2025 VA CECC SUMMIT INFORMATION

Quick Info

Date: May 20, 2025

Time: 9:30 am-3:50 pm (Check-in: 9:00 am – 9:30 am)

Summit Agenda

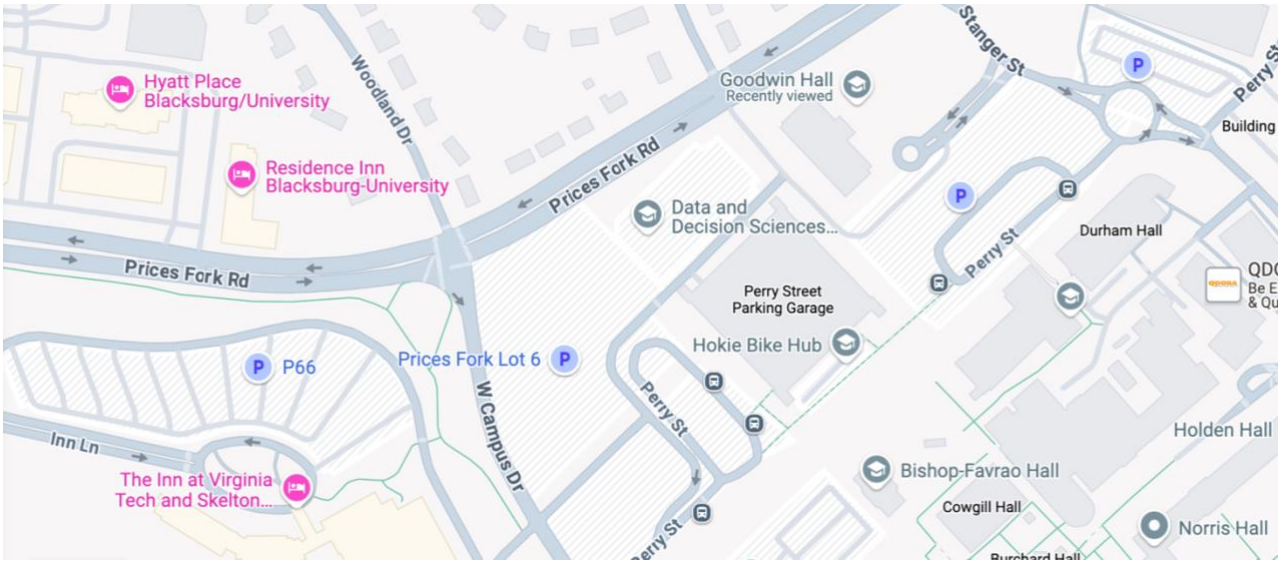
Morning Session (Goodwin 190)	
9:00am-9:30am	Check-in begins
9:30am-9:40am	Opening Remark | Steve McKnight, Vice President for Strategic Research Alliances, Virginia Tech
9:40am-10:40am	**Distinguished Lecturer | Johannes Lercher, Technische Universität München**
10:40am-11:05am	Sen Zhang, University of Virginia
11:05am-11:20am	Break
11:20am-11:45am	Jie Chen, Virginia Tech
11:45am-12:10pm	Samji Samira, Virginia Tech
12:10pm-2:10pm	**Lunch and Poster Session** (at Goodwin 125 and Goodwin Atrium)
Afternoon Session (Goodwin 190)	
2:10pm-3:10pm	**Distinguished Lecturer | Natalia Shustova, University of South Carolina**
3:10pm-3:40pm	Moumita Bhattacharya, RTI International
3:40pm-3:50pm	Closing remarks

Check-in and Day Information

Check-in will begin at 9:00am in the Atrium in Goodwin Hall at Virginia Tech. Poster session participants should hand off their posters at this time. After checking in, participants will be directed to the Goodwin 190, where the summit seminars will be held. At lunch time, the summit will move to Goodwin 125 for food, and later for networking at the poster session to be held in the Goodwin Atrium. After poster awards are selected, the summit will move back Goodwin 190 until 3:45pm, the scheduled end time of the event.

Parking 🅿

Parking Lot: Perry St Parking Garage beside Goodwin Hall
Parking can be paid using the app in the following link:
https://parking.vt.edu/parking/parkmobile.html



Addresses

Key Locations

- Goodwin Hall: 635 Prices Fork Rd, Blacksburg, VA 24061
- Perry Street Parking Garage: 1330 Perry St, Blacksburg, VA 24061

Nearby Hotels

- The Inn at Virginia Tech and Skelton Conference Center: 901 Prices Fork Road, Blacksburg, VA 24061
- Hyatt Place Blacksburg/University: 650 University City Boulevard, Blacksburg, VA 24061

Program

Distinguished Speakers

Johannes Lercher

Title: Catalysis for a future carbon-based industry

Abstract: The marked decentralization of power harvesting, the storage of the harvested power in fuels and chemicals and the implementation of carbon recycling are the key elements in the ongoing changes of power harvesting and energy storage. Catalysis will be the central element in this transition that will be characterized by a gradual evolution of today's petroleum and chemical processes and the necessity to develop conversion strategies that can be economically used at widely varying scale of implementation. Especially for decentralized concepts, novel principles, low reaction temperatures and the presence of water will be mandatory for safe and reliable operation.

Realizing such a radical change from centralized specialized industrial complexes requires a fundamental understanding of the underlying interactions and transformations between catalysts and substrates. In addition to the primary conversion of electric power to hydrogen, hydrogen addition and removal as well as carbon-carbon bond manipulation are the critical elementary steps to reach eventually a carbon-balanced chemical and energy industry.

For both acid-base and metal catalyzed reactions, the lecture will show the links between underlying physicochemical causes for the observed changes in catalytic rates. The impact of water and protic solvents on oxide materials leads to a complex reaction environment in which catalysis takes place at relatively high ionic strength. It will be shown that in the extreme case of ionic liquids, C-C bonds can be manipulated close to ambient temperature and that even macromolecules can be converted to small molecules. Together, the fundamental insight helps enabling new strategies to foster a sustainable future in chemical transformations.

Bio: Johannes Lercher studied Chemistry at the TU Wien, completing doctoral studies in 1980 and spent 1982 at Yale University. After a decade at TU Wien, he joined the University of Twente, Netherlands as Professor of Chemical Technology. Since 1998, he was Professor of Chemistry at the TU München (retired 2023), and between 2011 and 2025 also Director of the Institute of Integrated Catalysis at the Pacific Northwest National Laboratory. His research addresses fundamental aspects of catalysis lowering the carbon footprint via radically new approaches to synthesize energy carriers and intermediates. He was Editor-in-Chief of the Journal of Catalysis, President of the International Zeolite Association and the European Federation of Catalysis Societies. He is member of the Austrian Academy of Sciences, the US National Academy of Engineering, the German National Academy of Science and Engineering, the Spanish Academy of Science, the Academia Europaea, the European Academy of Sciences. His contributions to research have been recognized by awards such as the Michel Boudart Award of the North American Catalysis Society and the European Federation of Catalysis Societies, the Alwin Mittasch Prize of DECHEMA, and the ENI Award for Hydrocarbon Research.

Natalia Shustova

Title: MOF Reactivity

Abstract: Heterogeneous catalysts are widely used in the chemical and pharmaceutical industries due to their high efficiency, recyclability, and resistance to contaminants, all of which have a significant global economic impact annually. One strategy to achieve the mentioned benefits of heterogeneous catalysis with the convenience of homogeneous molecular systems is through coordinative and non-coordinative integration of the molecular catalysts within porous hosts. Metal-organic frameworks (MOFs) have gained attention in this area due to their modularity, versatile methods for introducing catalytic sites, and selective pore size capabilities. In our study, we explored several MOFs as both cargo vehicles and catalysts for the first time, employing aromatization, aminocarbonylation, and carbonylative Suzuki–Miyaura coupling as model reactions. These reactions highlight that MOFs can serve a dual role as a gas cargo vehicle and a catalyst, leading to product formation with yields similar to reactions employing pure gases. Furthermore, the MOFs can be recycled without sacrificing product yield, while simultaneously maintaining crystallinity. We employ the resonance energy transfer approach to assess its distribution within porous matrices using various encapsulation methods. Thus, the reported findings were also supported crystallographically and spectroscopically (e.g., diffuse reflectance infrared Fourier transform spectroscopy), foreshadowing a pathway for the development of multifunctional MOF-based reagent-catalyst cargo vessels for reactive gas reagents as an attractive alternative to the use of toxic pure gases or gas generators.

Bio: Natalia B. Shustova is a Fred M. Weissman Palmetto Professor at the Department of the University of South Carolina (USC). She holds Ph.D. degrees in Physical Chemistry and Inorganic Chemistry and completed her postdoctoral training at the Massachusetts Institute of Technology. Dr. Currently, she serves as an Associate Editor at ACS Materials Letters, following her term as an Associate Editor of Materials Chemistry Frontiers. Dr. Shustova is a recipient of international and national awards, including the Friedrich Wilhelm Bessel Research Award from the Humboldt Foundation, IAS Hans Fischer Fellowship, the National Science Foundation Career Award, the Cottrell Scholar Award, the Alfred P. Sloan Research Award, the Breakthrough Award, the McCausland Fellowship, Breakthrough Award, and Camille Dreyfus Teaching-Scholar Award. Dr. Shustova was named a Scialog Fellow of the Research Corporation for Science Advancement (RSCA), which accelerates 21st-century transformational science through research, dialog, and community outreach. She also serves on the RSCA Selection Committee, which assesses the research and educational performance of Assistant Professors across institutions in the USA, selecting the next generation of candidates for the Cottrell Scholar Award. She is a member of the executive committee for the Arnold and Mabel Beckman Foundation and also serves as a Chair on the International MOF Committee, comprising 14 scientists from eight countries. Her current research interests include graphitic hybrid materials for sustainable energy conversion, the chemistry of *f*-block elements, stimuli-responsive materials, sensors, and gas-phase heterogeneous catalysts.

Invited Speakers

Sen Zhang

Title: Well-Defined Nanocrystal Surfaces and Interfaces for Heterogeneous Catalysis

Abstract: Crucial to sustainable energy future is the ability to manipulate important chemical reactions for the production and conversion of hydrogen and renewable carbon-based chemicals through the development of advanced catalysts. Well-defined nanocrystals with atomically precise surfaces and interfaces allow us to bridge the knowledge gap between conventional single-crystal bulk materials and powder catalysts to achieve a new and in-depth understanding of structure-catalytic property relationships. In this talk, I will first highlight how the surfaces and interfaces of nano- and sub-nano catalysts can be precisely controlled at the atomic level to optimize catalytic performance in the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), both of which are integral to water electrolyzers. I will also report how constructing core/shell heterostructured and multi-interface nanocrystals can enhance the oxidation of biorenewable ethanol. The integration of controlled synthesis of nanocrystals, in-situ structural/catalytic characterization, and advanced theoretical calculation for electrocatalyst optimization will be discussed, which will also be extended to thermocatalytic processes (e.g., CO2 hydrogenation).

Bio: Sen Zhang is currently an Associate Professor of Chemistry and Materials Science and Chemistry, and Commonwealth of Virginia Eminent Researcher at the University of Virginia. He received his B.Sc. in polymer science and engineering from the University of Science and Technology of China in 2008 and his Ph.D. in inorganic chemistry from Brown University in 2013. Prior to joining the University of Virginia, he was a NatureNet postdoctoral fellow at the University of Pennsylvania from 2013 to 2016. His research interests are in nanomaterials controlled synthesis, assembly, and catalysis for reactions involved in energy and environmental applications, such as fuel cells reactions, water splitting, CO_2-to-fuel conversion and biomass conversion. He has received Sloan Research Fellowship (2022), NSF CAREER award (2022), Scialog Collaborative Innovation Award (2021), Chinese-American Chemistry & Chemical Biology Professors Association (CAPA) Distinguished Junior Faculty Award (2021), and University of Virginia Research Excellence Award (2021).

Jie Chen

Title: Physics-based Uncertainty-aware Data-driven Analysis and Design

Abstract: The advancement of science and technology has come to the data era, with Machine Learning (ML) exerting a profound influence. A gap exists in harnessing advanced machine learning for addressing complex engineering analysis and design challenges, primarily because many of these approaches have been developed in isolation from engineering analysis and design practices. Also, knowledge accumulated in engineering needs deeper integration with data science. This talk is two-fold: first, it involves incorporating domain expertise from science and engineering into the development of ML algorithms (*Physics for ML*). Second, it applies ML techniques to solve intricate problems in science and engineering (*ML for Physics*). Moreover, this talk discusses quantifying and utilizing uncertainties in engineering analysis and design. Data-driven methods provide a powerful aid to describe and understand uncertainties. Among all the data-driven methods, this talk focuses on physics-based and multi-fidelity machine learning for analysis and design under uncertainties. The main engineering field on which this talk focuses is mechanical properties of materials and structures including additive manufacturing, and high-throughput materials data analysis and discovery.

Bio: Dr. Jie Chen is an Assistant Professor in Mechanical Engineering at Virginia Tech. He was a Postdoctoral Fellow in Mechanical Engineering at Northwestern University (IDEAL Lab) after gaining PhD from Mechanical Engineering at Arizona State University (PARA Lab). His research focuses on physics-based uncertainty-aware data-driven analysis and design under uncertainty applied in advanced manufacturing, advanced materials systems, and fatigue & fracture.

Samji Samira

Title: Influence of visible photon flux on reactions of co-adsorbed CO and H on Pt surfaces

Abstract: Photoexcitation of small (<5 nm), adsorbate covered metal nanoparticles (NPs) has been shown to result in bond specific, wavelength dependent photochemical reaction pathways. Such processes have the potential enable access to excited state chemical transformations that are inaccessible by purely thermal processes. For instance, the use of 440 nm visible photon flux on sub 5 nm Pt NPs has been shown to enhance: (i) CO desorption kinetics [1], (ii) CO oxidation kinetics [2], and (iii) methanol decomposition to CO and H_2 [3]. In these examples, the primary effect of the visible photon flux has been ascribed to driving CO desorption from the surface, with minimal effects from co-adsorbates.

Herein, we investigate the influence of visible photon flux on the kinetics of reactions between co-adsorbed CO* and H* on 1.5±0.3 nm Pt NPs via *in situ* FITR spectroscopy and detailed kinetic studies. Visible photon fluxes promote the rate of methane formation during reactions between co-adsorbed CO and H with maximum rate enhancement observed for 440 nm illumination, consistent with the direct photoexcitation of Pt–CO bonds [1-3]. Measurements of apparent activation barriers, reaction orders, and KIE indicate that the 440 nm photon flux promote the rate of CO desorption thereby increasing the rate of the competitive H_2 adsorption and thus the overall rate of methane formation [4]. Further, degree of rate control analysis suggests that the visible photon flux also increases the rate of the rate controlling step of CO* hydrogenation. These studies demonstrate that photons channel new reaction pathways and coverages, that are distinct and cannot be purely accessed by thermal routes.

References:

[1] Alvarez, I. B., Le, T., Hosseini, H., Samira, S., Beck, A., Marlowe, J., Montemore, M. M., Wang, B., Christopher, P. *J. Am. Chem. Soc.* **2020,** *146,* 12431-12443.
[2] Kale, M. J., Avanesian, T., Xin, H., Yan, J., Christopher, P. *Nano Lett.* **2014,** 14, 5405-5412.
[3] Qi, J., Resasco, J., Robtajazi, H., Alvarez, I. B., Abdelrahman, O., Dauenhauer, P., Christopher, P. *ACS Energy Lett.* **2020**, *5* 3518-3525.
[4] Samira, S., Marino, S., Jalil, A., Gordon, M., Christopher, P. (2025) *In preparation*

Bio: Samji Samira is an Assistant Professor in the Department of Chemical Engineering at Virginia Tech. Samji's research interests include: (i) design of electrocatalytic active site environments via precise engineering of the electrode-electrolyte interfaces, and (ii) development of manipulatable materials which can serve as both light harvesters, as well as active centers. Prior to joining Virginia Tech, Samji was a Postdoctoral Scholar at the Department of Chemical Engineering, University of California, Santa Barbara. Samji earned his Ph.D. in Chemical Engineering from Wayne State University. His previous research has been recognized with various awards including the Ralph H. Kummler Award for distinguished achievement in graduate student research, Young Scientist Presenter Award from the International Congress on Catalysis and Kokes award from the North American Catalysis Society.

Moumita Bhattacharya

Title: Development of Novel Non-aqueous Carbon Capture Solvents: From Lab to Commercial Scale

Abstract: Dr. Moumita Bhattacharya will present on the development of RTI International's novel non-aqueous solvents for carbon capture, with a particular focus on advancing the technology from the lab scale toward commercial deployment. In addition to discussing the technical aspects and progress of this innovative work, Dr. Bhattacharya will briefly share her professional journey and the key insights she has gained throughout her career in carbon capture and conversion research.

Bio: Dr. Moumita Bhattacharya received her bachelor's and master's degrees in chemistry from Jadavpur University in India. She later moved to the United States for her graduate studies, initially working on C–H functionalization under the mentorship of Dr. Sid Das at Utah State University. She then joined Dr. Caroline Sauma's lab at the University of Utah, where her research focused on the role of amines in integrated carbon dioxide capture and its photo- and electrochemical conversion to alternative fuels. After earning her Ph.D. from the University of Utah, Dr. Bhattacharya joined XploSafe LLC., a spin-off from Oklahoma State University. There, she contributed to several NASA- and DoD-funded projects by developing and optimizing solid sorbents for the mitigation of toxic volatile organic compounds (VOCs). She was also actively involved in the development of Small Business Innovation Research (SBIR) grant proposals and engaged regularly with project stakeholders. Following her time in Oklahoma, Dr. Bhattacharya moved to the Research Triangle Institute in North Carolina, where she resumed her work in carbon capture and conversion. Her current research centers on lab- and pilot-scale CO_2 capture technologies, with a focus on exploring carbon conversion pathways that utilize commercially available amines.

Posters

Poster #	Poster Title	Presenting Author
1	Investigation and Development of p—block Catalysts for Electrocatalytic Carbon—Nitrogen Coupling	Parker Ballard-Kyle
2	Methane Activation on Mo-Fe/ZSM-5: Insights into Bimetallic Active Sites and Deactivation Mechanisms for Aromatization	Md Sifat Hossain
3	Elucidating a Solid-Molecular Mechanism of Oxygen Evolution in NiFe (Oxy)hydroxides	Liping Liu
4	Interpretable Deep Learning for Predicting Electronic Descriptors	Shih-Han Wang
5	Aminophenol Ligated Mn for Transfer and Electrocatalytic Hydrogenations	Sayantani Saha
6	Sustainable Acetylene Removal from Ethylene via Electrified Semi-Hydrogenation in Flow Reactors	Libang Xu
7	Elucidating structural evolution of CuNi catalysts in CO2 reduction and its enhanced C2+ products selectivity	Wenjin Sun
8	Structure-Sensitivity of CO Oxidation over Supported Pt Catalysts in the Subnanometer Regime and Its Origin	Md Raian Yousuf
9	Tuning Catalytic Reactivity via Spin Crossover: Design and Study of Mn Complexes with Tailored Ligands	Sreenivasulu Chinnabattigalla
10	Functionalizing Ru-UiO-67 to Incorporate Charge Transport Groups for Water Oxidation	Sumanta Basak
11	Explorations of high-spin and low-spin transition metals in long-lived charge separated states	Tzu Ching Cheng
12	Probabilistic Machine Learning for Uncertainty Quantification in Materials Science and Beyond	Jun Li
13	Insights into metal speciation, distribution and activation of Mo-modified zeolites for methane aromatization	Emanuele Joy
14	Ni-Based Perovskites for Clean Hydrogen Production and Carbon Nanotube Formation.	Silvanus Junior Darkey
15	Unraveling Particle Size and Electronic Effects in C_2H_2 and C_2H_4 Hydrogenation over Ceria-Supported Platinum	Sara Haidar
16	Improving Charge Transfer in Zirconium MOF Films for Electrochemical Water Oxidation	Claudio Amaya-Santos
17	Controlled Synthesis of Co2P-Pt Heterostructure Nanocrystals for the Alkaline Hydrogen Evolution Reaction	Daniel Musikanth
18	Production of a Sustainable Biomass-Derived Monomer using Porous-Organic Frameworks	Emma Blanco
19	Elucidating a Solid-Molecular Mechanism of Oxygen Evolution in NiFe (Oxy)hydroxides	Liping Liu
20	Automated Synthesis Procedure Generation in Heterogeneous Catalysis Via Fine-Tuned Large Language Model	Raul Bernardo Diaz Aquino
21	Unveiling the Interplay of Electronic and Phononic Excitations in Laser-Induced Catalytic Processes	Xiangrui Wang
22	Theory-infused neural network for interpretable reactivity prediction	Shih-Han Wang