2023 VA CECC SUMMIT INFORMATION

Quick Info

Date: August 7, 2023

Time: 9:00 am-5:00 pm (Check-in: 8:30 am – 9:00 am)

Summit Agenda

Morning Session (VCU ERB1313)	
8:30am-9:00am	Check-in begins
9:00am-9:10am	Opening Remark | P. Srirama Rao, VCU Vice President for Research and Innovation
9:10am-9:40am	Katharine Tibbetts, Virginia Commonwealth University
9:40am-10:10am	Pei Dong, George Mason University
10:10am-10:20am	Break
10:20am-10:50am	Jason Bates, University of Virginia
10:50am-11:50am	**Distinguished Lecturer | Susannah Scott, UC Santa Barbara**
11:50am-1:50pm	Lunch and Poster Session (at VCU ERB Collaboration Hub)
Afternoon Session (VCU ERB1313)	
1:50pm-2:50pm	**Distinguished Lecturer | Carsten Sievers, Georgia Tech**
2:50pm-3:20pm	Hongliang Xin, Virginia Tech
3:20pm-3:50pm	Puru Jena, Virginia Commonwealth University
3:50pm-4:00pm	Break
4:00pm-4:30pm	Chelsea Jenkins, Deputy Secretary of Commerce and Trade, Virginia
4:30pm-5:00pm	Bruce Vlk, Electric Vehicle Program Manager and Communications Director at Virginia Clean Cities

Check-in and Day Information

Check-in will begin at 8:30am at the collaboration hub of the engineering research building (ERB) at VCU. Poster session participants should hand off their posters at this time. After checking in, participants will be directed to the multipurpose room ERB1313, where the summit seminars will be held. At lunch time, the summit will move to the collaboration hub for food and networking at the poster session. After poster awards are selected, the summit will move back to the ERB1313 until 5:30pm, the scheduled end time of the event.

Parking

JL Parking Lot, 200 W Cary St

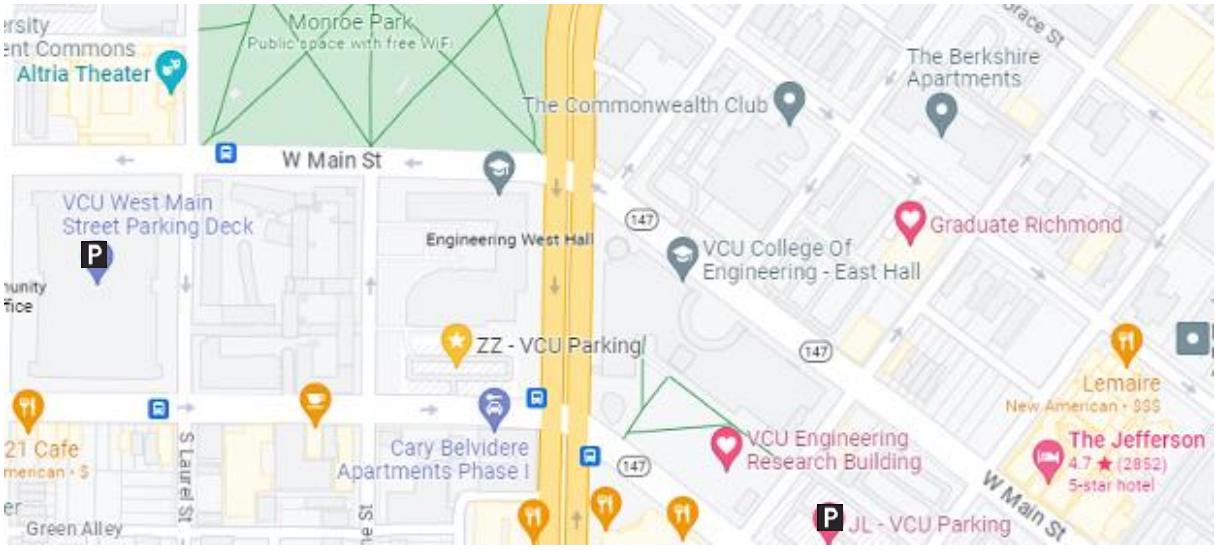
About 🅿

Pay-by-space meters are available 7 days a week at the JL Parking Lot. Rates are $2 per hour for the first hour, $4 for two hours and $2 per hour for each additional hour for a maximum daily rate of $16 per day.

West Main Street Parking Deck, 801 W Main St

About 🅿

Parking costs: $2 for the first hour, $4 for two hours and $2 per hour for each additional hour for a maximum rate of $16 per day. Credit cards, debit cards and cash are accepted.



Addresses

Key Locations

1. VCU Engineering Research Building: 401 W Cary St, Richmond, VA 23284
2. JL Parking Lot: 200 W Cary St, Richmond, VA 23284
3. West Main Street Parking Deck: 801 W Main St, Richmond, VA 23284

Nearby Hotels

4. Graduate Richmond: 301 W Franklin St, Richmond, VA 23220
5. The Jefferson Hotel: 101 W Franklin St, Richmond, VA 23220

Program

Distinguished Speakers

1. Susannah Scott

Title: Imagining a chemical industry based on renewable and recycled carbon

Abstract: The widespread adoption of renewable chemical feedstocks and the transition to circular carbon is likely to require a major transition away from catalytic processing of volatile hydrocarbons towards condensed phase reactions of non-volatile biomass and post-consumer plastics. Adapting heterogeneous catalysts optimized for converting fossil-fuel-derived hydrocarbons to upgrade renewable and recycled carbon is a major challenge, due to vast differences in volatility and solubility. Solvent effects arising from covalent and non-covalent interactions alter behaviours at solid surfaces and in porous catalytic materials, where interactions are strongly influenced by partitioning of molecules between the bulk liquid phase and the surface or pore volume. Nanoscale structuring of solvent molecules near these surfaces alters mobility and promotes or prevents adsorption of reactive molecules near active sites. This lecture will describe effects at the molecular level by probing the molecular composition at the solid-liquid interface, while simultaneously observing the kinetics of catalytic reactions that transform energy-rich carbon-based molecules.

Bio: Susannah Scott is a Distinguished Professor in both Chemical Engineering and in Chemistry & Biochemistry at the University of California, Santa Barbara. She received her Ph.D. in Inorganic Chemistry from Iowa State University, under the direction of Jim Espenson and Andreja Bakac, for her work on the activation of O_2 and transition metal-catalyzed oxidation mechanisms. She was awarded a NATO Postdoctoral Fellowship for work with Jean-Marie Basset at the Institut de recherches sur la catalyse (CNRS) in Lyon, France. In 1994, she joined the faculty of the University of Ottawa (Canada), where she was named a Canada Research Chair. In 2003, she moved to the University of California, Santa Barbara, where she currently holds the Duncan and Suzanne Mellichamp Chair in Sustainable Catalysis and is Chair of the Santa Barbara Division of the University of California's Academic Senate. She is an Executive Editor for ACS Catalysis, and a member of the Board of Reviewing Editors for Science. Her research interests include the design of heterogeneous catalysts with well-defined active sites for the conversion of conventional and unconventional carbon-based feedstocks, as well as environmental catalysts to promote air and water quality.

2. Carsten Sievers

Title: Fundamentals and Applications of Mechanocatalytic Processes

Abstract: Mechanochemical processes use mechanical collisions in a ball mill or similar device to drive chemical reactions. The collisions can create transient surface sites with extraordinary catalytic activity and hot spots that are characterized by rapid local temperature rises followed by dissipation of heat to the environment. In addition, mechanical forces can create intimate contact between two solids, so that the conversion of a solid reactant over a solid catalysts becomes viable. The formation of hot spots is analyzed in a fundamental study of the conversion of $CaCO_3$ to CaO. Based on models for the impact of the milling ball and heat dissipation, each collision can be modeled as a transient batch reactor. The rates of CO_2 formation in a flow-through milling vessels are determined at different milling frequencies to validate the model. The impact of a 20 mm steel ball with a net velocity of 4.5 m/s results in a hot spot temperature of above 800 °C. These dynamic environments can be used for ammonia synthesis from the elements. During milling in a mixture of N_2 and H_2, titanium metal is converted into TiN. Additional collisions lead to the formation of reactive nitride species. During the decay of the hot spot, the system passes through a regime in which hydrogenation of reactive nitrides to ammonia is thermodynamically and kinetically feasible. The ability to convert solid feedstock opens new possibilities for converting lignin and waste plastics. For example, the depolymerization of poly(ethylene terephthalate) (PET) occurs readily when the polymer is milled with NaOH. After an initial period, in which monomers are produced at a constant rate, the reaction mixture is converted into a wax that coats the milling balls or is pressed into the sites of the milling vessel. After wax formation, the remaining polymers are converted much faster. The reaction kinetics are explained with a modified shrinking core model. For depolymerization of poly(ethylene), we demonstrate a process, in which the polymer is partially oxidized in random positions of the backbone to facilitate cleavage of C-C bonds.

Bio: Carsten Sievers obtained his Diplom and Dr. rer nat. degrees in Technical Chemistry at the Technical University of Munich, Germany. Under the guidance of Prof. Johannes A. Lercher, he worked on heterogeneous catalysts for various petrochemical processes. In 2007, he moved to the Georgia Institute of Technology to work with Profs. Christopher W. Jones and Pradeep K. Agrawal as a postdoctoral fellow. His primary focus was the development of catalytic processes for biomass depolymerization and synthesis of biofuels. He joined the faculty at the Georgia Institute of Technology in 2009. His research group is developing catalytic processes for the sustainable production of fuels and chemicals. Specific interests are catalyst deactivation and regeneration, mechanocatalysis, plastics upcycling, catalytic processes in aqueous phase, surface chemistry of complex molecules, production of value-added chemicals from biomass, operando spectroscopy, and CO_2 capture and conversion. He published over 100 peer-reviewed papers. He is Director of the Southeastern Catalysis Society and Editor of Applied Catalysis A: General.

Invited Speakers

1. Katharine Tibbetts

Title: Laser synthesis of transition metal composite nanomaterials as catalysts for energy conversion

Abstract: Catalysts containing first-row transition metals are widely sought for applications in energy conversion due to the high abundance and low cost of metals such as Fe, Ni, Cu, and Zn. Laser synthesis methods have emerged in the last decade as promising routes to myriad transition metal-based catalysts that can outperform similar materials synthesized with traditional wet-chemical methods. Laser-induced decomposition of transition metal complexes in solution initiates the self-assembly of complex nanostructures in a single step without added chemical reducing agents or surfactants, thereby generating little chemical waste and satisfying "green chemistry" principles. This presentation will highlight recent advances in my group towards the controlled laser synthesis of two classes of transition metal nanocomposites: copper-based phyllosilicate nanosheets and nickel dispersed on porous carbon. Manipulation of the laser conditions and adding promotor complexes such as zinc nitrate to copper nitrate precursor solution enables extensive control over the amount of Cu_2O present in laser-synthesized copper phyllosilicate nanosheets, which enhances their catalytic activity towards reduction of CO_2 to CO and methanol. Low-density plasma formed by loosely focusing femtosecond laser pulses into a solution of nickelocene forms well-dispersed nickel species supported on porous carbon that exhibit high activity towards the electrochemical Oxygen Reduction Reaction (ORR) for applications in fuel cells and Zn-air batteries.

Bio: Katharine Moore Tibbetts is an Associate Professor of Chemistry at Virginia Commonwealth University. She received an AB in Chemistry from Princeton University in 2005, where she received a Fulbright fellowship to study in Germany following graduation. She returned to Princeton for doctoral studies in 2006, where she received a NSF Graduate Research Fellowship. She obtained her Ph.D. in Chemistry in 2012 under the direction of Prof. Herschel Rabitz and worked as a postdoctoral researcher at Temple University under the direction of Prof. Robert Levis from 2012-2015. Since coming to VCU in 2015, she was the recipient of the Presidential Early Career Award in Science and Engineering in 2019 and the VCU Outstanding Early Career Faculty Award in 2020. Her current research interests focus on two areas: (1) ultrafast dynamics organic cations with a focus on energetic and biologically relevant molecules, and (2) laser synthesis of nanomaterials for catalysis and energy conversion applications. Webpage link: https://chemistry.vcu.edu/people/faculty/tibbetts.html

2. Pei Dong

Title: TBA

Abstract: TBA

Bio: TBA

3. Jason Bates

Title: Quantification of Catalytically Relevant Fe Species in Nitrogen-Doped Carbon

Abstract: Heterogeneous catalysts consisting of iron cations incorporated into nitrogen-doped carbon ("Fe-N-C") have received extensive attention as leading alternatives to Pt for the electrochemical oxygen reduction reaction (ORR), and additionally catalyze the thermal oxidation of organic molecules with O_2 as the oxidant. Fe-N-C catalysts host mononuclear nitrogen-ligated active centers, FeN_x, that frequently coexist with agglomerated Fe species. Although FeN_x are the dominant active centers for ORR electrocatalysis and many aerobic oxidations, the accuracies of methods to quantify them are still debated. Here, we develop a kinetic probe-reaction approach to quantify FeN_x centers and compare it with spectroscopic and probe-molecular methods. Model Fe-N-C catalysts were synthesized to contain mononuclear FeN_x species at low loadings (0.1–0.4 wt% bulk Fe) on solvent-accessible surfaces using a postsynthetic metalation approach and their Fe speciation was confirmed by low-temperature ^{57}Fe Mössbauer spectroscopy. The initial rate of oxidation of a water-soluble hydroquinone molecule (per $g_{catalyst}$) catalyzed by these model materials correlates linearly with their density of FeN_x centers, reflecting their intrinsic turnover frequency (TOF) for this reaction. This TOF, in turn, enables the estimation of the active-site density on any other Fe-N-C catalyst through a simple rate measurement. Kinetically determined FeN_x site densities are measured on a suite of fourteen Fe-N-C catalysts with diverse synthetic origins and Fe speciation (0.3–8.4 wt% bulk Fe) and are compared with those estimated by low-temperature ^{57}Fe Mössbauer spectroscopy, CO pulse chemisorption, and electrochemical stripping of NO derived from NO_2^-. Kinetic quantifications of FeN_x centers correlate well with those obtained from the CO pulse chemisorption method and Mössbauer spectroscopy. The broad survey of Fe-N-C materials also reveals the presence of outliers and challenges associated with each site quantification method. The kinetic method developed here does not require pretreatments that may alter active-site distributions nor specialized equipment beyond reaction vessels and analytical instrumentation (e.g., NMR), offering an attractive complementary approach.

Bio: Jason Bates received his B.S. in Chemical Engineering at the University of Kansas in 2014 and a Ph.D. in Chemical Engineering at Purdue University in 2019. After a postdoctoral stay in the Department of Chemistry at the University of Wisconsin–Madison, he began his independent career at the University of Virginia in August of 2023. His research explores the fundamentals of heterogeneous thermal and electrocatalysis in areas relevant to decarbonization of the energy and chemical industries.

4. Hongliang Xin

Title: Machine Learning for Catalytic Materials Design toward Sustainability

Abstract: Finding catalytic materials with optimal properties for sustainable chemical and energy transformations is one of the pressing challenges faced by our society today. Traditionally, the discovery of catalysts or the philosopher's stone of alchemists relies on a trial-and-error approach with physicochemical intuition. Decades-long advances in science and engineering, particularly in quantum chemistry and computing infrastructures, popularize a paradigm of computational science for materials discovery. However, the brute-force search through a vast chemical space is hampered by its formidable cost. In recent years, machine learning (ML) has emerged as a promising approach to streamline the design of active sites by learning from data. In this talk, we present an interpretable ML framework for accelerating catalytic materials design, particularly in driving a sustainable nitrogen cycle. We will discuss existing challenges and opportunities of ML in predicting catalytic materials, and more importantly, on advancing catalysis theory beyond conventional wisdom. We envision future directions in developing highly accurate, easily explainable, and trustworthy ML strategies, facilitating the maturation of the data science paradigm for sustainability through catalysis.

Bio: Hongliang Xin is an Associate Professor of Chemical Engineering at Virginia Polytechnic Institute and State University. He received his Ph.D. in Chemical Engineering from the University of Michigan in 2011. Dr. Xin joined the ChE faculty in August 2014 after postdoc at Stanford/SLAC. At Virginia Tech, his research focus is the development of an interpretable machine learning framework for tackling problems in fundamental surface science and catalysis. He received the recognition from the Journal of Materials Chemistry A as one of the 2017 Emerging Investigators. He received the Dean's award for Outstanding New Assistant Professor in 2018 and Engineering Faculty Fellow in 2019. He is one of the 2019 Class Influential Researchers from ACS Industrial & Engineering Chemistry Research. He is the recipient of the prestigious NSF CAREER Award (2019).

5. Puru Jena

Title: Catalytic Potential of Borane-based Clusters

Abstract: Boron, due to its electron deficient character, forms unusual structures and bonds. Predicted in 1955 and synthesized five years later, dodecaborate anion, $B_{12}H_{12}^{2-}$, is such an example where the B atoms occupy the vertices of an icosahedron with radially bonded hydrogen. Of the four electrons in a BH pair, two are involved in a covalent bond between B and H while the other two are contributed to the cage bonding. Wade's theory provided the first understanding of the stability of $B_{12}H_{12}^{2-}$ in terms of skeletal electron pairs where (n+1) pairs of electrons are needed to stabilize the dodecaborate anion, n being the number of B atoms. The rich chemistry of this class of clusters has been exploited by replacing H with other ligands such as halogens and superhalogens as well as by replacing B atoms with C and Be. The potential of this class of clusters in hydrogen storage, electrolytes in metal-ion batteries, and promoting unusual reactions has been explored. While dianions of the size of $B_{12}H_{12}^{2-}$ are usually unstable in the gas phase due to electron-electron repulsion, the unusual stability of these species particularly when H atoms are replaced by CN moieties has led to the discovery of highly reactive species. For example, when one of the ligands in $B_{12}(CN)_{12}^{2-}$ is detached, the naked B in the resulting $B_{12}(CN)_{11}^{-}$ becomes super-electrophilic and binds to noble gas atom, Ar, at room temperature. The present talk will discuss the potential of dodecaborates and their derivatives in activating molecules such as H_2, CO_2, N_2, CO, and H_2O. In addition, I will discuss the interesting chemistry of $B_{12}X_{11}^{2-}$ (X=F, Cl, Br, I, CN) dianions that defy the Wade's rule and has greater potential in activating CO_2 and N_2. Time permitting, I will introduce the concept of single superatom catalysis versus single atom catalysis.

Bio: Puru Jena, Distinguished Professor of Physics and Founding Director of the Institute of Sustainable Energy and Environment at Virginia Commonwealth University (VCU) received his Ph. D. in Physics from the University of California in 1970. After postdoctoral and visiting appointments at Dalhousie University, University of British Columbia, Northwestern University, and Argonne National Laboratory, he joined Michigan Technological University as an Associate Professor of Physics in 1978. He moved to VCU in 1980 where he has remained ever since, except for a year (1986-87) at the National Science Foundation as a Program Director and a year (2007-08) at the US Department of State as Jefferson Science Fellow and Senior Science Adviser. Author of more than 650 papers and 14 edited books, Prof. Jena works at the interface of Physics, Chemistry, and Materials Science. He has given over 550 invited lectures at international conferences and institutions in 34 countries and 6 continents. His Google Scholar citations and H-index stand at 34,500 and 92, respectively. His many honors include Member of the National Academy of Inventors, Prof. A. K. Chandra Memorial Award of the Indian Chemical Society, Outstanding Scientist of Virginia and Outstanding Faculty of Virginia awarded by the Governor of Virginia, Presidential Medallion, Outstanding Scholar and University Award of Excellence from VCU, and David Hare Professorship Lecture. He has served on scientific panels at the National Science Foundation, Department of Energy, National Academy of Science, Virginia Governor's Task Force on Renewable Energy and Presidential Commission on Nanoscience and Energy between Russia and USA.

6. Chelsea Jenkins

Title: TBA

Abstract: TBA

Bio: TBA

7. Bruce Vlk

Title: Electrification and Alternative Fuels: Federal Policy Implementation in Virginia

Abstract: Clean Cities organizations are spread throughout the United States and are funded by the U.S. Department of Energy in accordance with the Energy Policy Act of 1992. Virginia Clean Cities is based at James Madison University where it advances air quality improvement, economic opportunity, and energy security through deployment of alternative fuel vehicles and infrastructure, education programs and other petroleum reduction activities. Program Manager Bruce Vlk will discuss their work in alternative fuels, electric vehicles, and other advancements in transportation technology. VCC's work engages all levels of government, private industry, academia, and the nonprofit sector.

Bio: Bruce Vlk (pronounced VELK) is Program Manager and Communications Director at JMU's Virginia Clean Cities. He spent 13 years at the University of Virginia in a variety of administrative leadership roles. Prior to this experience, he worked in Virginia state government, and currently serves as an appointed member of the Virginia Land Conservation Foundation board of trustees. He has published articles in the subjects of history and public administration. He serves as a vice president of the Czechoslovak Society of Arts and Sciences, an interdisciplinary academic association.