BERKELEY CATALYSIS CENTER

Distinguished Lecture Series Seminar

Friday, October 29, 2004
The McCollum Room
775A&B Tan Hall
10 am to 12 pm

Dr. Jens K. Nørskov

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"Heterogeneous Catalysis from First Principles"

ABSTRACT:

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 gives an unprecedented insight into these processes, and it allows us to pinpoint the origin of the catalytic activity of a metal in terms of its electronic structure. The ammonia synthesis is used to exemplify the approach. It will be shown that by combining density functional calculations with kinetic modeling we can now predict relative catalytic activities of different metals. The generality of the approach is illustrated by including a number of other catalytic reactions into a universal property-activity scheme, which identifies the surface properties that determine the catalytic activity for a whole class of reactions.