

### **344c A Systematic Microkinetic and Mechanistic Analysis of the Water-Gas-Shift Reaction Kinetics on Low and High Temperature Shift Catalysts**

*Caitlin A. Callaghan, Ilie Fishtik, and Ravindra Datta*

Interest in fuel cells as an alternative power sources has increased dramatically in recent years. The lack of an immediately available hydrogen infrastructure has inspired the study of fuel processing reactions, including the water-gas-shift (WGS), in an attempt to better understand the mechanism and kinetics, thus allowing for a more systematic design of reformers and their catalysts. Here, a 17-step microkinetic model for the WGS reaction on both low temperature shift (LTS) and high temperature shift (HTS) catalysts is examined. A reaction pathway structure is constructed that provides a global view of the reaction's topological structure as well as its predictive kinetic analysis. The theoretical estimations of the reaction energetics are determined from the Unity Bond Index-Quadratic Exponential Potential Method (UBI-QEP) and the pre-exponential factors are based on transition state theory. Simplification and reduction of the mechanism is performed based on the results from a rigorous De Donder affinity analysis, coupled with quasi-steady state and quasi-equilibrium assumptions. An analytical rate expression is derived based on the simplified mechanism and is validated experimentally for both catalysts. The LTS and HTS catalyst mechanisms are compared energetically and mechanistically.