CHEMICAL ENGINEERING

SEMINAR SERIES

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Monday, March 28, 2016

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Quantitative Assessment of Channeling Mechanisms in Nanoscale Catalytic Architectures

ABSTRACT: Our research group is focused on materials for electrocatalysis, particularly non-precious electrocatalysts for fuel cell reactions. We approach this challenge in two ways: using transition metal catalyst centers and redox enzymes. These approaches are similar in that catalytic turnover is much lower than precious metal catalysts such as platinum, and transport limitations becomes important when catalyst loadings are increased to compensate for low activity.

Natural and technological instances of enzyme catalysis often feature multistep reaction cascades. The throughput and yield of such nanoscale catalytic architectures is limited by the ability to retain reaction intermediates and direct them toward downstream reaction steps. Nature has settled on several approaches to intermediate channelling, including electrostatic attraction, confinement, and surface affinity. This presentation will discuss the limits of such approaches through modeling, from the molecular dynamics to continuum scales. The extent to which intermediate transport limits overall reaction flux is defined by a flux control coefficient, calculated from numerical results. The extent to which individual and combined channeling approach can enhance overall flux and/or reaction yield under idealized circumstances are predicted, and the various complications introduced by nonidealities are discussed. becomes important when catalysts loadings are increased to compensate for low activity.

RECEPTION 3:30 • LECTURE 4:00 – 5:00
PHYSICS ASTRONOMY BLDG. (PAA) A110

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BIOGRAPHY: Scott Calabrese Barton is an Associate Professor of Chemical Engineering at Michigan State University. His research focuses on engineering and materials issues in fuel cells, particularly kinetics and mass transport in fuel cell electrodes. His work has covered a range of systems, including direct methanol fuel cells, zinc-air batteries, biofuel cell electrodes and transition metal catalysts for oxygen reduction. He is the recipient of a CAREER award from the National Science Foundation and a Petroleum Research Fund award from the American Chemical Society. He currently serves as Chair of the Energy Technology Division of the Electrochemical Society.