reactivity of the Hydrated Electron with CO_2. *J. Phys. Chem. B* **2024**, *128* (2), 567-575. doi:10.1021/acs.jpcb.3c06935

Nilles, C. K.; Borkowski, A. K.; Bartlett, E. R.; Stalcup, M. A.; Lee, H.-J.; Leonard, K. C.; Subramaniam, B.; Thompson, W. H.; Blakemore, J. D., Mechanistic Basis of Conductivity in Carbon Dioxide-Expanded Electrolytes: A Joint Experimental-Theoretical Study. *J. Am. Chem. Soc.* **2024**, *146* (4), 2398-2410. doi:10.1021/jacs.3c08145

Osei, D.; Gurrala, L.; Sheldon, A.; Mayuga, J.; Lincoln, C.; Rorrer, N. A.; Morais, A. R. C., Subcritical CO_2-H_2O hydrolysis of polyethylene terephthalate as a sustainable chemical recycling platform. *Green Chem.* **2024**, *26* (11), 6436-6445. doi:10.1039/d3gc04576e

Penland, L. N.; Hirushan, H. H.; Dissanayake, N.; Farber, R. G., Influence of hydrogen-bonded 3-mercaptopropionic acid bilayers on binary self-assembled monolayer formation. *J. Vac. Sci. Technol., A* **2024**, *42* (6), 063205. doi:10.1116/6.0003926

Piskulich, Z. A.; Laage, D.; Thompson, W. H., A structure-dynamics relationship enables prediction of the water hydrogen bond exchange activation energy from experimental data. *Chem. Sci.* **2024**, *15* (6), 2197-2204. doi:10.1039/d3sc04495e

Rosser, D. A.; Farris, B. R.; Leonard, K. C., Predictive machine learning models trained on experimental datasets for electrochemical nitrogen reduction. *Digital Discovery* **2024**, *3* (4), 667-673. doi:10.1039/d3dd00151b

Sharma, V. K.; Binder, T. P.; Allgeier, A. M., Conceptual Process Design and Techno-Economic Analysis of Biocatalytic Furfural Hydrogenation Using Ethanol as the Terminal Reductant. *ACS Sustainable Chem. Eng.* **2024**, *12* (29), 10776-10785. doi:10.1021/acssuschemeng.4c01718

Siakpebru, O. K.; Uchagawkar, A.; Gurrala, L.; Bartlett, J.; Adamson, P.; Gorschak, N.; Hassiba, A.; Niphadkar, P.; Bokade, V.; Morais, A. R. C., One-Pot Production of Liquid Hydrocarbons by Catalytic Hydrodeoxygenation of Lignocellulosic Biomass Using Nickel Loaded on Zeolite-Based Supports. *Energy Fuels* **2024**, *38* (14), 13029-13038. doi:10.1021/acs.energyfuels.4c00659

Singh, P.; Massie, A. A.; Denler, M. C.; Lee, Y.; Mayfield, J. R.; Lomax, M. J. A.; Singh, R.; Nordlander, E.; Jackson, T. A., C-H Bond Oxidation by MnIV-Oxo Complexes: Hydrogen-Atom Tunneling and Multistate Reactivity. *Inorg. Chem.* **2024**, *63* (17), 7754-7769. doi:10.1021/acs.inorgchem.4c00186

Singh, S.; Binder, T.; Hagberg, E.; Subramaniam, B., High-Performance Resin Formulations with Ozone-Pretreated Corn Cob Lignin and Lysine. *ACS Sustainable Chem. Eng.* **2024**, *12* (38), 14305-14318. doi:10.1021/acssuschemeng.4c05369

Stiel, J. P.; Henke, W. C.; Moore, W. N. G.; Barker, N. M.; Oliver, A. G.; Day, V. W.; Blakemore, J. D., Redox properties of [Cp*Rh] complexes supported by mono-substituted 2,2′-bipyridyl ligands. *Dalton Trans.* **2024**, *53* (41), 16956-16965. doi:10.1039/d4dt01766h

Suekuni, M. T.; Ezazi, M.; Kwon, G.; Craddock, P. R.; Allgeier, A. M., Assessment of Kerogen Wettability from Contact Angle Goniometry. *Energy Fuels* **2024**, *38* (3), 1864-1872. doi:10.1021/acs.energyfuels.3c03175

T. Melfi, D.; Scurto, A. M., Carbon Dioxide-Induced Separations of Terephthalic Acid from Aqueous Disodium Terephthalate Solutions for Polyester Upcycling. *ACS Sustainable Chem. Eng.* **2024**, *12* (50), 17977-17981. doi:10.1021/acssuschemeng.4c05645

Torres-Velasco, A.; Patil, B. S.; Zhu, H.; Qi, Y.; Podkolzin, S. G.; Bravo-Suarez, J. J., A general method for studying reactive surface species, CT-SKAn: Charge-transfer spectrokinetic analysis. *J. Catal. 2024,* **434**, 115508. doi:10.1016/j.jcat.2024.115508

Uchagawkar, A.; Ramanathan, A.; Zhu, H.; Chen, L.; Hu, Y.; Douglas, J.; Mais, M.; Kobayashi, T.; Subramaniam, B., Insights into Dopant-Mediated Tuning of Silica-Supported Mo Metal Centers for Enhanced Olefin Metathesis. *ACS Catal.* **2024**, *14* (11), 8317-8329. doi:10.1021/acscatal.4c01700

Yu, M.-M.; Zhang, Z.; Guan, G.-L.; Patil, B.; Srinivasan, P. D.; Wang, G.; Feng, W.-H.; Miao, Y.-T.; Wang, L.-J.; Zhu, H.; Shakouri, M.; Huang, R.; Ding, D.; Sun, W.; Bravo-Suarez, J. J.; Hu, Y.; Yu, S.-M.; Cui, Y.; Wang, Q.; Yang, J.-H.; Wu, J.-F.; Chou, L., Insights into a Nitrogen-Doped Cobalt Oxide Catalyst for Enhanced Hydrogenation of CO_2 to C_{2+} Hydrocarbons. *ACS Sustainable Chem. Eng.* **2024**, *12* (14), 5496-5508. doi:10.1021/acssuschemeng.3c07908

Zhu, H.; Douglas, J. T.; Subramaniam, B., Influence of Trace Metal in Plastics on Catalyst Activity and Reusability during Polyolefins Upcycling with Polyoxometalates. *ACS Catal.* **2024**, *14* (20), 15633-15644. doi:10.1021/acscatal.4c04719