LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

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Catalysis: Making the Quantum Leap to Tomorrow's Fuels

by

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Most long-term energy policies include the conversion of renewable organic matter into chemicals and fuels, such as ethanol. A promising approach for converting organics into fuels involves their conversion into syngas (a mixture of CO and H_2), followed by the selective recombination of these intermediates into specific fuel components. A major challenge associated with the synthesis of ethanol from syngas is an inability to find a low-cost catalyst that promotes the proper combination of CO dissociation and CO insertion steps, so as to yield ethanol as the primary reaction product and inhibit the formation of methane, longer chain alkanes, and other coking reaction products. To identify promising new catalysts, quantum mechanical based simulations were used to evaluate the catalytic activity of a series of bimetallic clusters that range in size from 13 to 38 metal atoms. Density Functional Theory (DFT) simulations and Bronsted-Evans-Polanyi (BEP) relations were used to map out the full reaction mechanism from syngas to ethanol for each of these materials. Microkinetic models were built, considering the reaction steps as well as the diffusion of intermediate species between different metal surface sites. These simulations provided valuable information about the stability of specific metal combinations and more importantly, which combinations of metals are ideally suited for ethanol production.

David A. Bruce is a Professor in the Department of Chemical and Biomolecular Engineering at Clemson University. Prof. Bruce's research interests are in the areas of catalysis, renewable fuels and chemicals, pollution abatement, and molecular modeling. Prior experimental research efforts include the development of mesoporous oxide catalysts, heterogeneous chiral catalysts, lignin based separation and chemical conversion processes, and advanced waste treatment processes, including sonochemical and supercritical water oxidation processes. Prof. Bruce also leads computational efforts focused on the prediction of transport properties and structure-activity relationships for catalyst materials and biodegradable polymers via quantum mechanics and parallelized molecular dynamics methods. Prof. Bruce was named the Sigma Xi Researcher of the Year (2012, CU chapter) and received an NSF CAREER award for his work on the polymer templating of mesoporous oxide catalysts. Prof. Bruce is the holder of several material and processing patents, actively consults with numerous companies in the fuels and chemicals industry, and is on the Scientific Advisory Board of multiple start-up companies in the biofuels and renewable materials areas.

This seminar will be broadcast at the following venues: Johnston Hall 338 (LSU), Liberal Arts Building 234 (UNO), Qatar Pavilion Conference Room 226 (Xavier University), JB Moore Hall Room 211 (Southern University), and via Adobe Connect at https://connect.lsu.edu/la-sigma/ .