

CORE-CM SEMINAR

Michigan State University

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Catalysis in the 21st Century: What Role Can/Will Theory Play

Abstract:

Catalysis has a tremendous impact on the global economy. By some estimates, the value of industrial products whose manufacture depends on catalysis is on the order of several trillion dollars per annum. Despite this economic incentive, few new catalysts have traversed the great chasm that exists between the academic bench top and the industrial plant. This talk will focus on several aspects of catalyst-design from the computational chemist's perspective, focusing on examples from homogeneous catalysis in our group's research. Integration of theory with experiment will be highlighted. Current challenges in catalyst design, and hence opportunities for future research, will be discussed. Of particular interest are examples relevant to the activation and functionalization of light alkane C-H bonds resources that are found in natural gas and petroleum feedstocks.

Thursday, September 1, 2016
12:00 NOON
Room 1400 – Biomedical & Physical Sciences
Professor Mitch Smith - Host