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 2010 – 2011 Seminar Series

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Will present a seminar on

"ELECTRONIC STRUCTURE METHODS IN HETEROGENEOUS CATALYSIS: REACTION MECHANISMS AND NOVEL MATERIALS"

The detailed *reaction mechanism* and the nature of the *active site* in catalytic chemical transformations have been at the heart of understanding and improving heterogeneous catalysis. Unfortunately, and despite significant advances accomplished so far, determining the nature of the active site for a given reaction under realistic experimental conditions is non-trivial. Similarly, *in-situ* identification of key reactive intermediates is not always possible. In this talk, we will attempt to demonstrate how first-principles electronic structure *theory* can offer important insights on active sites and reaction mechanisms. These insights, combined with critical information from *experiments* and *microkinetic modeling*, offer new opportunities for an improved understanding of heterogeneous catalysis and can guide the quest for determining the nature of the active site. In addition, we will show how theory can assist with identifying and designing at the atomic-scale promising, sometimes metastable, catalytic sites with improved catalytic properties. It is then up to modern *inorganic synthesis* to meet the challenge of constructing the predicted catalytic sites.

Examples of catalytic reactions to be discussed include the low temperature Water-Gas-Shift (WGS) 1,2 reaction and the Preferential Oxidation (PROX) of CO in the presence of hydrogen 3,4 , both relevant to H₂ production and purification.

THURSDAY, SEPTEMBER 9, 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