Sustainable Aviation Fuels from Biomass Derived Ethanol

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Objectives: The objective of this work is to advance the commercial readiness of a new catalyst technology and enable higher efficiency production of sustainable aviation fuel (SAF) from ethanol. The novelty of the proposed concept lies in manipulation of catalyst length scales – from single-unit cell to fully-formulated catalysts, to study catalyst performance and deactivation. In ethanol to olefins conversion (ETO), a critical challenge is decoupling kinetics and transport in the complex series reaction pathway. We will use high space velocity measurements in ultrasmall crystallites (as small as single unit cell) to learn the intrinsic kinetics of olefins formation as well as coke formation. We will use atomistic modeling to further understand these phenomena to develop improved industrial catalyst formulations. The success of this project has strong potential to lead to increased adoption of ethanol to jet technologies.

Methods: State-of-the-art catalysts for ETO include zeolite-supported metal single atoms whose structures are presently unknown and for which quantitative comparisons of reactivity are hindered by the inability to quantify turnover frequencies (TOFs). In this project, we will synthesize promising formulations for powder scale testing, industrial formulation, and lab scale testing at realistic conditions over extended times on stream, and model the performance at the atomic, particle, and reactor scales.

Impact: The novel, multi-dimensional approach to studying deactivation in ethanol to olefins conversion is essential to the further development of this promising catalyst technology. The improved time on stream stability engendered will enable improved process efficiency that in turn reduce environmental impact and operational costs. In partnership with ORNL researchers, we will integrate the proposed work into existing DOE efforts, leverage experimental and simulation capabilities at ORNL, and foster growing collaborations between UA and ORNL. Support from EERE to fund this proposed work will enable a holistic collaboration between catalysis formulation and manufacturing experts and catalysis experts at UA, Johns Hopkins, Clariant and DOE Labs.

Major Participants: This project represents a collaborative effort between The University of Alabama, Johns Hopkins University, Oak Ridge National Laboratory, and Clariant. UA will lead the effort through novel catalyst formulation development, characterization, and bench scale testing with support of lifecycle analysis and technoeconomic analysis. Johns Hopkins University will synthesize single-unit cell zeolites and perform atomistic modeling activities. ORNL will support with long term testing, provision of real feedstocks, and olefin upgrading tests. Clariant will provide fully formulated/engineered catalysts for ETO, olefins oligomerization, and hydrotreating.