MAR12-2011-000400

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Tailoring Surface Chemical Properties Using Electronic Structure Theory

JENS NORSKOV, Stanford University

Electronic structure methods based on density functional theory have reached a level of sophistication where they can be used to describe complete catalytic reactions on transition metal surfaces. This opens the possibility that computational methods can be used to tailor surfaces with desired chemical properties. Recent progress in this direction for transition metal catalysts will be discussed. A series of concepts will be introduced to describe and understand trends in reactivity from one metal surface to the next. It is shown how these concepts can be used to identify the factors determining the catalytic activity of a given transition metal surface, and how this can form the basis for screening of a large number of metals and alloys for catalytic properties.