SCHOOL OF CHEMICAL, BIOLOGICAL & MATERIALS ENGINEERING

And

UNIVERSITY OF OKLAHOMA BIOENGINEERING CENTER

100 E. Boyd, Sarkeys Energy Center, T-335 405-325-5811 The University of Oklahoma Norman, Oklahoma 2009 – 2010 Seminar Series

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DR. ADITYA BHAN

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DEPARTMENT OF CHEMICAL ENGINEERING AND MATERIALS SCIENCE
UNIVERSITY OF MINNESOTA
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Will present a seminar on

"SHAPE SELECTIVE CHEMICAL CONVERSION OF OXYGEN CONTAINING MOLECULES"

We compare and contrast in this talk the effects of local zeolite structure on the dynamics of the carbonylation of surface methyl groups and of the parallel dehydration reactions of ethanol to produce diethyl ether and ethylene. We show that the apparent effects of proton density and of hydroxyl group environment on DME carbonylation turnover rates reflect instead the remarkable specificity of eight-membered ring zeolite channels in accelerating kinetically relevant *CH₃-CO reaction steps. In independent reaction studies, ethylene production via monomolecular ethanol dehydration reactions was observed on H-MOR materials because small 8-MR side pockets prevent the formation of bulky ethanol dimeric species and enable the selective stabilization and activation of ethanol monomers. These conclusions are consistent with the low rates of ethylene production on larger pore MFI and BEA zeolites where the absence of spatial constraints leads to the predominant prevalence of energetically favorable ethanol dimer species and the selective catalytic synthesis of diethyl ether. These studies extend the scope of shape selectivity concepts beyond those reflecting size exclusion and preferential adsorption.

THURSDAY, MARCH 4, 2010 COOKIES AND COFFEE -- 2:45 P.M. SEMINAR -- 3:00 P.M. SARKEYS ENERGY CENTER, ROOM M-204

THIS IS A REQUIRED SEMINAR FOR CHE 5971