School of Chemical, Biological and Materials Engineering

Phillips 66
Seminar Series
2019-2020

Tuesday, March 3, 2020
3:00 p.m. - 4:00 p.m.
Sarkeys Energy Center A-235

Dr. Eric McFarland

Professor
Department of Chemical Engineering
University of California Santa Barbara

"Decarbonizing Natural Gas by Reactive Separation on High Temperature Liquids"

Pyrolysis of abundant methane is the lowest cost, CO_2-free, process for producing molecular hydrogen and solid carbon. Practical deployment requires solution of several difficult problems. A high temperature liquid-based process is under investigation using catalytic molten salts. CH_4 molecular adsorption and dehydrogenation on liquid surfaces with high rates of molecular motion introduces unusual and interesting aspects of surface chemistry. In the liquid environment the carbon may be readily separated and removed continuously. The turnover frequency of methane on liquid surfaces is observed to strongly depend on the melt composition. The relative reactivities of different melt compositions were investigated both experimentally and by density functional theory (DFT) and *ab initio* molecular dynamics (AIMD) simulations. Experiments performed in bubble column reactors are compared to theory. Monovalent halide salt mixtures are found to be relatively inactive; however, polyvalent halide molten salt surfaces are catalytic with apparent activation energies of 90-200 kJ/mole. The catalytic liquid surfaces are found to facilitate both complete dehydrogenation, and the production of methyl radicals to increase the gas phase methane decomposition.

****Required Graduate Student Seminar for ChE 5971****

Refreshments served before Seminar

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