

# Sixth Irving Shain Chemistry Colloquium

## Helmut Schwarz

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Universität Berlin; and President,  
Alexander von Humboldt Foundation

**Friday, April 17, 2009; 3:30 PM**

**Room 1315 Chemistry**

**From Bare  $\text{FeO}^+$  to Cytochrome P-450:  
New Insight in the Intriguing Mechanisms  
of C-H Bond Oxygenation.**



This presentation begins with a mechanistic scheme for the oxygenation of hydrocarbons, based on detailed ion-molecule reactions in the gas phase and electronic structure calculations of binary transition-metal oxides. A result of this combined experimental / computational approach is a new paradigm, called two-state reactivity (TSR). We will apply TSR to the hydroxylation of alkanes and related processes. We propose that in thermal reactions spin-crossing effects can dramatically affect reaction mechanisms, rate constants, branching ratios and temperature behaviors of organometallic transformations [1-8]. Actually, spin-changes can accelerate and promote otherwise extremely inefficient processes, and this concept suggests a novel mechanism involving the catalytic action of P-450.

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Helmut Schwarz has been Professor of Organic Chemistry at Berlin University of Technology (TU) since 1983. Beyond his research in Berlin, Schwarz has been a visiting professor at several research institutions abroad. Since 1989 his research has been recognized by over a dozen prestigious awards, including three Honorary Doctorates. He serves on several editorial boards and is in demand as a Science Policy expert.

In 2008, Prof. Schwarz took on the presidency of the Alexander von Humboldt Foundation. Established in 1861, that society was dedicated to the support of German scientists doing research abroad. The Foundation now funds 1800 researchers a year, from 130 countries, while they conduct research in Germany. A network now connects some 23,000 researchers – including 40 Nobel winners – who call themselves Humboldt scholars.

**Please stay for refreshments in the Shain Tower Atrium at 4:30**