

## 2022 VA CECC SUMMIT INFORMATION

### Quick Info

Date: August 8, 2022

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

### Summit Agenda

Morning Session (at UVA Rotunda)	
8:30am-9:00am	Check-in begins
9:00am-9:10am	Opening Remark   Melur K. "Ram" Ramasubramanian (UVA VPR)
9:10am-9:45am	Ram Gupta, Virginia Commonwealth University*
9:45am-10:20am	Brent Gunnoe, University of Virginia*
10:20am-10:30am	Break
10:30am-11:05am	Amanda Morris, Virginia Tech*
11:05am-11:55am	<b>Distinguished Lecturer   Mahdi Abu-Omar, UC Santa Barbara*</b>
11:55am-2:00pm	<b>Lunch and Poster Session (at UVA Chemistry Department lobby)</b>
Afternoon Session (at UVA Rotunda)	
2:00pm-2:35pm	Chris Paolucci, University of Virginia*
2:35pm-3:20pm	Tutorial Seminar   Hua Zhou, Argonne National Lab*
3:20pm-4:00pm	Tutorial Seminar   Qian He, National University of Singapore*
4:00pm-4:10am	Break
4:10pm-5:00pm	<b>Distinguished Lecturer   Christophe Copéret, ETH Zürich*</b>
5:00pm-5:30pm	Conversation with Cell Press Editors (Stacey Chin, Matter; Michelle Muzzio, iScience)

\*Last 5-10 minutes allotted for Q&A

## Check-in and Day Information

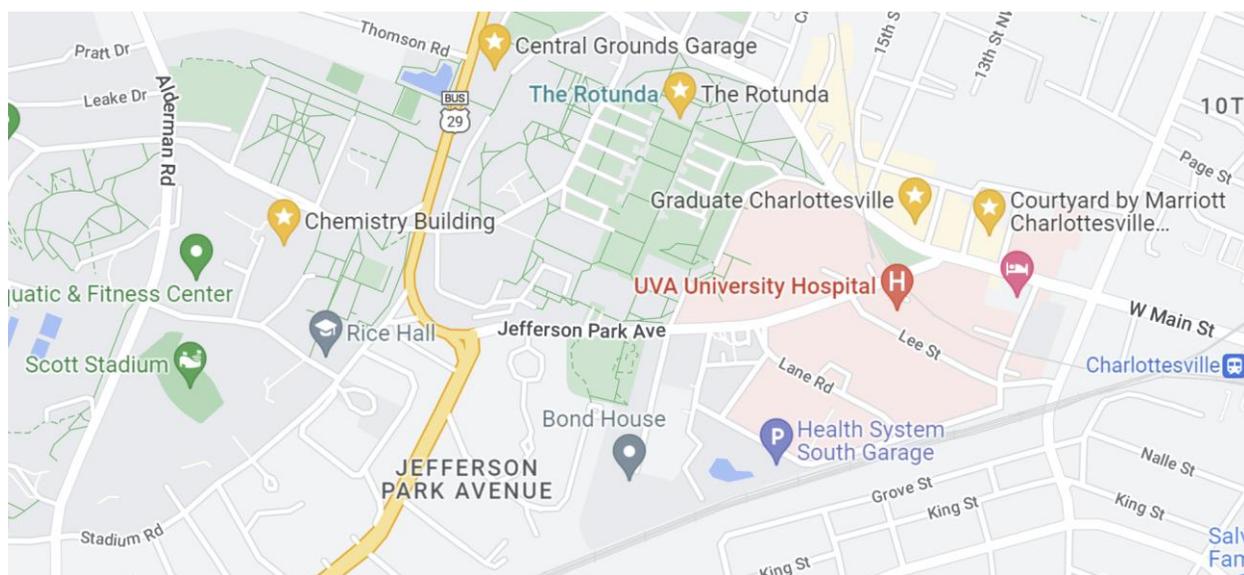
Check-in will begin at 8:30am at the main Rotunda entrance (facing the lawn). Poster session participants should hand off their posters at this time. After checking in, participants will be directed to the Rotunda Dome Room, where the summit seminars will be held. At lunch time, the summit will move to the Chemistry Building lobby for food and networking at the poster session. After poster awards are selected, the summit will move back to the Rotunda until 5:30pm, the scheduled end time of the event.

## Parking

The closest parking garage to the Rotunda is the Central Grounds Garage, located under the University Bookstore at 400 Emmet Street. Hourly parking may be paid via the [ParkMobile](#) app – ParkMobile charges a \$0.45 convenience fee per transaction, with hourly rates shown below.

Location	Time	Hourly Rate	Max Daily Rate
Central Grounds Garage	Monday through Saturday 7:30AM - 5:00PM	\$2.50	No Maximum
Central Grounds Garage	Monday through Saturday 5:00PM - 10:00PM	\$1.50	No Maximum

Overnight parking is not permitted. Visitors needing overnight parking accommodations may purchase a temporary BLUE permit to park in the lots at John Paul Jones Arena. Please contact the Parking and Transportation Office at [parking@virginia.edu](mailto:parking@virginia.edu) or by calling 434-924-7231 for more information. More information regarding hourly parking locations and payments can be found here: <https://parking.virginia.edu/parkmobile>.



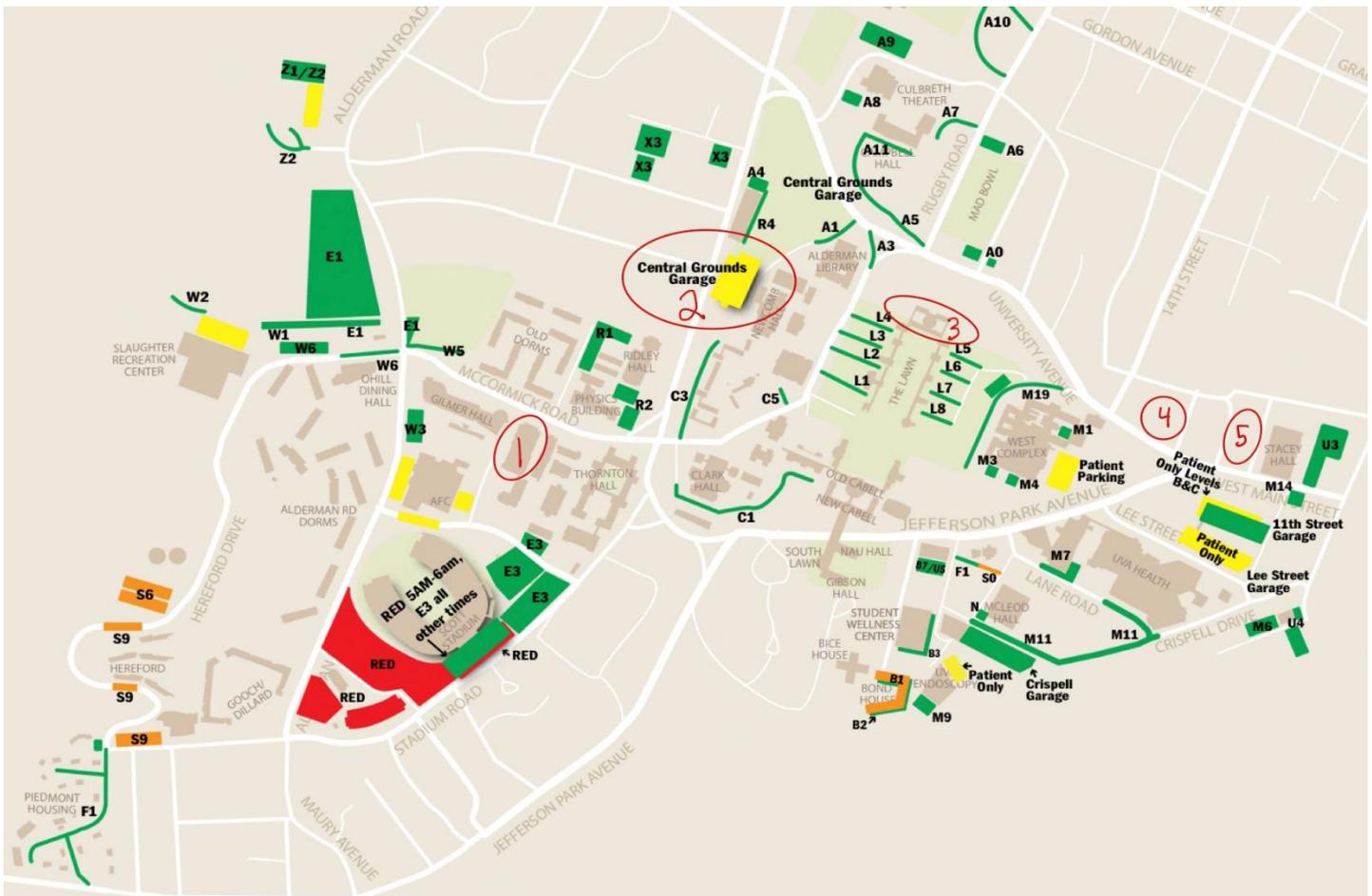
## Addresses

### Key Locations

1. Chemistry Building: 409 McCormick Rd, Charlottesville, VA 22904
2. Central Grounds Garage: 400 Emmet St S, Charlottesville, VA 22903
3. The Rotunda: 1826 University Ave, Charlottesville, VA 22904

### Nearby Hotels

4. Graduate Charlottesville: 1309 W Main St, Charlottesville, VA 22903
5. Courtyard by Marriott: 1201 W Main St, Charlottesville, VA 22903



# Program

### Distinguished Speakers

1. Mahdi M. Abu-Omar

**Title:** Catalysis for the circular economy: How to use nonconventional feedstocks from biomass to waste plastics

**Abstract:** Non-edible lignocellulosic biomass is the most abundant renewable carbon source on our planet. It offers an alternative and a complementary source to petrochemical refining for chemical production. However, utilization of biomass is underdeveloped. The biorefinery uses only the sugar components from biomass and lignin is a waste byproduct. Transition metal catalysts have been an integral part of the success story of the petrochemical industry in the 20th Century and will continue to play an important role in advancing green and sustainable chemistry into the 21st Century. Lignin conversion can improve the economics of biorefining by producing value-added products. Our research group has developed selective reaction chemistries that convert lignin into phenolic synthons while preserving all other components of the biomass. The renewable bio-phenols can be upgraded to polymers with advanced thermo-mechanical properties that rival those from petroleum. The implication and use of lignin synthons to make renewable and recyclable thermoset polymers will be discussed. A newly recognized emerging problem is the rise in plastics waste, more than 6 billion tons. Less than 7% of plastics is recycled. A better vision is to reclaim the carbon in waste plastics and upcycle it via catalysis to commodity chemicals. In this presentation, I will discuss the UCSB process for making biodegradable detergents from waste polyethylene using bifunctional catalysts.

**Bio:** Mahdi M. Abu-Omar is the Mellichamp Chair in Green Chemistry and Professor at the University of California, Santa Barbara (UCSB). His research accomplishments include selective conversion of biomass lignin to biophenols and the creation of renewable plastics based on lignin. He has authored/co-authored 200 original research articles in peer-reviewed scientific journals, mentored more than 50 Ph.D. and postdoctoral students, and held faculty appointments at Purdue University and UCLA. Mahdi is the Founder of Spero Renewables, a clean tech company that provides cost-effective and renewable substitutes to petrochemicals ([sperorenewables.com/](http://sperorenewables.com/)). He is the recipient of the American Chemical Society (ACS) Affordable Green Chemistry Award in 2022. Mahdi was elected Fellow of the American Association for Advancement of Science (AAAS) in 2012 and was a Senior Fulbright Fellow in 2008. Dr. Abu-Omar completed a Ph.D. from Iowa State University (1996) and a postdoc from Caltech.

### 2. Christophe Copéret

**Title:** Bridging the gap between well-defined and industrial catalysts via a molecular approach

**Abstract:** Industrial processes, in particular large-scale ones, mostly rely on heterogeneous catalysts. The search for more sustainable processes and the changes in environmental policies impose the continuous development of improved catalyst performances and catalytic processes, as well as the exploration of alternative routes. However, due to their inherent complexity, heterogeneous catalysts are mostly developed empirically rather than through detailed structure – activity relationships as the nature of the active sites are rarely known.

In this context, our group has been interested in understanding and controlling chemistry on surfaces, with the ultimate goal to generate isolated metal sites with defined chemical environment. <sup>1</sup> This approach has been used to develop highly active and selective single-site catalysts that can overperformed their homogeneous counterparts, but it can also provide useful information to understand and further develop industrial catalysts <sup>2</sup> or to study much more complex systems such as supported nanoparticles, where support effects, interfaces, alloying... remain complex to understand at the molecular level.

This lecture will be developed around these themes and will show that a careful characterization of surface sites on a molecular level is key to develop high performance catalysts and to bridge the gap between fundamental and applied catalysis.

**Bio:** Prof. Christophe Copéret (CCH) was trained in chemistry and chemical engineering at CPE Lyon, France, and carried out a PhD in chemistry with Prof. E.i. Negishi (Purdue University, USA – 1991-1996), where he investigated the synthesis of complex molecules via Pd-catalyzed carbonylation reactions. After a postdoctoral stay with Prof. K.B. Sharpless (Scripps), CCH was offered a research position at CNRS in 1998 and was promoted CNRS Research Director in 2008. Since 2010, CCH is Professor in the Department of Chemistry and Applied Biosciences, ETH Zürich. His scientific interest lies at the frontiers of molecular, material and surface chemistry as well as NMR spectroscopy with the aims to design molecularly-defined solid catalysts through detailed mechanistic studies and structure-activity relationships. CCH is a member of the Board of the Swiss Chemical Society, the Chair of SwissCat+, Member of NCCR Catalysis and an Associate Editor for the Journal of the American Chemical Society. Webpage: <http://www.coperetgroup.ethz.ch>

### Invited Speakers

#### 1. Ram Gupta

**Title:** Clean Energy for a Growing and Prospering World

**Abstract:** Over the last 10,000 years, the human population has increased from 4 million people to currently 7.8 billion. This 2000-fold increase in the population coupled with a 30-fold increase in the per capita energy consumption has put a significant pressure on the energy use, mostly for moving, heating, lighting, cooling, and information processing. In the meantime, due to research and innovation, the efficiencies of energy convertors have significantly improved, and the world has moved from using wood to more-energy dense fossil fuels. Unfortunately, the fossil gas and oil resources are depleting at an alarmingly fast rate which can cause a major disruption in the world economy. A sustainable source of energy is the one that can satisfy our present need without jeopardizing the future supply. Biomass, solar photovoltaic, solar thermal, wind, and hydrokinetic energies are being development to address and shortfall as well to provide a less polluting energy. Significant recent innovations have been made in these technologies, which will be discussed. However, some key challenges remain for technologies to become economically competitive.

#### 2. T. Brent Gunnoe

**Title:** Cu(II) Carboxylate Arene C–H Functionalization: Tuning for Non-Radical Pathways

**Abstract:** The C–H acetoxylation of non-directed arenes benzene and toluene, as well as related functionalization with OPiv and OHex ester groups (OPiv = pivalate; OHex = 2-ethylhexanoate), using simple Cu(II) salts with over 80% yield will be presented. Combined experimental and computational studies results indicate that the arene C–H functionalization likely occurs by a non-radical Cu(II)-mediated organometallic pathway. The Cu(II) salts used in the reaction can be isolated, recycled, and reused with little change in reactivity. Also, the Cu(II) salts can be regenerated in situ using O<sub>2</sub> and, after the removal of the generated water, the arene C–H acetoxylation and related esterification reactions can be continued, which leads to a process that enables recycling of Cu(II). The inclusion of coordinating ligands, including water, switches the reaction to an alternative, non-organometallic pathway that likely involves the generation of free-radical intermediates.

### 3. Amanda Morris

**Title:** Metal-Organic Frameworks for Energy Applications

**Abstract:** Metal-organic frameworks (MOFs) are supramolecular architectures comprised of metal nodes connected by multi-dentate organic/inorganic linkers. Incorporation of molecular chromophores into these solid-state structures has been exploited to develop luminescent sensors, light emitting diodes, photovoltaics, and photo/electro-catalysts. In terms of catalysis, the high surface area of MOFs can be exploited to produce a higher catalytic rate per geometric area than those realized by other approaches. The crux of catalysis, however, is diffusion. The Morris group has explored the diffusion of electrons and ions through MOFs as a function of an applied electric field. The results indicate that in most cases, as expected, ion motion is restricted through the 3D MOF networks. The effect of ion size and electronic self-exchange rates will be presented. Additionally, the effect of 3D MOF structure and pore size will be discussed. We place this discussion in the context of electrocatalytic water oxidation by MOFs through a detailed study of a ruthenium terpyridine bipyridine aquo catalyst modified UiO-67-type MOF. The MOF was competent at water oxidation with a rate constant on par with the homogeneous catalyst. Additionally, the stability of the catalyst was greatly enhanced, and the MOF could be recycled at least 3 times without loss in activity. Follow-up experiments indicate that the catalysis occurs throughout the MOF particles and is not confined to the surface. Ultimately, the catalyst operated at a rate 100 times that of a monolayer of the same catalysts on electrochemical supports. The design parameters for next-generation MOF water oxidation catalysts will be presented.

### 4. Christopher Paolucci

**Title:** Cation and Nanoparticle Interconversion in Metal-Exchanged Zeolites

**Abstract:** Metal cations and nanoparticles supported on oxides and zeolites are used as catalysts for a wide range of chemical reactions, with various and distinct active site requirements. Consequently, sintering and redispersion processes that interconvert cations and agglomerated nanoparticles underpin catalyst activation and deactivation phenomena, yet the influence of the nanoparticle size distribution, gas conditions, zeolite topology, and cation identity on the thermodynamic and kinetic factors influencing such interconversion are not well-understood. Here, we use density functional theory calculations and mathematical modeling to elucidate the conditions that generate a favorable thermodynamic driving force for agglomeration or redispersion and use kinetic Monte Carlo simulations to estimate the rates of interconversion. We show that redispersion of Pd nanoparticles proceeds through a different mechanism than for Pt nanoparticles, and cationic Pt and Pd have different stability windows with respect to gas conditions and zeolite topology. Our results show that water, a ubiquitous molecule in practical applications of these materials, promotes agglomeration of cations into nanoparticles for both Pt and Pd.

### Tutorial Seminars

1. Qian He

**Title:** Electron Microscopy for Better Catalysts

**Abstract:** In this tutorial, I will introduce how electron microscopy techniques can help the design or optimization of catalytic nanomaterials. Some examples include precious metal catalysts and oxide catalysts. I will also share my personal experience of how a microscopist can work better with the catalysis community (and vice versa). I will also talk about some emerging opportunities in electron microscopy that can potentially help catalyst research, including 4D-STEM, environmental electron microscopy etc.

2. Hua Zhou

**Topic:** Synchrotron X-ray Techniques for Catalysis

**Abstract:** TBA