

# On the role of hydrogen in heterogeneously catalyzed reactions

## Frontiers in Catalysis Science and Engineering Seminar Series

### Presented by...

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### Abstract

Hydrogen is a frequent participant in several heterogeneously catalyzed reactions, including Fischer-Tropsch Synthesis (FTS) of fuels, ammonia synthesis, oxygen reduction reaction (ORR), NO reduction, preferential oxidation of CO in the presence of H<sub>2</sub> (PROX), etc. Having analyzed the detailed aspects of the reaction mechanism for a number of these reactions on various transition metal and alloy surfaces using first-principles methods, some common principles governing the role of hydrogen in a wide range of catalytic transformations begin to emerge. In this presentation, we will discuss these common mechanistic principles by examples, including FTS<sup>1,2</sup>, NO-reduction, ORR<sup>3</sup>, PROX<sup>4,5</sup>, through an analysis of the energetics of alternative elementary reaction steps and the resulting potential energy diagrams. Connections to observations from experimental studies provide an invaluable perspective for the evaluation of our theoretical assessments.

### More info?

See <http://iic.pnl.gov>

[http://www.engr.wisc.edu/che/faculty/mavrikakis\\_manos.html#address](http://www.engr.wisc.edu/che/faculty/mavrikakis_manos.html#address)

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