William F. Schneider, Atomic-Scale Structural Evolution of Rh(110) during Catalysis

The paper is organized as follows: Section II reports the...
Our mission is straightforward:
Invent cleaner, safer, energy-efficient technologies that protect the planet and human health.

Our approach is unique:
Students and researchers collaborate at the CEBC to design cleaner, safer, economically viable chemical technologies.

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

As the chemical industry’s global output continues to expand—nearly doubling its 2010 volume by 2020—the Center’s mission is more relevant than ever.
A Community for Collaboration

Looking back over the past year, I am struck by the CEBC’s tremendous achievements, as highlighted in the following pages. The center’s strong foundation of engaging effectively with stakeholders has contributed significantly to its successes. I’m proud to say that we have fostered a space for collaboration that reaches across boundaries — within and beyond the university. Seeing our community of researchers continue to grow is both gratifying and inspiring.

In October 2016, the University of Kansas conducted a five-year external review of the CEBC. The overall assessment was very positive, with top marks for the quality of faculty, staff and leadership, as well as funding, research and partnerships. The report also provided valuable suggestions for continued growth and vibrancy, which will guide the center’s strategic planning for the future.

A surge in industry-sponsored projects this year brings the total to five company-sponsored projects, with three more contracts nearing finalization — a record number for the center. In addition, four companies became members, including DuPont, Chevron Phillips Chemical Co., W. R. Grace and Chemours.

Exciting R&D advances from federally funded projects continue to provide leveraging opportunities for CEBC’s member companies. Much of the research addresses challenges related to the complex water-energy-food nexus. Our researchers are creating novel solutions to problems such as sustainable energy production, energy-efficient water purification, and resource-efficient ways to make fuels and chemicals from biomass, CO$_2$ and shale gas components.

CEBC’s unique education program is training the future workforce with the skills they need to be successful in industry and academia. Frequent interactions with company representatives help students gain insight into corporate research and development. In the past five years, a dozen graduates and postdocs have been hired by chemical companies, including some CEBC partner companies. Several have also taken university positions worldwide.

Since 2003, the CEBC has become a leading catalysis center that serves both the mission of the University of Kansas and offers unique value to chemical and related industries. As confirmed by the recent external review, the center’s strong community for collaboration shows much promise for a bright future. Our successes are made possible by the accomplishments of faculty, students and staff with exceptional guidance from the Industry and Science Advisory Boards. We are also grateful to the visionary leaders of the University of Kansas who facilitate such accomplishments.

Bala Subramaniam
Dr. Bala Subramaniam
CEBC Director
2016 Invited Talks

James Blakemore
Two plenary talks at Advancing Energy Sustainability by Governance Leadership in Artificial Photosynthesis, Australian National University, Sept. 2-13

R.V. Chaudhari
Green Chemistry Gordon Research Conference, Vermont, July 31 - Aug. 5

Bala Subramaniam
• American-Russian Chemical Engineering Scientific School, Russia, May 23-25
• inPROMPT 2016: Tunable Solvents for Green Processing, Germany, June 2-3
• Vice chair, Green Chemistry Gordon Research Conference, Vermont, July 31 - Aug. 5

Franklin Tao
• International Workshop on Single-Atom Catalysis, China, June 30 - July 2
• National University of Singapore, June 28
• World Congress on Petroleum and Refinery, Austria, July 21-23
• ACS Symposium: In Situ & Operando Spectroscopy of Catalysts, Aug. 19-25
• Symposia: 1) Electronic and Ionic Dynamics at Solid-Liquid Interfaces; 2) Catalytic Materials for Energy and Sustainability, Boston, Nov. 27 - Dec. 2

Funding successes

$20,000,000+ in federal grants garnered since 2009

$3,000,000+ average annual funding level 2009-2016

21% funding from industry sources

New Grants, Awards & Recognition, Pages 5-6

Partnering with research institutions

21 institutions worldwide have worked with the CEBC since the center’s inception

7 have partnered with CEBC on federally funded projects

4 core partners have helped shape research focus and scale-up potential

New Research Partners, Page 7

Engaging with industry

25 companies have partnered with CEBC since the center’s inception

9 current industry partners, with more in discussion

5 current industry-sponsored projects, a record number for CEBC, with several more in planning

New Industry Partners, Page 8
Ten years of Research Experiences for Teachers

2 Kansas high school teachers participated in 2006 when the RET program was launched using CEBC funds (NSF funding awarded 2009)

32 total high school teachers (22) and undergraduate students (10) have worked with KU faculty mentors from several departments

1000+ high school students across Kansas have benefited from the 40 original lessons created

More on Education & Outreach, Page 9

Diverse Trainees

162 researchers have trained at CEBC since 2009

43 Postdocs & Associate Researchers
Many have embarked on industry careers or have earned professorships

19 Visiting Scholars
From China, Columbia, India, Germany, Poland and South Africa

50 Graduate Students
12 hired by chemical companies
12 hired as postdoctoral researchers
6 to academia & other pursuits
20 current students

More on Students & Researchers, Page 10

Discovery and innovation

336 manuscripts published since CEBC’s 2003 inception

53 total invention disclosures (38) and patents (15)

5 license options negotiated, one currently in discussion

2016-2017 publications list, back cover

Spotlight on Safety

At the CEBC, researchers are trained in safety procedures that go well above most university standards. A key feature is monthly mandatory safety meetings, covering topics such as how to perform risk assessments, manage waste appropriately, ensure electrical safety, and use gas cylinders properly.

CEBC’s lab inspection process was updated in January 2017. Instead of individual peer-to-peer inspections, a team inspects the labs each month to promote greater accountability, constructive dialogue and safer experiments. Findings are recorded and presented at monthly safety meetings.

There are also leadership opportunities for researchers as part of the CEBC Laboratory Safety Committee, composed of students, postdocs and staff, with faculty engagement.
Raghunath Chaudhari, CEBC Deputy Director and Deane E. Ackers Distinguished Professor of Chemical & Petroleum Engineering, has been named a Fellow of the National Academy of Inventors in recognition of his innovative work in catalysis, reaction engineering, multiphase reactors and kinetic modeling. His research has led to many discoveries — including a smart, energy-efficient method for turning plant sugars into the building blocks for plastics, paints, fibers and many other everyday items.

Chaudhari becomes the third KU professor to be named an NAI Fellow. Last year, Bala Subramaniam, CEBC Director and Dan F. Servey Distinguished Professor of Chemical and Petroleum Engineering, and Val Stella, a University Distinguished Professor of Pharmaceutical Chemistry, became KU’s first NAI Fellows. According to the NAI, election to Fellow status is a high professional distinction accorded to “academic inventors who have demonstrated a prolific spirit of innovation in creating or facilitating outstanding inventions that have made a tangible impact on quality of life, economic development and the welfare of society.”

Mark Shiflett, who has worked at DuPont since 1987, joined KU in August as a Foundation Distinguished Professor in the Department of Chemical and Petroleum Engineering. He will conduct research at CEBC in separations, ionic liquids and green chemistry.

At DuPont, his research resulted in three environmentally safe refrigerant mixtures, one of which has generated more than $1 billion in revenue. He holds 44 patents and has several patent applications pending. He has published more than 70 scholarly articles and is frequently an invited lecturer at conferences.

Mark Shiflett received a national award from the American Institute for Chemical Engineers November 13, 2016, in San Francisco, California. The AIChE Industrial Research and Development Award recognizes several of Shiflett’s pioneering discoveries at DuPont, where he was a Technical Fellow for more than 20 years before joining KU in August. His work has led to non-ozone-depleting refrigerants, as well as new applications with ionic liquids and an environmentally friendly process for making highly durable grades of titanium dioxide. He also was recognized for his valuable efforts mentoring and educating chemical engineers.
Marco Caricato wins NSF Career Award

Marco Caricato, Assistant Professor of Chemistry, was selected to receive a National Science Foundation Faculty Early Career Development (CAREER) award. The prestigious five-year, $625,000 award recognizes junior faculty who are rising stars in research and education.

The award will support Caricato’s research to develop new theoretical models and computer software to simulate how light interacts with solid chiral materials. Chiral objects are mirror images of each other. Caricato’s models will help scientists characterize and design new chiral materials that could be useful for electronics, catalysis and many other applications.

Caricato also has plans for an ambitious outreach program. His goal: Bring computational chemistry into Kansas high school classrooms. “Computer simulations have enormous educational potential in this technological age,” said Caricato, who started this project as part of the CEBC’s NSF-funded Research Experiences for Teachers. Working with Stan Spurlin, chemistry teacher at Olathe East High School, the team began developing novel tools that allow pre-college-aged students to explore bonding and intermolecular forces. Ultimately, this project will help inspire the next generation of rising stars in science, technology, and engineering careers.

New NSF grant: From CO₂ to useful products

Kevin Leonard, Assistant Professor of Chemical and Petroleum Engineering, James Blakemore, Assistant Professor of Chemistry, and Bala Subramaniam, Dan F. Servey Distinguished Professor of Chemical and Petroleum Engineering, recently received an award from the National Science Foundation to fund research in sustainable chemistry, engineering and materials. The three-year, $450,000 award is part of an initiative organized by NSF known as SusChEM.

The team will develop a first-of-its-kind apparatus to perform electrocatalysis in liquid carbon dioxide. They hope to invent a new way to convert carbon dioxide waste into useful fuels and chemicals. Pressurized carbon dioxide pumped into the reactor will dissolve in a liquid mixture of other ingredients needed for the electrochemical reaction, “expanding” its volume. In this manner, the carbon dioxide not only speeds up the reaction but is also more readily available for conversion into methanol or other fuels and chemicals, with the help of suitable catalysts and electricity.

Leonard wins young investigator award

Kevin Leonard was chosen by the Army Research Office (ARO) for a $150,000 grant to intelligently design earth-abundant water splitting electrocatalysts. The three-year award will help Leonard’s research group study how inexpensive, readily available catalysts can be used to generate hydrogen or oxygen. The ARO program consists primarily of single investigator research efforts, university-affiliated research centers, and specially tailored outreach programs.
Zeolite library donated to CEBC

A new library of innovative materials will accelerate fundamental research and catalyze industry engagement at the University of Kansas.

The DuPont Company and Dr. David Corbin (pictured at left) recently donated a library of microporous materials containing over 3,000 unique zeolites, carbons and ion-exchange resins to be housed at CEBC. Many of these materials are commonly used as commercial adsorbents and catalysts for chemical processes. Access to this library gives the CEBC a unique resource for a variety of chemical catalysis and separation projects.

“We gratefully acknowledge this donation from Dr. Corbin and DuPont,” said CEBC Director, Bala Subramaniam. “We feel privileged that the CEBC was chosen to house this extensive library, allowing CEBC researchers to investigate these unique materials for novel applications in separations and catalysis.”

Corbin, a 35-year DuPont veteran, was recently appointed as a senior research scientist at KU. He will work with CEBC industry partners on proprietary projects.

CEBC initiates partnership with German scientists

The CEBC hosted five scientists from Friedrich-Alexander Universität of Erlangen-Nürnberg (FAU) in June. The goal of the visit was to identify high risk/high reward collaboration opportunities.

The FAU team was led by Peter Wasserscheid (below left). He and his collaborators at FAU, including Hannsjörg Freund (below right), are among the world leaders in ionic liquids, hydrogen storage, and process optimization. Wasserscheid directs major research efforts in Germany’s quest for a renewable energy economy.

Following the visit, preliminary research was initiated with Bala Subramaniam (below center) and R.V. Chaudhari, distinguished professors of chemical engineering at the University of Kansas. Currently, the team is exploring funding options to expand this collaborative international partnership.

PNAS, C&E News feature Blakemore research

In June 2016, KU Assistant Professor of Chemistry James Blakemore (above) reported in the Proceedings of the National Academy of Sciences how his research group isolated an unusual intermediate in a reaction pathway that leads to hydrogen production. His unexpected finding was also highlighted in Chemical & Engineering News in June. These reports show that a popular ligand present during hydrogen production reactions, called pentamethylycyclo-pentadienyl, or Cp*, can be actively involved in the reaction, briefly bonding to hydrogen before the hydrogen moves on to its ultimate destination. Remarkably, another team of researchers at the University of North Carolina at Chapel Hill also observed the unusual intermediate in the context of their work.

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Two former industry members rejoin CEBC

CEBC welcomes back Chevron Phillips Chemical Company and DuPont Company as industry partners. Both of these companies were charter members of CEBC, joining at the center’s launch in 2003.

Chevron Phillips Chemical Company, a flagship petrochemical company, was formed in 2000 after the merger of Chevron Corporation and Phillips Petroleum Company. One of the world’s top producers of olefins and polyolefins, aromatics, specialty chemicals, piping and proprietary plastics, it operates 35 manufacturing centers with 5,000 employees globally.

DuPont is one of the most successful and sustained enterprises in the world. For more than two centuries, it has delivered a multitude of innovations, including products that work to grow healthy crops, transform the sun’s rays into clean energy, keep food fresher longer, make cars lighter and more efficient, and protect the lives of soldiers and police officers.

Photo: Albert Tam, IAB member representing DuPont, discusses postdoc Pablo Palafox’s poster at the CEBC Fall 2016 Advisory Board Meeting

Meet our two newest industry partners

W. R. Grace is a leading global supplier of catalysts and engineered materials, built on talent, technology and trust. The company’s two industry-leading business segments — Catalysts and Materials — provide innovative products, technologies and services that enhance products and processes worldwide. Grace employs approximately 3,700 people in more than 30 countries.

Chemours Titanium Technologies in 1931 pioneered the chemistry on which their Ti-Pure™ formulations are based. The company continues as the global leader in TiO₂ production today. Chemours titanium dioxide is a key component of some of the whitest, brightest, and most efficient applications — brilliant paints, pristine plastic, gleaming laminates, and durable automotive and aerospace coatings.

Photo: Dorai Ramprasad, IAB member representing W.R. Grace

Industry recruitment forum a success

The “Emerging Feedstocks Forum” was organized at CEBC in May 2016 to enhance industry partnerships. Ten representatives from nine companies attended the forum. Discussion at the event led two companies to sponsor projects at the CEBC, hence becoming dues-paying members. The event featured presentations from several CEBC faculty members. In addition, Dan Ginosar, Distinguished Staff Scientist at Idaho National Laboratory (INL) and KU alumnus, shared opportunities at INL to scale up CEBC’s catalytic advances.

Photo: Dan Ginosar, INL

Photo: Prof. Franklin Tao gives a presentation on single-site catalyst synthesis at the Emerging Feedstocks Forum, attended by representatives from Archer Daniels Midland, Burns & McDonnell, Chevron Phillips Chemical, Chiyoda International, DuPont, Evonik, Flint Hills Resources, W.R. Grace, and Noritake
Article in chemical education journal

Environmental impact studies for chemical processes tend to be highly technical. Education Director Claudia Bode sought to simplify a few such impact studies performed at the CEBC. Together with Bala Subramaniam and two undergraduates, Bode summarized five key takeaways from data for several industrial processes. Their work was published this February in the *Journal of Chemical Education*. The practical lessons help college students think about ecological burdens in the context of economics, building skills critical for their future careers.

New middle school science club

Emporia, Kansas, middle school students have a new after-school club this year, thanks to the efforts of James Blakemore, assistant professor of chemistry at KU. Blakemore started the club in October. The goal is to engage students in hands-on chemistry, ultimately building long-term relationships that help to inspire students to seek careers in science. Blakemore’s research assistant, Tyler Kerr, has since traveled 12 times along an 80-mile stretch of highway to lead the club activities. To see Blakemore’s lab first-hand, the club traveled to KU along with teachers, parents and several other students — 65 in all — over the course of two days.

Elements of surprise for all ages

Is your wedding ring really 14 carat gold? An x-ray fluorescence device can reveal the answer — and promote science to the public. In early 2016, the CEBC purchased one of these devices with a grant from NSF. It has been demonstrated at more than half a dozen events this year at schools, museums and libraries for hundreds of people, including the group of middle schoolers from Emporia, Kansas, during their tour of Blakemore’s laboratory.

Events in Lawrence, Kansas, featuring the XRF device:

- Public library’s summer reading kick-off, June 4
- Lied Center’s ticket sales kick-off event, June 6
- High school teachers at CEBC, June 30
- Undergraduates at KU, July 12
- Hillcrest Elementary School science fair, January 26
- Cordley Elementary School science fair, February 2
- Emporia middle schoolers at KU, March 20-21

Beyond Research

New postdoc adds teaching training

Last fall the CEBC recruited Julian Silverman to serve in a unique postdoctoral position that integrates teaching and research training. The three-year position is funded through a $4 million interstate grant from the National Science Foundation Experimental Program to Stimulate Competitive Research (EPSCoR). Silverman obtained his PhD in chemistry in 2016 from the City University in New York. He currently works with Professor Bala Subramaniam in lignin deconstruction research. He also is helping incorporate meaningful sustainability-related exercises in the curriculum for a graduate-level course, “Industrial Development of Catalytic Process.”
Undergraduate student Truman Scholarship finalist

Undergraduate Tomas Green, a student in the Subramaniam group, is one of two KU students named as finalists for the prestigious Harry S. Truman Scholarships, which provide up to $30,000 for graduate study. Winners must show a strong track record of campus and community service, a commitment to a career in government or nonprofit sectors, and a high probability of becoming a “change agent.”

Graduate student wins Kokes Award

Yuting Li won a 2017 Kokes Award from the North American Catalysis Society (NACS). The award covers hotel and registration fees at the 25th annual NACS meeting in Denver, Colorado, June 4-9. Li is the third student in Professor Franklin Tao’s research group to be selected for this award. Luan Nguyen and Shiran Zhang, who both earned PhDs last spring, also were recipients.

Industry partners share professional insights

Peter Coughlin, Director Of Catalysis & Materials Research at Honeywell UOP, shared career advice with students and postdocs at the CEBC Industry Advisory Board meeting last spring. As for traits that make an ideal employee, Dr. Coughlin advocated for being patient, flexible, thoughtful and curious. He added, “Learn the fundamentals; they’ll always have a place in research.”

Scott Bloomer, Patent Agent with Archer Daniels Midland, presented a patent workshop for more than two dozen students and postdocs last fall. Bloomer discussed the differences between patenting in a university and corporate setting and the different types of intellectual property. He also shared a wealth of advice about what to patent and how to go about it.

ACS accolade

Anand Ramanathan, CEBC associate researcher, was recognized for the best presentation in the session, “Heterogeneous Catalysis for Selective Oxidation and Reduction toward a Green Production,” at the American Chemical Society National Meeting in Philadelphia, PA in August 2016.

ISCRE 24 Travel Awards

CEBC researchers and students received travel awards to attend the International Symposium for Chemical Reaction Engineering in Minneapolis, Minnesota, June 12-15, 2016, including graduate students Dupeng Liu, Kakasaheb Nandiwale and Ziwei Song, postdoctoral researcher Jian-Feng Wu, and associate researchers Anand Ramanathan and Xiaobin Zuo.

Newly Employed

Xin Jin, former CEBC postdoc
China University of Petroleum, Associate Professor

Tapan Maji, former CEBC postdoc
Hired by Zoetis, India

Pansy Patel, former CEBC postdoc
Hired by PPG Industries, Pennsylvania

Arely Torres, former CEBC postdoc
Hired by Archer Daniels Midland, Illinois

Wenjuan Yan, former grad student
Postdoc at China University of Petroleum

Zhenxing Wang, former CEBC postdoc
Hired by Contemporary Amperex Technology, China