

MIT Chemical Engineering Department

Fall 2018 Seminar Series

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Engineering Active Sites and Their Environments to Guide Catalytic Molecular Transformations in Sustainable Energy Systems



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**Friday, September 28, 2018
3:00pm (Reception at 2:45 pm)
66-110**

Abstract: Future strategies for energy production will undoubtedly require processes and materials that can efficiently convert sustainable resources into fuels and chemicals. While enzymes elegantly integrate highly active centers together with adaptive nanoscale environments to exquisitely control catalytic transformation involved in such processes, they limited industrially by their durability and stability. Advances in theoretical methods, computing and spectroscopy now allow one to track the molecular transformations and how they proceed in heterogeneous catalytic systems at specific sites and within particular environments. We present recent advances in computational catalysis and their application to engineering molecular transformations for energy conversion and chemical synthesis. We discuss the sites and nanoscale environments necessary to carry out specific bond-making and breaking reactions as well as proton and electron transfer processes important in the catalytic reduction and oxidation processes that control the catalytic conversion of biomass to chemicals as well as the electrocatalytic transformations of fuels to energy. More specifically, we discuss the heterogeneous catalytic hydrogenation of oxygenates to value-added chemicals and the electrocatalytic reduction of oxygen and carbon dioxide to water and CO, respectively.