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Department of Chemistry

Student Seminar Series

9:45 a.m. Tuesday, April 16, 2013 • 331 Smith Hall

Professor

John T. Yates Jr.

Department of Chemistry
University of Virginia

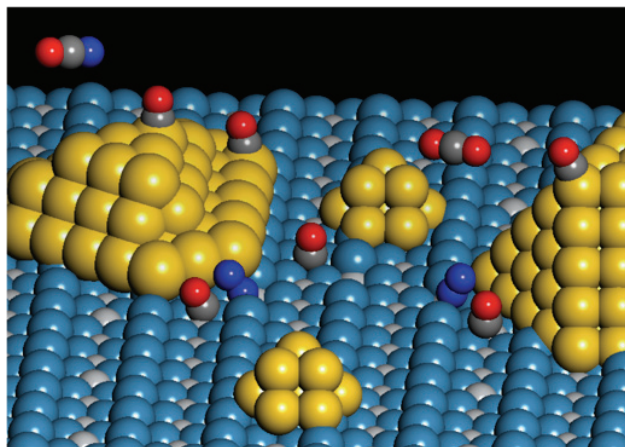
A New Kind of Active Site in Heterogeneous Catalysis on Au Nanoparticles

Website:

<http://chem.virginia.edu/faculty-research/faculty/john-t-yates-jr/>

Abstract

Gold, usually considered to be inactive chemically, becomes very active for heterogeneous catalysis when subdivided into nanometer-sized clusters and supported on reducible oxides such as TiO_2 . Such supported nanoparticles of Au feature sites at the interface between the Au and the TiO_2 support, which exhibit high catalytic activity for oxidation reactions. We have used transmission IR spectroscopy combined with DFT calculations to investigate the catalytic oxidation of CO and ethylene, finding that the sites responsible for activity are on the perimeter of the Au particles. Oxygen- molecule activation occurs by adsorption of an O_2 molecule between a perimeter Au atom and a neighbor Ti^{4+} site, producing a $\text{Ti}^{4+}\text{-O-O-Au}$ species which is a strong oxidizer analogous to a peroxy species. These special surface sites are called dual-catalytic sites. I will show a combination of experimental and theoretical results which all point to the unique activity of the dual-catalytic sites at the Au particle perimeter. In addition, an exotic surface species, the ketylidene species, $\text{Au}_2\text{C}=\text{C}=\text{O}$, has been discovered when C_2H_4 is first oxidized to acetate and then to $\text{Au}_2\text{C}=\text{C}=\text{O}$.



Host: Emily Pelton

John T. Yates Jr. is one of the world's leading investigators in the field of surface chemistry and physics, including both the structure and spectroscopy of atoms and molecules on surfaces, the dynamics of surface processes, and the development of new methods for research in surface chemistry.



He earned his bachelor's degree from Juniata College, and his doctorate from the Massachusetts Institute of Technology. Following three years as assistant professor at Antioch College, he joined the National Bureau of Standards, first as a postdoctoral research fellow and then, from 1965 until 1982, as a member of its scientific staff.

Yates joined the University of Pittsburgh in 1982 as a professor of chemistry and as the founding director of the university's Surface Science Center. In 1994, he was jointly appointed to the Department of Physics. He moved to the University of Virginia in 2006 as a professor and research fellow, and established a new research program in surface science.

He has received many honors and awards, including being elected a fellow of the American Chemical Society (ACS); Gerhard Ertl Lecturer Award for Surface Science and Catalysis; five ACS award in chemistry and surface chemistry, including the ACS Peter Debye Award in Physical Chemistry; the Arthur W. Adamson Award for Distinguished Service in the Advancement of Surface Chemistry; the American Vacuum Society Medard Welch Award; and being elected a member of the National Academy of Sciences.

He has served on editorial boards for six journals, and has written books and more than 720 research papers.

Yates' research interests include imaging chemical bond directions in adsorbed molecules; photochemistry on semiconductor surfaces; adsorption on carbon single wall nanotubes; adsorption on ionic solid surfaces.