**Bridging the Gap between Heterogeneous Catalysts and Bioinorganic Enzymes**

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**Abstract:**

To better understand why enzymes are able to perform redox reactions at mild reaction conditions and heterogeneous solid oxide catalysts require elevated reaction temperatures for oxidation reactions, the mechanisms and kinetics of methanol oxidation by bioinorganic enzyme mimics and heterogeneous solid oxide catalysts were compared at the molecular level both experimentally and theoretically. The experimental studies employed time-resolved *in situ* spectroscopy to monitor the molecular chemical transformations of the enzyme mimic and solid oxide catalysts as well as the methanol reactant and reaction intermediates. Both reactions proceed via the same V-OCH3 intermediate. The origin of the difference in reactivity between bioinorganic enzymes and solid oxide catalysts is related to the highly reactive peroxo VO2 sites only present in bioinorganic enzymes and not present in heterogeneous solid oxide catalysts under high temperature reaction conditions. The DFT calculated normal vibrational modes and reaction steps are in line with the experimental findings. This study bridges the gap between heterogeneous solid oxide catalysts and protein-based vanadate enzymes for methanol oxidation as well as other oxidation reactions.

**Speaker Bio:**

**Ozgen Yalcin** is a post-doctoral researcher in the *Operando* Molecular Spectroscopy and Catalysis Research Laboratory under the supervision of Prof. Israel E. Wachs at Lehigh University. She received her B.S. and M.Sc. in Chemical Engineering from Middle East Technical University (METU), Ankara, Turkey. She received dual PhD degrees from both the Department of Chemical & Biomolecular Engineering at Lehigh University and the Department of Chemical Engineering at Middle East Technical University. Her principal research interests are in heterogeneous catalysis and can be categorized as computational studies of water-gas shift reaction over inorganic metal oxides, and experimental studies of non-carcinogenic alternatives of solid oxide catalysts for high temperature water-gas shift reaction systems. She also has experience in methanol oxidation by bioinorganic enzyme mimics and supported vanadium oxide catalysts. In the future, she wants to contribute to the field of heterogeneous catalysis by applying the rich experiences she gained from academia.