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Catalysis Club of Philadelphia

Webinar: 7 pm, Thursday, September 23rd, 2021

Zoom link shared after registration

Speaker: Prof. Eranda Nikolla

*Department of Chemical Engineering and Materials Science
Wayne State University*

**Embracing the Complexity of Catalytic Structures:
Engineering Nonstoichiometric Mixed Metal Oxides for
Oxygen Electrocatalysis**

Student Speaker: Chae Jeong-Potter

Meeting Schedule:

6:30 PM: Welcome

7:00 PM: Talk by Chae Jeong-
Potter

7:30 PM: Talk by Prof. Nikolla

Meeting Fees:

Free to all who register

Meeting Etiquette:

Please remember to mute your
microphone and arrive early to
solve any technical issues.

Camera sharing prior to the talks
is encouraged.

Online Registration – Please
register online by Wednesday,
September 22nd at
[http://catalysisclubphilly.org/w
ebinar-registration/](http://catalysisclubphilly.org/webinar-registration/) or Chair-
Elect Udayshankar Singh,
udayshankar.singh@grace.com.

A Zoom meeting invite will be
provided through the
confirmation email. If you do
not receive a confirmation
email immediately after
registration, please contact
Renjing Huang,
hrenjing@seas.upenn.edu.

Membership – Dues for the
2021-22 season will be \$25 (\$5
for the local chapter and \$20
for the national club). Dues for
students, post-docs and
retirees will be \$10 (\$5 for the
local club and \$5 for the
national club).

Embracing the Complexity of Catalytic Structures: Engineering Nonstoichiometric Mixed Metal Oxides for Oxygen Electrocatalysis

Eranda Nikolla

*Department of Chemical Engineering and Materials Science
Wayne State University, Detroit, MI*

Dwindling fuel resources and high levels of CO₂ emissions have accelerated the need for renewable energy resources and more efficient energy conversion and storage systems. The goal of our research group is to design active, selective and stable catalysts/electrocatalysts for chemical and electrochemical transformations related to energy and chemical conversion. We focus on engineering complex, non-stoichiometric mixed metal oxides and controlling the 3-dimensional environment of metal catalysts through inverted catalytic structures and surface bound ligands as potential avenues for addressing limitations with the current state-of-the-art catalytic structures for energy and chemical conversion.

In this talk, I will mainly discuss our work on designing non-stoichiometric mixed metal oxide electrocatalysts for electrochemical reactions involving oxygen. These processes play an important role in energy conversion and storage technologies such as fuel cells, electrolyzers and metal-air batteries. The compositional versatility of non-stoichiometric metal oxides belonging to the perovskite family, of the general form $A_{n+1}B_nO_{3n+1}$ ($n = 1, 2, 3... \infty$; A = rare earth/alkaline earth metal; B = transition metal), presents numerous opportunities to tune the catalytic performance of these oxides for targeted reactions. However, identification of non-stoichiometric metal oxides for these reactions is often limited by their complexity and lack of effective descriptors of their activity and stability. We have combined theory, advanced characterization, controlled synthesis and electrochemical studies to shed light on the factors that govern oxygen electrocatalysis on these oxides and have identify ways to tailor their activity and stability. These studies have open avenues for engineering active and stable cationic centers in non-stoichiometric mixed metal oxide electrocatalysts for targeted reaction chemistries.

Bio



Eranda Nikolla is a Professor in the Department of Chemical Engineering and Materials Science at Wayne State University. Her research interests lie in the development of heterogeneous catalysts and electrocatalysts for chemical conversion processes and electrochemical systems (i.e., fuel cells, electrolyzers) using a combination of experimental and theoretical techniques. Dr. Nikolla received her Ph.D. in Chemical Engineering from University of Michigan in 2009 working with Prof. Suljo Linic and Prof. Johannes Schwank in the area of solid-state electrocatalysis. She conducted a two-year postdoctoral work at California Institute of Technology with Prof. Mark E. Davis prior to joining Wayne State University. At Caltech, she developed expertise in synthesis and characterization of meso/microporous materials and functionalized surfaces. Her group's impact to catalytic science has been recognized through the National Science Foundation CAREER Award, the Department of Energy Early Career

Research Award, Camille Dreyfus Teacher-Scholar Award, the Young Scientist Award from the International Congress on Catalysis, the 2019 ACS Women Chemists Committee (WCC) Rising Star Award, and the 2021 The Michigan Catalysis Society Parravano Award for Excellence in Catalysis Research and Development.

Feasibility Study of Combining Direct Air Capture of CO₂ and Methanation with Dual Function Materials (DFM)

Chae Jeong-Potter, Monica Abdallah, Robert J. Farrauto

Earth and Environmental Engineering, Columbia University in the City of New York

A dual function material (DFM) is comprised of an alkaline adsorbent and catalytic metal supported on the same porous carrier. It was originally developed in our group for CO₂ capture from power plant effluents with subsequent catalytic methanation using renewable H₂. Methane is a useful feedstock for fuel and/or chemicals. The DFM allows for the capture and conversion of CO₂ to occur using a single material in a single reactor. This eliminates the need to transport the captured CO₂ for utilization, reducing energy requirements and costs associated with CO₂ compression. In the power plant application, the capture/catalytic conversion operation is carried out isothermally at flue gas temperature (320°C), further reducing energy requirements.

We have demonstrated that the DFM is also able to selectively chemisorb the dilute CO₂ (~400 ppm) from ambient filtered air which can be subsequently catalytically hydrogenated to methane (Figure 1). Because direct air capture (DAC) technologies have free-range of geography, this technology has the added advantage of being aptly placed at emerging power-to-gas facilities or facilities with waste H₂ to eliminate the requirement for transporting H₂. Consequently, DFM relies solely on existing natural gas infrastructure for distribution.

Given the large volumes of ambient air that require processing, the cycle of CO₂ adsorption and methanation must be conducted in a temperature swing operation. We capture CO₂ at ambient temperature (i.e. 25°C) followed by heating to T>200°C in H₂ for methanation. Successful cyclic capture of 400 ppm CO₂/air at 25°C and subsequent methanation has been demonstrated. We also demonstrate that feed flowrates and cycle durations can be tailored to achieve high adsorption kinetics and high capture capacities, allowing for high rates of methane production. Cyclic operation with the DFM is also possible in the presence of humid ambient air, proving that DFM has further potential for DAC application.

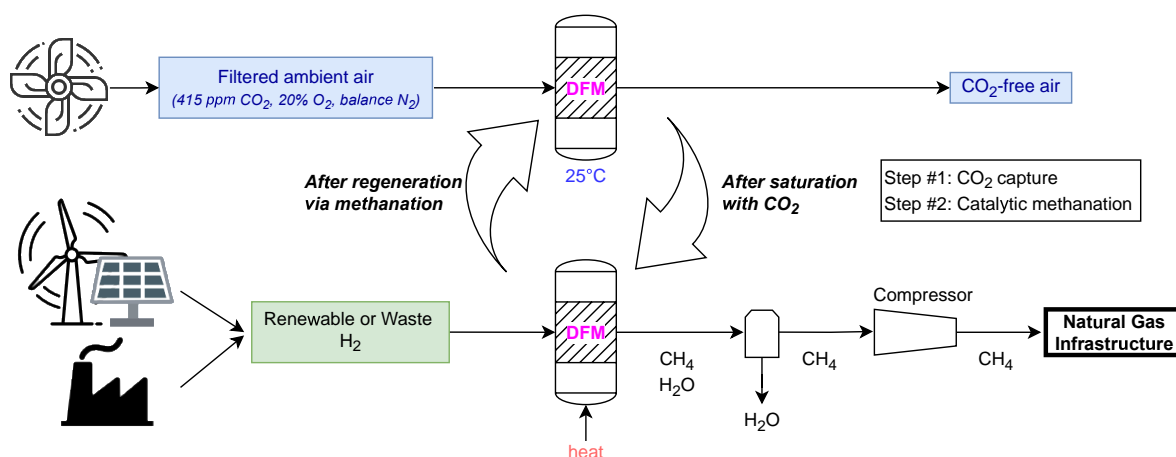


Figure 1: Process flow diagram for CO₂ capture and renewable natural gas (CH₄) generation for recycle back to the natural gas infrastructure. The CO₂ is captured on the DFM from filtered ambient air (step 1) at 25°C and catalytically methanated with the introduction of renewable or waste H₂ (step 2) at an elevated temperature in the same reactor. Parallel reactors will be required for continuous operation.

Bio

Chae Jeong-Potter is a senior Ph.D. candidate in the Earth and Environmental Engineering Department at Columbia University. She is currently advised by Professor Robert Farrauto, a Professor of Practice with over 40 years of catalytic industry experience. Chae's Ph.D. research focuses on investigating dual function materials (DFM) for selective capture of CO₂ from both ambient air and power plant flue gases and subsequent catalytic conversion to methane. She has contributed significantly to three U.S. DOE grants on DFM for direct air capture (DAC), all of which have been awarded. Chae will be completing her Ph.D. at the end of 2021 and in her post-graduate work hopes to continue research in catalysis for sustainable fuel synthesis.

Before joining Columbia, Chae graduated with her Bachelor's of Engineering (2016) and Master's of Engineering (2018) in Chemical Engineering from The Cooper Union, a prestigious specialized engineering and art college in NYC. She was awarded a full tuition scholarship for all 6 years of her studies and received the Henry Ender's Fellowship during her Master's.