Ultrahigh Vacuum Investigations of Bimetallic Catalysts and the Development of Nanoparticle Catalysts for High-Pressure Applications

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Planned Completion = December 31, 2006

Research Goals and Objectives

- Determine Structure-Reactivity Relationships of Model Pt-Bimetallic Catalysts
  - structural characterization with *in situ* STM
- Characterize Reaction Mechanism for Hydrogen Generation from Methanol on Bimetallic Catalysts
  - relevant surface oxygen phases prepared and studied in UHV
  - kinetic investigations using mass spectrometric methods
- Develop Efficient Nanoparticle Catalysts to Produce Hydrogen via Steam Reforming of Methanol
  - Low Reaction Temperature
  - High Hydrogen Yields
  - Low CO Content

Relevance to Current State-of-the-Art

- ★ Atomically Resolved Structures of Bimetallic Surfaces
- ★ UHV Preparation and Characterization of High Concentration Surface Oxygen Phases
- ★ Design of Nanoparticle Catalysts and Possibility for Enhanced Catalysis Mediated by Particle Size

Relevance to NASA

- ★ Potential for Efficient On-Site Hydrogen Production
- ★ Rational Design of Nanoparticle Catalysts for Other Applications

Budget, Schedule and Deliverables

- 2005 Budget: $132,367
- 2006 Budget: $70,000

Task	Q1	Q2	Q3	Q4	Q5
Characterize Structures of Pt-Ru Surfaces	X	X			
Kinetic and STM Studies of Methanol Oxidation		X	X		
Identify Property Trends in Pt-M Surfaces				X	X
Design & Calibration of Reactor System	X				
Catalytic Activity Measurements		X	X	X	X
Catalyst Formulation Improvements				X	X

Deliverables:

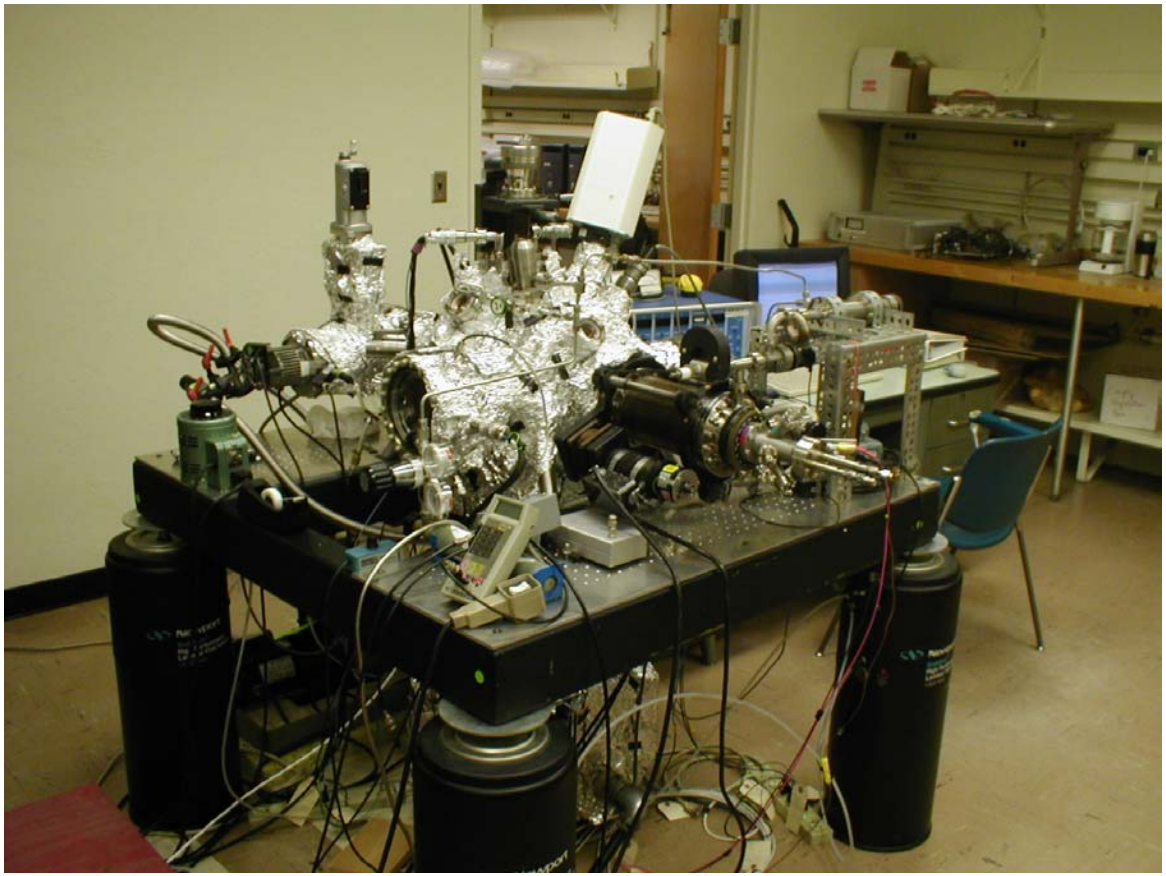
- Mechanistic Insight of Reactions and Catalysts
  - Rational Catalyst Design
- New Low-T Catalyst: High Hydrogen Yield + Low CO

Q1	Oct-Dec 05
Q2	Jan-Mar 06
Q3	Apr-Jun 06
Q4	Jul-Sep 06
Q5	Oct-Dec 06

Anticipated Technology End Use

- Catalytic Hydrogen Production from Hydrocarbon Feedstocks (for use in fuel cells or as rocket fuel)
- Flexible Catalyst ➡ Variable Feedstock for Hydrogen Production
  - Potential for Biomass or Waste Utilization
- Nanoparticle Catalysts for Other Applications
  - CO oxidation for CO_2 lasers
  - CO_2 decomposition for O_2 generation

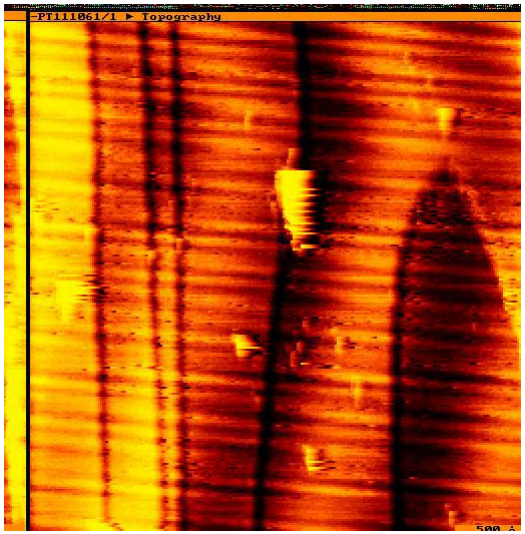
Accomplishments and Results, J. Weaver



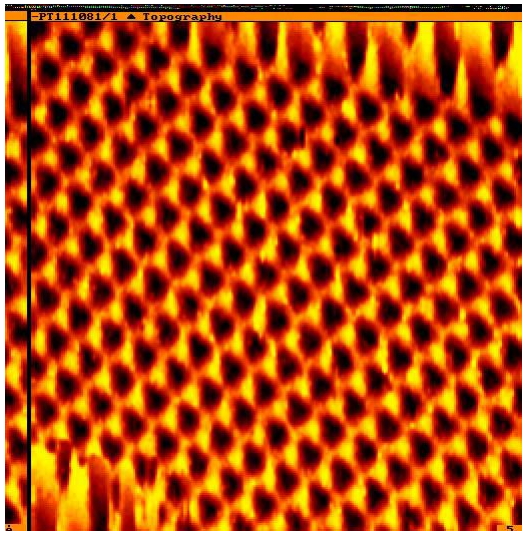
Modification and Development of Ultrahigh Vacuum System with Scanning Tunneling Microscope (STM)

Accomplishments and Results, J. Weaver

- STM modification successful in enabling surface features to be resolved over nanoscopic and atomic dimensions



Monatomic steps on Pt(111)



Adsorbed S atoms on Pt(111)

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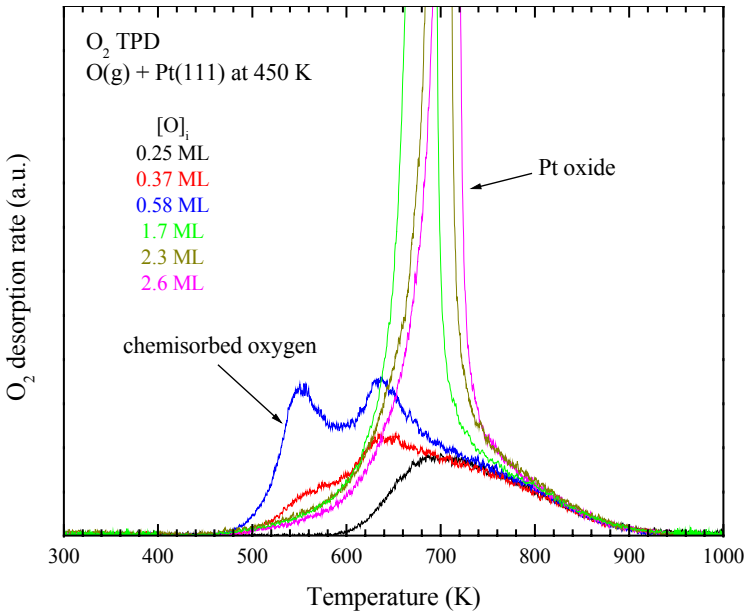
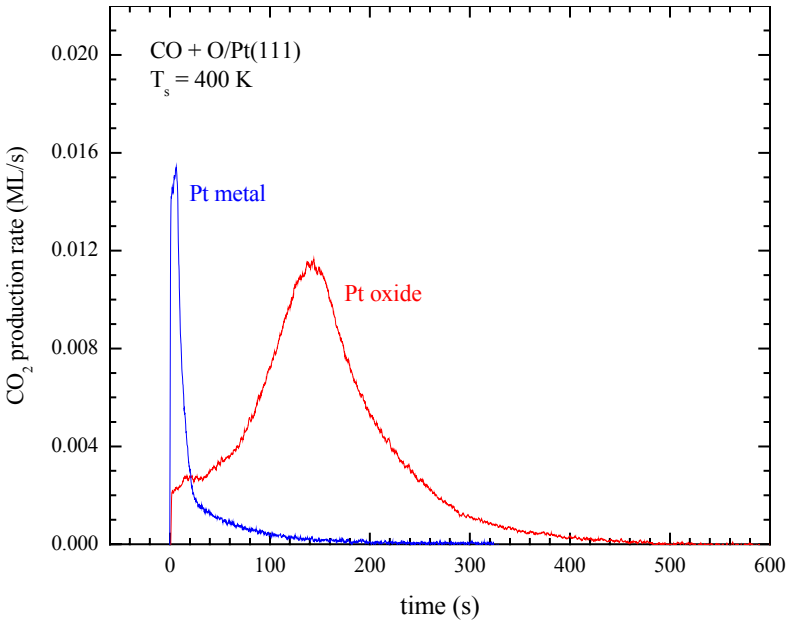
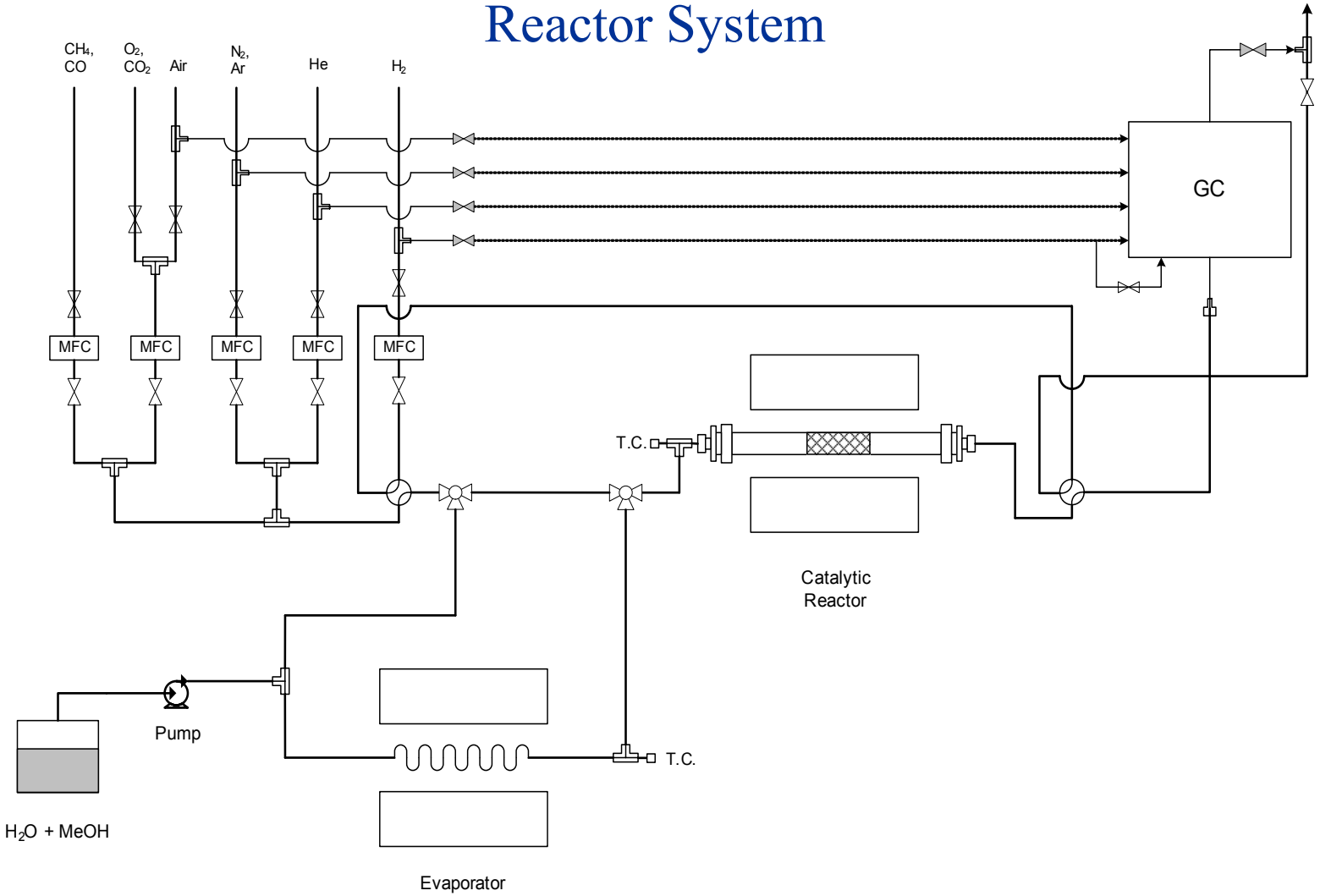




- First demonstration of Pt oxide growth in UHV using beams of oxygen atoms
- Enables detailed characterization of relevant surface oxygen phases
- Direct measurements of CO oxidation kinetics on Pt
- Low activity of Pt oxide

Accomplishments and Results, H. Weaver

Reactor System



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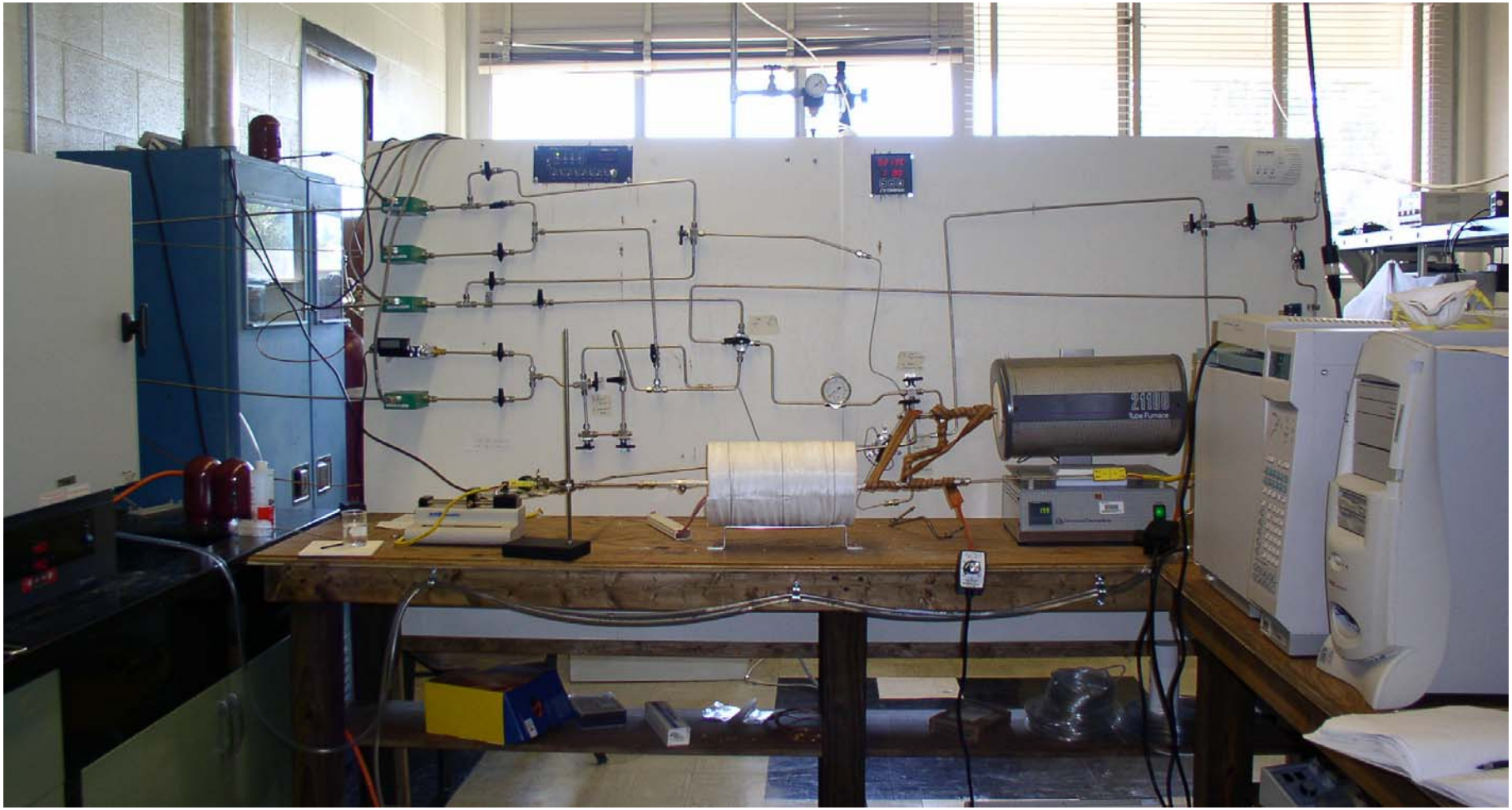
Reactor System



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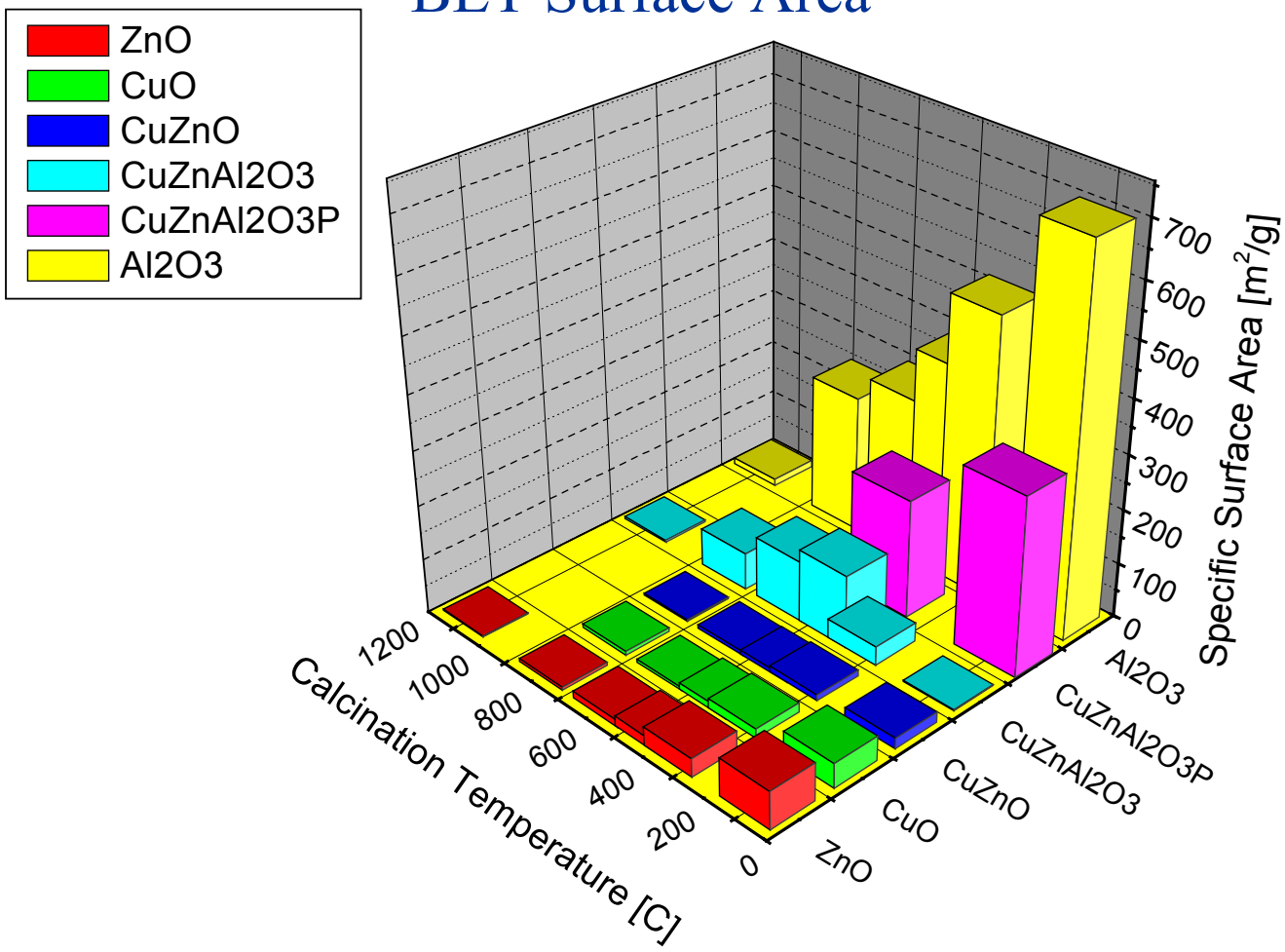
BET Surface Area



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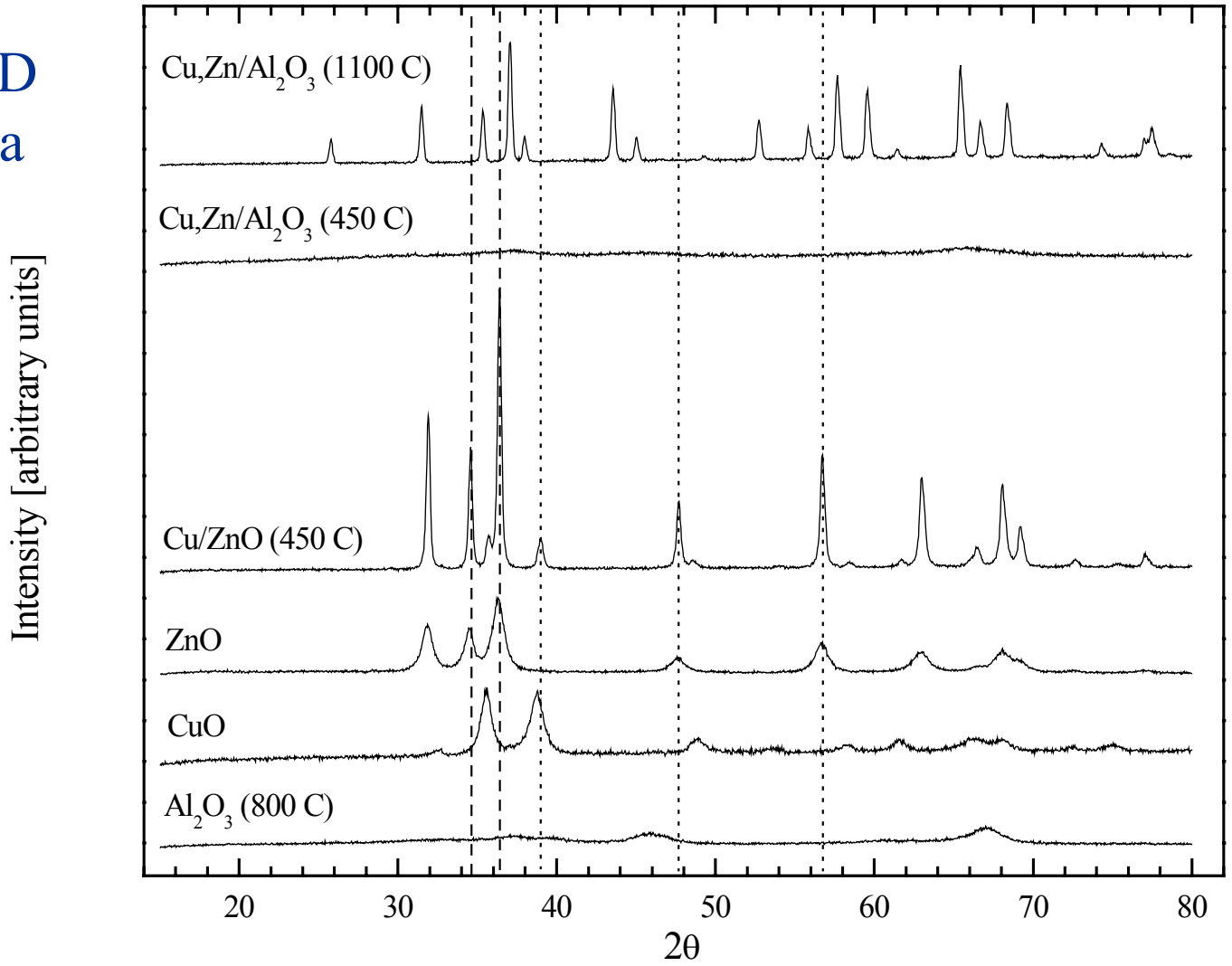
XRD Data



Future Plans

- Characterize structure and reactivity of Pt-Ru nanoclusters on oxide surfaces in UHV/STM system
- Examine properties of other Pt-bimetallics (Pd, Rh, Ag) to identify structure-property relations
- Activity measurements of prepared catalysts in reactor system
- Modify catalyst formulation according to activity measurements
- Determine how the catalytic activity is influenced by different factors:
  - Calcination temperature
  - Catalyst pretreatment
  - Catalyst preparation method
  - Catalyst support
  - Active metal particle size