Catalysis Club of Philadelphia

Webinar: 6:30pm EST, Thursday, February 25th, 2021

Webinar link shared after registration

Speaker : Prof. Fanxing Li

Chemical and Biomolecular Engineering Department
North Carolina State University

Tailoring Metal Oxide Redox and Surface Properties for Sustainable Energy Conversion

Graduate Student Speaker: Sagar Sourav

Department of Chemical and Biomolecular Engineering, Lehigh University
Biological and Chemical Science and Engineering, EES&T, Idaho National Laboratory

New Mechanistic Insights into Oxidative Coupling of Methane Reaction over Supported Na_2WO_4/SiO_2 Catalysts

Meeting Schedule:
6:30 PM: Networking Time
7:00 PM: Opening Remarks
7:05 PM: Student Speaker
7:20 PM: Main Speaker

Meeting Fees:
Free to CCP Members

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

Webinar Registration:
Please register online by **Wednesday, *February 24th*** using this **LINK** or notify Arrangements Chair Jian Chang (CJ).

A webinar meeting invite will be provided on February 24th to all those who register.

Membership:
Dues for the 2020-21 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 local club and $5 for national club). Use this **LINK** for membership registration.

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Tailoring Metal Oxide Redox and Surface Properties for Sustainable Energy Conversion

Prof. Fanxing Li

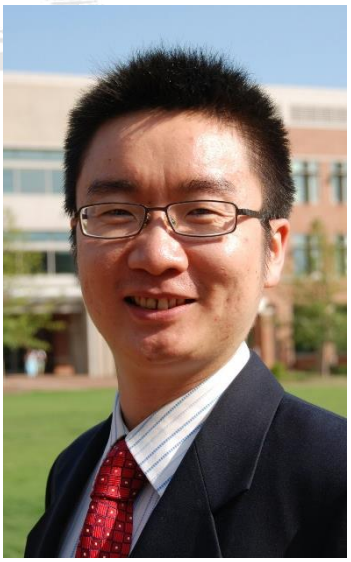
Alcoa Professor, Chemical and Biomolecular Engineering Department, North Carolina State University

Abstract:

Unlike conventional fuel conversion processes which oxidize carbonaceous molecules with gaseous oxidants, the chemical looping strategy seeks to intensify fossil fuel conversion processes using lattice oxygen of transition metal oxides. In a typical chemical looping scheme, carbonaceous molecules are oxidized by active lattice oxygen (O^{2-}) in the transition metal oxide, which functions as an oxygen carrier, a.k.a. redox catalyst. In a subsequent step, the O^{2}- deprived oxygen carrier is replenished by a gaseous oxidant. In addition to fossil fuel combustions, tailored redox catalysts can be applied for a variety of applications including selective oxidation, water-splitting, and CO_2 reduction.

This presentation exemplifies the use of iron and manganese containing mixed oxides for methane partial oxidation, oxidative dehydrogenation (ODH) of ethane, water-splitting, and CO_2 reduction. A number of redox catalysts composed of iron and/or manganese oxides are synthesized and characterized. Rational strategies to improve the redox activity, product selectivity, and/or water-splitting and CO_2 reduction conversions are investigated through the assistance of ab-initio calculation tools and mechanistic investigations. Compared to traditional heterogeneous catalysts, the redox catalysts in the current study show the potential to be more selective. They also possess excellent redox stability. Close to 100% water and CO_2 reduction efficiencies are shown to be achievable through rational selection of mixed metal oxides.

Speaker's Biography:



Dr. Fanxing Li is Alcoa Professor in the Chemical and Biomolecular Engineering Department at North Carolina State University. Dr. Li received his BS and MS degrees in chemical engineering from Tsinghua University in 2001 and 2004, respectively. He received his PhD at the Ohio State University in 2009. Dr. Li has published over 90 journal articles and book chapters. He is also an inventor/co-inventor of 11 issued patents and 3 patent applications. He has won numerous awards including the *"20 under 40" by the American Society for Engineering Education, the U.S. National Science Foundation CAREER Award, Humboldt Fellowship for Experienced Researchers, SABIC Young Professional Award, the NC State Sigma Xi Faculty Research Award, and was named as a NC State University Faculty Scholar and a winner of the Chancellor's Innovation Fund.*

New Mechanistic Insights into Oxidative Coupling of Methane Reaction over Supported Na_2WO_4/SiO_2 Catalysts

Sagar Sourav

Department of Chemical and Biomolecular Engineering, Lehigh University

Biological and Chemical Science and Engineering, EES&T, Idaho National Laboratory

Abstract:

The oxidative coupling of methane (OCM) to form C_2 products is a promising technique for conversion of natural gas into value-added chemicals. Among many catalysts tested for the OCM reaction, the supported Mn-Na_2WO_4/SiO_2 catalysts exhibit superior performance due to their excellent on-stream stability. The complexity of the catalyst structure and dynamic nature of the oxide phases during the OCM reaction, however, have hindered the complete understanding of stable oxide phases and nature of catalytic active sites present in supported Mn-Na_2WO_4/SiO_2 catalysts. Additionally, lattice oxygen species present in supported Mn-Na_2WO_4/SiO_2 catalysts play crucial roles in the OCM reaction mechanism, but no consensus has been reached regarding the nature and origin of lattice oxygen species.

In this study, we have utilized in-situ Raman spectroscopy and chemical probe experiments (H_2-TPR, temporal analysis of products (TAP)) to understand the structure and associated lattice oxygen species present in supported Na_2WO_4/SiO_2 catalysts. Additionally, transient and steady-state kinetic experiments in controlled environment of TAP and fixed-bed reactors were undertaken to gain insights into the mechanism and reaction pathways of OCM over supported Na_2WO_4/SiO_2 catalysts.

We observed that the supported Na_2WO_4/SiO_2 catalysts contain both dispersed surface Na-WO_x sites and a molten Na_2WO_4 phase under OCM reaction conditions. A molecular O_2*-type lattice oxygen species originates from the molten Na_2WO_4 phase, while surface Na-WO_x sites possess atomic O*-type lattice oxygen species. Both the surface Na-WO_x sites and the molten Na_2WO_4 phase are catalytically active but are involved in different reaction steps. Our findings show that the molten Na_2WO_4 phase mostly over-oxidizes CH_4 to form CO_2, but also assists in oxidative dehydrogenation of C_2H_6 to C_2H_4. On the other hand, the surface Na-WO_x sites were found responsible for selective oxidation of CH_4 to C_2 hydrocarbon products and over-oxidization of CH_y to CO

Speaker Biography:

Sagar Sourav earned his Bachelor of Technology from National Institute of Technology (NIT) Rourkela and Master of Technology from Indian Institute of Technology (IIT) Kanpur, both in Chemical Engineering. Currently, he is a 5th year PhD graduate student in the Department of Chemical and Biomolecular Engineering, Lehigh University. He is also the recipient of the Graduate Fellowship Award from Idaho National Laboratory (INL). His research interest includes understanding the molecular structural dynamics of supported W-oxide catalysts for oxidative coupling of methane and design of Cr-free high-temperature water-gas shift bulk mixed oxide catalysts.