

Live

Reaction Pathway Discovery and Analysis: Bringing Biological and Chemical Catalysis Together

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Abstract: Reaction pathway analysis is a powerful tool to design novel routes to chemicals, identify optimal processing conditions, and suggest strategies for catalyst design. We have developed methods for the assembly of kinetic models of substantive detail that enable linking of the atomic and process scales. We have applied our methodology to a range of different problems, including production of silicon nanoparticles, biochemical transformations, polymerization/depolymerization, and tropospheric ozone formation. While the chemistries are seemingly very disparate, applying a common methodology to study them reveals that there are many features of complex reaction networks that are ubiquitous. This talk will focus on mechanistic modeling of a range of conditions for converting hydrocarbons derived from renewable sources, starting with quantitative analysis of chemical catalysis by native inorganic constituents and transitioning to mechanistic understanding of how enzymes achieve exquisite selectivity for similar chemistries, leading to the potential for the design of novel pathways.

Biography: Linda Broadbelt is Sarah Rebecca Roland Professor in and Chair of the Department of Chemical and Biological Engineering University at Northwestern University. She was also appointed the Donald and June Brewer Junior Professor from 1994-1996. She has completed the short course Business for Scientists and Engineers through the Kellogg Graduate School of Management. Her research and teaching interests are in the areas of multiscale modeling, complex kinetics modeling, environmental catalysis, novel biochemical pathways, and polymerization/depolymerization kinetics. She is currently the Chair of the Catalysis and Reaction Engineering Division of AIChE, and also previously served on the Executive Board of the National Program Committee of AIChE. She is currently an Associate Editor for *Industrial & Engineering Chemistry Research*. Her honors include selection as the AIChE Women's Initiative Committee Mentorship Excellence Award winner, a Fellow of the American Association for the Advancement of Science, a Fulbright Distinguished Scholar Award, a CAREER Award from the National Science Foundation, appointment to the Defense Science Study Group of the Institute for Defense Analyses, and selection as the Ernest W. Thiele Lecturer at the University of Notre Dame and the Allan P. Colburn Lecturer at the University of Delaware.

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Where: CB#204W