

CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES: Surface Reaction Mechanisms on Single Atom Alloys and in Zirconium Diboride Thin Film Growth

Abstract:

The mechanisms of surface chemical reactions are relevant to a variety of technological fields including heterogeneous catalysis and thin film growth by chemical vapor deposition (CVD). This talk will cover the mechanisms of two distinct areas of surface chemical reactions. The first area is selective hydrogenation reactions over Pd/Cu(111) single-atom-alloy model catalysts. The second area is the growth of ZrB₂ thin films by the thermal decomposition of Zr(BH₄)₄. Low coverages of catalytically active metals deposited onto the surfaces of less active host metals can form single atom alloys (SAAs), which often display unique catalytic properties. The catalytic properties of SAAs are ultimately determined by their surface structure. We have used polarization dependent reflection absorption infrared spectroscopy to study the selective hydrogenation reactions of acetylene, propyne, 1,3-butadiene and styrene over a Pd/Cu(111) SAA surface. Reactants and products were monitored in the gas phase with s-polarized spectra, while p-polarized spectra were obtained to identify surface species present during the reaction. In each case, no hydrogenation occurred over the Cu(111) surface, but selective hydrogenation occurred over the Pd/Cu(111) SAA. Full hydrogenation to the saturated alkane did not occur.

Zirconium diboride (ZrB₂) is an extremely hard material with a high melting point of 3246 °C, properties that make it suitable for applications as an ultrahigh temperature ceramic. In many applications, it is used in the form of coatings on other materials. Thin films of ZrB₂ can be grown conformally via chemical vapor deposition (CVD) using zirconium borohydride, Zr(BH₄)₄, as a precursor. Homoepitaxial growth of ZrB₂ on a ZrB₂(0001) single-crystal was studied using the techniques of reflection-absorption infrared spectroscopy (RAIRS), low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), and scanning tunnelling microscopy (STM). Exposure of Zr(BH₄)₄ to the ZrB₂(0001) surface at 90K led to the molecular adsorption of Zr(BH₄)₄, which desorbed without dissociation upon heating. However, exposure at 1250K led to homoepitaxial growth of ZrB₂ films. A variety of different structures were observed with STM, including compact hexagonal ZrB₂ islands, and a (√3×√3)-R 30° boron-terminated structure.

About the Speaker:

Education:

1978-1982: Massachusetts Institute of Technology. PhD in Physical Chemistry, 1982. Thesis title: "An Angle-Resolved Photoemission Study of CO on the Pt(111) and Pt(321) Surfaces" Thesis Advisor: Dr. F. Read McFeely
1974-1978: University of California, Berkeley. BS in Chemistry, with honors, 1978.

Professional Experience:

2026 and 2010, Short-term fellowships, Japanese Society for the Promotion of Science
January-June, 2004, Eminent Visiting Scientist, Institute for Physical and Chemical Research, Wako-shi, Japan
September-December 1998, Guest Professor, Tohoku University, Sendai, Japan
August 1994-August 1995, Visiting Scholar, Waseda University, Tokyo, Japan
1992-Present: Professor, University of Illinois Chicago
1989-1992: Associate Professor, University of Illinois Chicago
1984-1988: Assistant Professor, University of Illinois Chicago
1982-84: Postdoctoral research with Prof John T. Yates, Jr., University of Pittsburgh. Research on the vibrational properties of molecules chemisorbed on metal surfaces using the technique of infrared reflection absorption spectroscopy.
1978-82: Research assistant in the group of Dr. F. Read McFeely, Dep. of Chemistry, MIT. Research on the geometric and electronic structures of chemisorbed molecules.
1976-78: Undergraduate research with Prof. H. F. Schaefer III, using ab initio calculations to study small molecular complexes.

Professional Organizations:

American Chemical Society, member since 1981
American Vacuum Society, member since 1982

Awards and Honors:

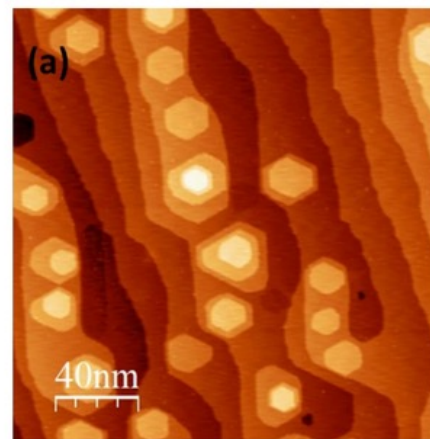
Dreyfus Teacher-Scholar Award, 1989
University of Illinois, University Scholar Award, 1990
Fellow of the American Vacuum Society, elected 2002
Teaching Recognition Award, University of Illinois at Chicago, 2008
Fellow of the American Association for the Advancement of Science, elected 2009
Fellow of the American Chemical Society, elected 2011
AVS Prairie Chapter Outstanding Researcher Award, 2022
UIC Researcher of the Year Award in Physical Sciences and Engineering, 2025



Michael Trenary

Professor

Department of Chemistry
University of Illinois Chicago



STM image after a 10 L exposure of Zr(BH₄)₄ to ZrB₂(0001) at 1200°C.