MAR14-2013-020447

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

First principles analysis of metal and oxide-metal interfacial catalysis for hydrogen production

JEFFREY GREELEY, Purdue University

Current and growing interest in the development of new catalytic materials for complex chemistries has challenged the methods traditionally employed by practitioners of computational catalysis. Explicit Density Functional Theory (DFT) analysis of all possible reaction pathways in biomass reaction networks, for example, is computationally prohibitive, and to make progress at a reasonable rate, strategies to accelerate the predictions made by DFT-based methods must be developed. In this talk, we will review some recent work in our group focusing on first principles analyses of the production of hydrogen from the decomposition of biomass-derived oxygenated hydrocarbons on heterogeneous catalytic surfaces. We will discuss, in particular, the development of accelerated DFT-based strategies to map the complex reaction networks associated with biomass decomposition at metal and oxide-metal interfaces, and we will show how these strategies can efficiently produce semi-quantitative predictions of activity and selectivity trends in hydrogen production on these surfaces. We will also briefly describe the development of reactivity trends for another chemical process that is relevant to biomass chemistry, the water-gas shift reaction, at metal-oxide interfaces, and will describe how bifunctional properties of these interfaces may promote this important chemistry.