جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology
Clean Combustion Research Center

Issue 6 | Fall 2021

KAUST Clean Combustion Research Center (CCRC) Newsletter

Cover Photo: The Corrosion Rig Photographed by Cedric Ghoussoub

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A MESSAGE

From the Center Director

William Roberts
Center Director,
Clean Combustion Research Center,
Professor of Mechanical Engineering

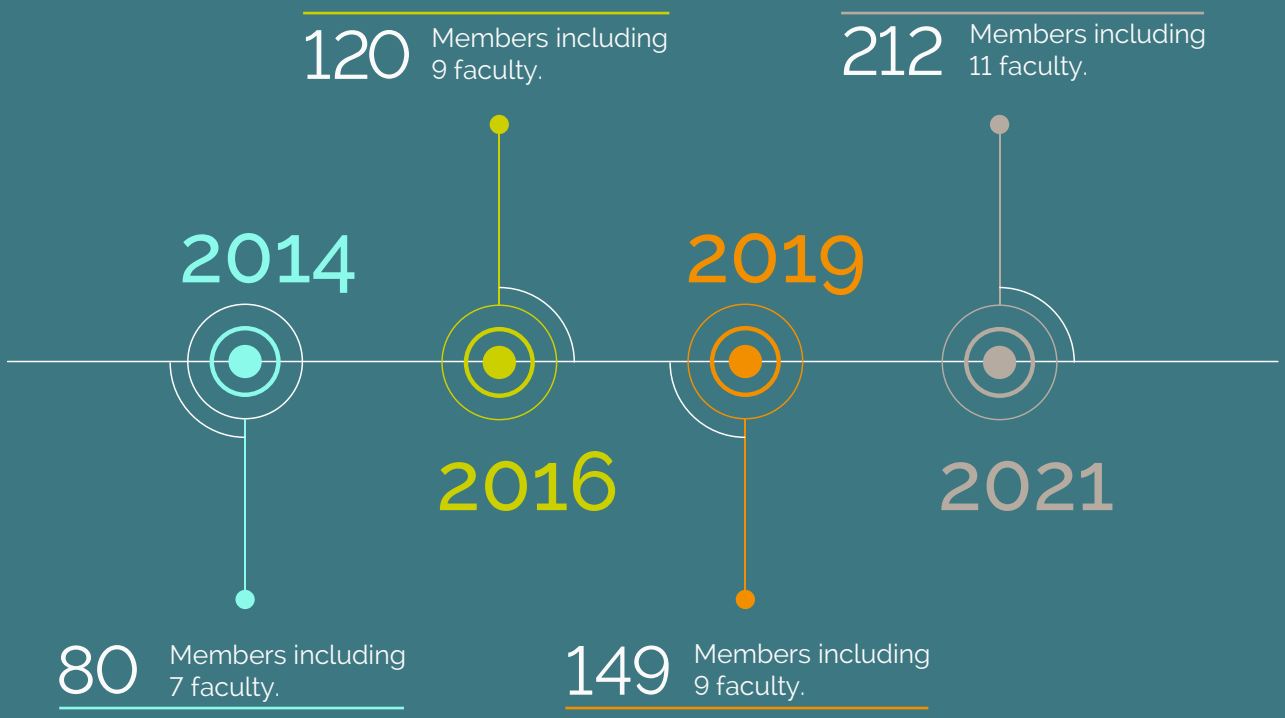
Dear all,

I hope this newsletter finds you and your families safe and healthy. As with everyone else, we have been adversely affected by the coronavirus, with many in the center losing loved ones and most of us not being able to travel to see family. The global slowdown in the movement of goods has also adversely affected our ability to deliver on some of our projects, but as will you, we will endure and overcome.

The center continues to grow in terms of faculty, students and postdocs, and external funding. In this edition of the newsletter, you will find articles on the retirement of Prof. Robert Dibble, and the welcoming of new members Prof. Bassam Dally from Adelaide and Prof. Jamie Turner from Bath. KAUST is reaching maturity in terms of the number of faculty, so it is getting more difficult to hire. We are very fortunate to have Bassam and Jamie join us, as well as new-to-the-Center Prof. Xu Lu. Xu came to KAUST without affiliation to any center (about half the faculty do not belong to one of KAUST's eleven centers), but saw the advantages of being a member of our team and joined as a full member. Additionally, we were successful in appointing Dr. Thibault Guiberti to a new role; Research Assistant Professor. I am very enthusiastic about these additions to the Center. We now have 100 Ph.D. students in the Center and our total population has crossed the 200 threshold!

We just completed an external evaluation at the request of the Vice President: Research, Prof. Donal Bradley. The three-day virtual evaluation was chaired by Prof. Margaret Wooldridge with five other exceptionally well-qualified evaluators from academia and industry. The evaluation was a very positive experience for faculty, staff, and students.

CCRC'S GROWTH THROUGH THE YEARS



Feedback from the review committee was uniformly positive and complementary, with recognition of our contributions and impact to combustion science and overall global footprint. In addition to an evaluation for the VPR, Prof. Wooldridge and colleagues provided valuable suggestions to us on how to maintain our leadership role in combustion and energy systems.
We are working to establish an Advisory Board, comprised of highly accomplished people from industry (both In-Kingdom and multi-national) and government.

We anticipate this Advisory Board will assist the Center in identifying research opportunities and help move our discoveries up the Technology Readiness Level scale where they can make an impact. The Kingdom is aggressively adopting a Circular Carbon Economy approach and we expect to be thought leaders and technology providers for this initiative.

Lastly, I would like to extend an invitation to participate in our next KAUST Research Conference on Hydrogen-Based Mobility and Power. These conferences are a great way to interact with the Center and find avenues to collaborate. The Conference will be held in hybrid mode on 7-10 of February 2022. Please watch our website for details.

Stay safe,
Bill Roberts

Prof. Robert Dibble becomes Professor Emeritus

Prof. Dibble with Prof. Sarathy at his home in Berkeley.

Towards the end of 2019, we said goodbye to Prof. Robert Dibble, who worked with the CCRC as a Full Professor of Mechanical Engineering since 2014. Now as a Professor Emeritus, he still provides support and guidance to the CCRC researchers and students. We caught up with him recently and here is what he shared.

"Helen and I came to the CCRC thinking we would stay a year or two. We stayed 5 years, a testimony as to how much fun and excitement we enjoyed. Leaving CCRC was a retirement accelerated by Covid. From the vibrant CCRC and KAUST I, like many other people, transitioned to staying in my home office for the last 2 years, as the Berkeley Campus was largely empty."

"I have been working on a design to convert the 100 million dead trees in Western North America to H2 and CO2. I remind you, on an atom basis, a tree is 50% hydrogen! The idea is to collect the trees and then gasify them to make hydrogen and carbon dioxide that you then store in the earth. What I discovered was the cost to do all of this was near a billion dollars and thus it is not obvious that converting trees to hydrogen is the best use of money that may be better invested into wind power and solar PV."

HIS ADVICE TO FUTURE ENGINEERS

"Sometimes you may hear that Science and Engineering are different career paths. But, long ago, I was lectured that Engineering is Science with a profit constraint. This definition has served me well. Thus a good engineer has to be well-founded in Science and also has to have an eye on Finance. A case in point, see above, my efforts on converting trees to hydrogen are held back by economics.

Engineers also discover that good writing skills are an important ingredient for Engineering success, the good news is the better writing emerges from better reading, thus it is good if you can read novels regularly, say once a month as a target."

Prof. Bassam Dally

Dr. Bassam Dally officially joined the CCRC as a Professor of Mechanical Engineering at the beginning of this year. Previously, the Deputy Director of the Centre for Energy Technology, CET, at the University of Adelaide, he has contributed to many public and scientific forums related to energy, co-authored three major review papers and more than 270 research papers.

Prof. Dally has received many awards over the years, and in 2016 he was named 'Energy Professional of the Year' by the SA Branch of the Australian Energy Institute. In 2019 he was named a Fellow of the Combustion Institute.

"I am excited about the opportunity to work collaboratively with world-leading researchers at CCRC and to conduct groundbreaking research that leads to impact on society, the environment, and academia," he noted.

Prof. James Turner

Dr. James Turner joined the CCRC in 2021 as a Professor of Mechanical Engineering.

"I am very excited about working collaboratively with the world-leading researchers at CCRC and to perform leading-edge research to help decarbonize transportation. I have a great deal of knowledge of automotive needs and requirements and I hope to use this to enable my research to be relevant both to industry and academia, and thus to benefit society and the environment," he said.

His interests are primarily in engines and powertrains of all types and the decarbonization of the fuels that they use. Dr. Turner is a Fellow of both the Institution of Mechanical Engineers and the Society of Automotive Engineers (SAE) and is the current Chairman of the Universities' Internal Combustion Engines Group (UnICEG) in the UK.

Prof. Xu Lu

Dr. Xu Lu joined the CCRC as an Assistant Professor of Mechanical Engineering in early 2021.

Prof. Xu Lu completed his B.Eng., M.Sc. and, Ph.D. degrees from the Department of Mechanical Engineering, the University of Hong Kong in 2012, 2013, and 2017, respectively. Before joining KAUST, he was a postdoctoral fellow at the Department of Chemistry and Energy Sciences Institute, Yale University. So far, he has 1 U.S. provisional patent and 25 publications in Journal of the American Chemical Society, Angewandte Chemie International Edition, ACS Energy Letters, Journal of Power Sources, Applied Energy, Renewable Energy, Nature etc.

Prof. Xu Lu's research focuses on reactor and material engineering for electrochemical CO2 conversion and long-term energy storage. He is also interested in hydrogen fuel cell, seawater electrolysis, and in-situ flow/material characterizations.

Prof. Thibault Guiberti

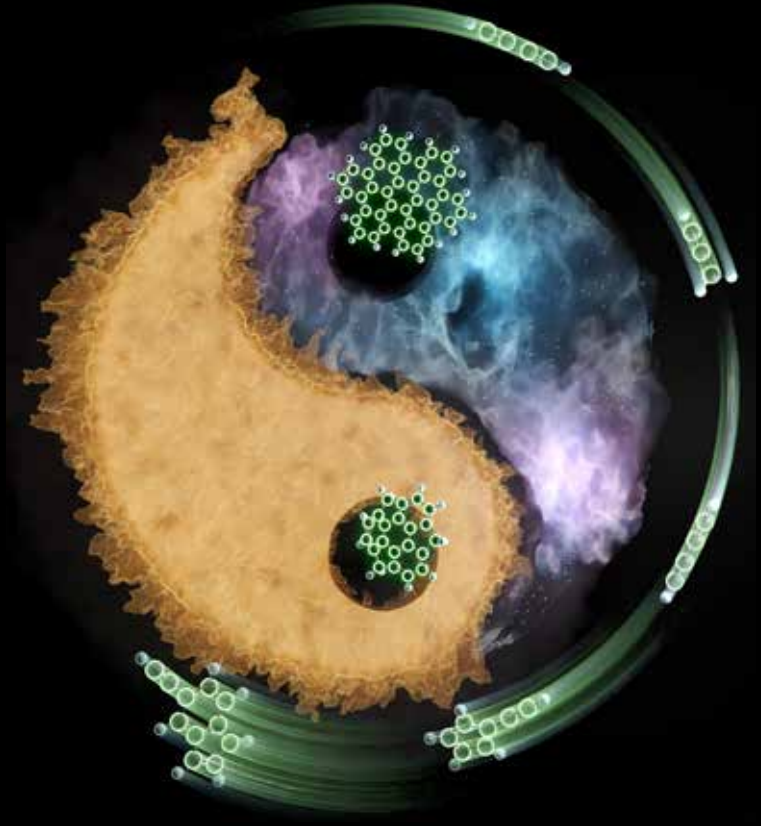
Dr. Thibault Guiberti was appointed as an Assistant Research Professor of Mechanical Engineering in July 2021.

Prof. Guiberti joined KAUST and CCRC in 2015 as a Postdoctoral fellow in the group of Prof. Roberts. In 2017, he became a Research Scientist and focused his research on turbulent reactive flows and optical diagnostics. With his research, Prof. Guiberti hopes to contribute to the promotion of carbon-free fuels, such as hydrogen and ammonia, in practical combustion devices. He has published 40 journal publications, contributed to many international conferences and workshops, and is a co-inventor on 3 new patents.

"In my new capacity, I look forward to further pushing the boundaries of experimental combustion at extreme conditions (high pressure and high levels of turbulence) and contributing to the emergence of CCRC as a world-leading center for hydrogen and ammonia utilization research," stated Prof. Guiberti.

Read more about new faculty appointments on the CCRC website

RSR Chain Reaction Towards Carbonaceous Nanostructures



Soot is a carbonaceous particle resulting from incomplete combustion of hydrocarbon fuels, and directly impacts combustion efficiency in practical combustion devices. Soot emission in the atmosphere has dire consequences to the human health and the environment. PM2.5 derived from soot can travel deeply in the lungs, deposit in the alveoli, enter the circulatory system, and finally reach other organs, causing potential health issues. Soot deposition promotes the melting of ice glaciers, while soot in the upper atmosphere affects weather in the form of clouds and precipitation by providing condensation nuclei.

Soot formation is one of the most complex phenomena in combustion, involving complicated interactions among combustion chemistry, fluid mechanics, mass/heat transport, and particle dynamics. The need to suppress soot emissions necessitates active control of soot formation processes, which in turn requires a fundamental understanding of the physicochemical pathways from fuel to soot. Sufficient experimental evidence has linked polycyclic aromatic hydrocarbons (PAH) to soot inception in combustion processes. A number of reaction mechanisms based on benzene and resonantly stabilized radicals (RSRs) have been proposed in literature to explain the formation and growth of PAHs. However, the fundamental formation mechanisms of carbonaceous nanostructures from PAH building blocks remain elusive.

We have deployed a wide range of theoretical and experimental methods to investigate the reaction chemistry of aromatic hydrocarbons to facilitate a comprehensive understanding of PAH and soot formation. In a recent work, we have shown that PAH formation may be driven by the RSR chain reaction of butadiyne and propargyl – termed continuous butadiyne addition cyclization (CBAC) mechanism. We found fulvenallenyl radical to be a critical intermediate in this RSR chain reaction. In addition, butadiyne is able to undergo continuous addition on RSRs without frequent H-elimination. Our findings challenge the conventional wisdom that radical site regeneration, being central to PAH growth, requires sequential hydrogen elimination and/or abstraction.

In the CBAC mechanism, PAH growth does not depend on abundant free radical consumption, and could, therefore, help explain carbonaceous nanoparticle coalescence in radical-deficient reaction environments, such as the post-combustion zone and interstellar medium. Our understanding of PAH growth also helps elucidate the evolution of carbon-rich galaxies, e.g., Wolf-Rayet stars.

FOR MORE DETAILS:

H. Jin, L. Xing, J. Yang, Z. Zhou, F. Qi, A. Farooq, Continuous Butadiyne Addition to Propargyl: A Radical-Efficient Pathway for Polycyclic Aromatic Hydrocarbons, J. Phys. Chem. Lett. 12 (2021) 8109-8114

Dr. Francesco Di Sabatino

Program: Ph.D. Student (Spring 2020)
PI: Prof. Deanna Lacoste
Current Position: Postdoctoral Appointee, Sandia National Laboratories in Livermore, U.S.A

"My journey at KAUST started in January 2016 and ended in June 2020. During the years at KAUST, I had the chance to meet amazing people and friends from around the world, work in state-of-the-art combustion laboratories, broaden my knowledge of combustion processes, laser diagnostics, and plasma-assisted combustion. Moreover, I had the chance to travel around the world and visit countries such as U.S.A., Australia, and Japan.

I am currently a Postdoctoral Appointee at the Combustion Research Facility at Sandia National Laboratories in Livermore, California, U.S.A."

Claudia Hernández

Program: M.S. Student (Fall 2020)
PI: Prof. William L. Roberts
Current Position: Technical Consultant, AspenTech, Germany

"During my masters at KAUST, Prof. Roberts led a consortium in which the main goal was to find an alternative to reduce the amount of sulfur in the preferred fuel in the maritime industry: heavy fuel oil. My task within this team consisted of creating a simulation able to mimic a process called "oxidative desulfurization" in a software called Aspen Plus.

After I graduated from KAUST, I worked in AspenTech as a technical consultant and during my time in the company, I was trained in Aspen PIMS, a planning solution software used by most refineries and olefins plants worldwide that allows economic evaluations and plant design and I helped several costumers with the management of the software."

KAUST Research Conference - Near Zero-Carbon Combustion Technology, 2021

The Clean Combustion Research Center hosted the first-ever hybrid conference on 'Near Zero-Carbon Combustion Technology' from 21-23, June 2021. With more than 700 registered online participants, the conference showcased talks from 30 experts from academia, government laboratories, and industry.

Chaired by Prof. Bassam Dally and Prof. Gaetano Magnotti of the CCRC, the conference focused on three main themes.

EFFICIENT POWER GENERATION WITH INTEGRATED CARBON CAPTURE

Talks and discussions were held on innovative power cycles, including supercritical CO2, coupled with cost-effective strategies for carbon capture for carbon-neutral power generation and the transportation sector. Keynote talks were by Prof. Jon Gibbins, the University of Sheffield on the "Global Picture on Carbon Capture" and by Dr. Jeremy Fetvedt, Chief Engineer at 8 Rivers Capital on the "Allam Cycle".

COMBUSTION OF CARBON-FREE FUELS FOR POWERGENERATIONANDTRANSPORTATION

Fuels such as ammonia and hydrogen hold the promise of combustion-free of greenhouse emissions. Experts speakers discussed the key challenges in the production, delivery, and combustion of these carbon-free fuels, and proposed strategies to overcome existing barriers to the development of a hydrogen economy. Keynote talks were by Prof. Jenny Larfeldt, Chalmers University on the "Combustion of carbon-free fuels for power generation with Siemens Energy's industrial gas turbines" and by Trevor Brown, the Executive Director of the Ammonia Energy Association on the "Role of Ammonia to decarbonize transport and industry".

CONFERENCE REPORT: LOW CARBON THERMAL ENERGY FOR INDUSTRIAL APPLICATIONS

This topic focused on the development of low carbon thermal energy for use in the production of cement, iron/steel, and Alumina. Experts discussed the viability and options of decarbonization through electrification, renewable thermal energy, energy storage, and renewable fuels internationally and in KSA. Keynote talks were by Dr. Cédric Philibert, IFRI on the "International Trends in Decarbonizing Heavy Industry" and by Prof. Alan Weimer, the University of Colorado on "Two-step Solarthermal Water Splitting".

Visit the conference website for more information and recorded talks.

SAUDI ARABIAN SECTION OF THE COMBUSTION INSTITUTE

11th SASCI MEETING

October 12-13, 2021

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CLEAN COMBUSTION WINTER SCHOOL

13 February to 3 March 2022

- Exciting lectures on combustion physics, chemistry, and diagnostics
- 3-weeks research experience with state of the art facilities
- Small class of 10 of the best engineering students

Successful applicants will receive full funding for round-trip airfare, health insurance, on campus hotel accommodations, visa costs and associated expenses, and a stipend.

DEADLINE FOR REGISTRATION OCTOBER 30, 2021
Visit the website below for details.

www.ccws.kaust.edu.sa

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KAUST RESEARCH CONFERENCE

Hydrogen-Based Mobility and Power

February 7-10, 2022

Travel fellowships are back this year for students and postdoctoral researchers and will be awarded on the basis of merit.

SAVE THE DATE

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CCRC Tropical Thursdays

Did you know Thursdays are the end of the workweek in Saudi Arabia?

To celebrate the end of another productive week, the CCRC has "Tropical Thursdays" where people are encouraged to wear their brightest and most tropical clothes to work. We also have fun activities and refreshments set up for the day.

What do you do to celebrate the end of your work week?