

# ***Solar Water Splitting:*** **Photocatalyst Materials** **Discovery and Systems** **Development**

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This presentation does not contain any proprietary or confidential information

Project ID #  
PDP34

# Overview

## Timeline

- Anticipated July 1, 2005 start
- December 31, 2007 completion

## Budget

- \$3.75MM total
  - \$3.0MM DoE
  - \$750k GE/Caltech
- \$1.25MM FY05

## Barriers

Usable semiconductor bandgap:

### Materials Development

- Materials Efficiency
- Materials Durability
- Bulk Materials Synthesis

### Systems Development

- Systems Design and Evaluation

## Partners

Caltech



# Objectives

## Program Objectives:

- Development of Photoelectrochemical system exhibiting:
  - 9% Solar to hydrogen efficiency
  - > 10,000 hrs durability
  - < \$5.00 gge hydrogen costs

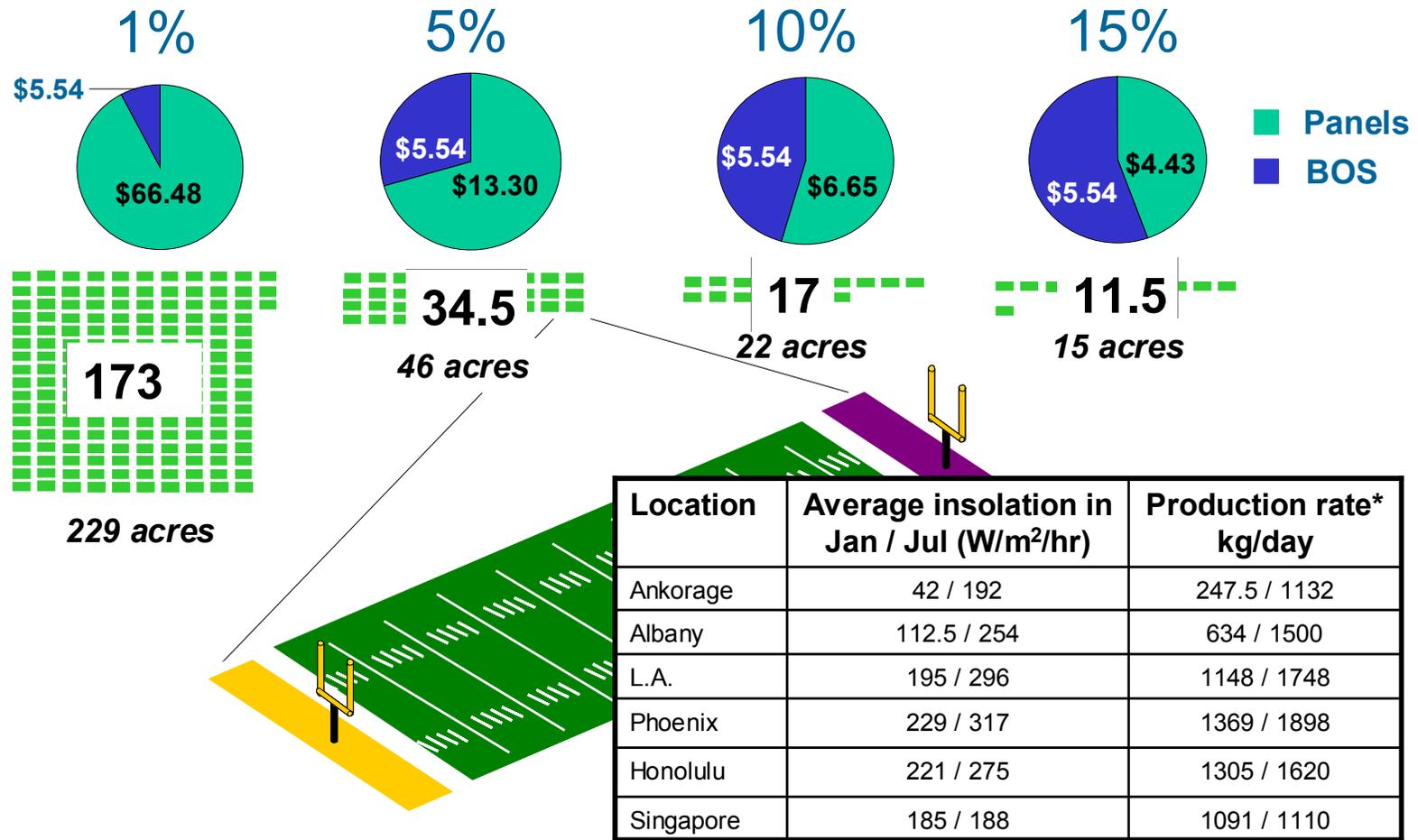
## FY05 Objectives:

- Increased materials efficiency through band-gap engineering
  - Valence band modification through anionic doping of oxides
  - Optimization of composition through high-throughput screening (HTS)
  - Optimization of particle morphology for cell design/manufacture
- Development of robust membrane technology



# Background

Example: 1000 kg/day remote refueling station in Albany, NY



\*assumes 10% efficiency

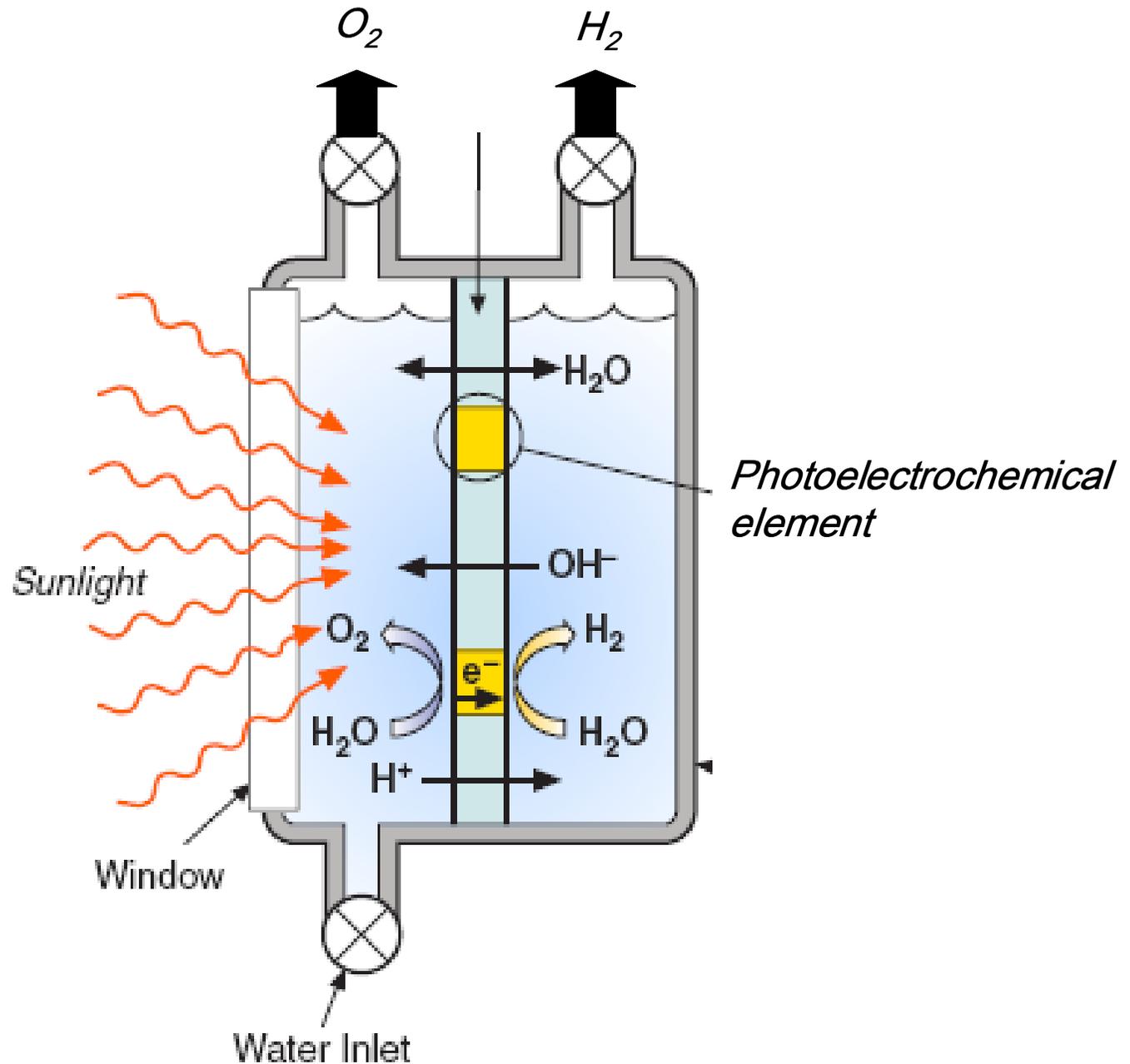
- System cost / efficiency critical technology drivers
- Performance regional



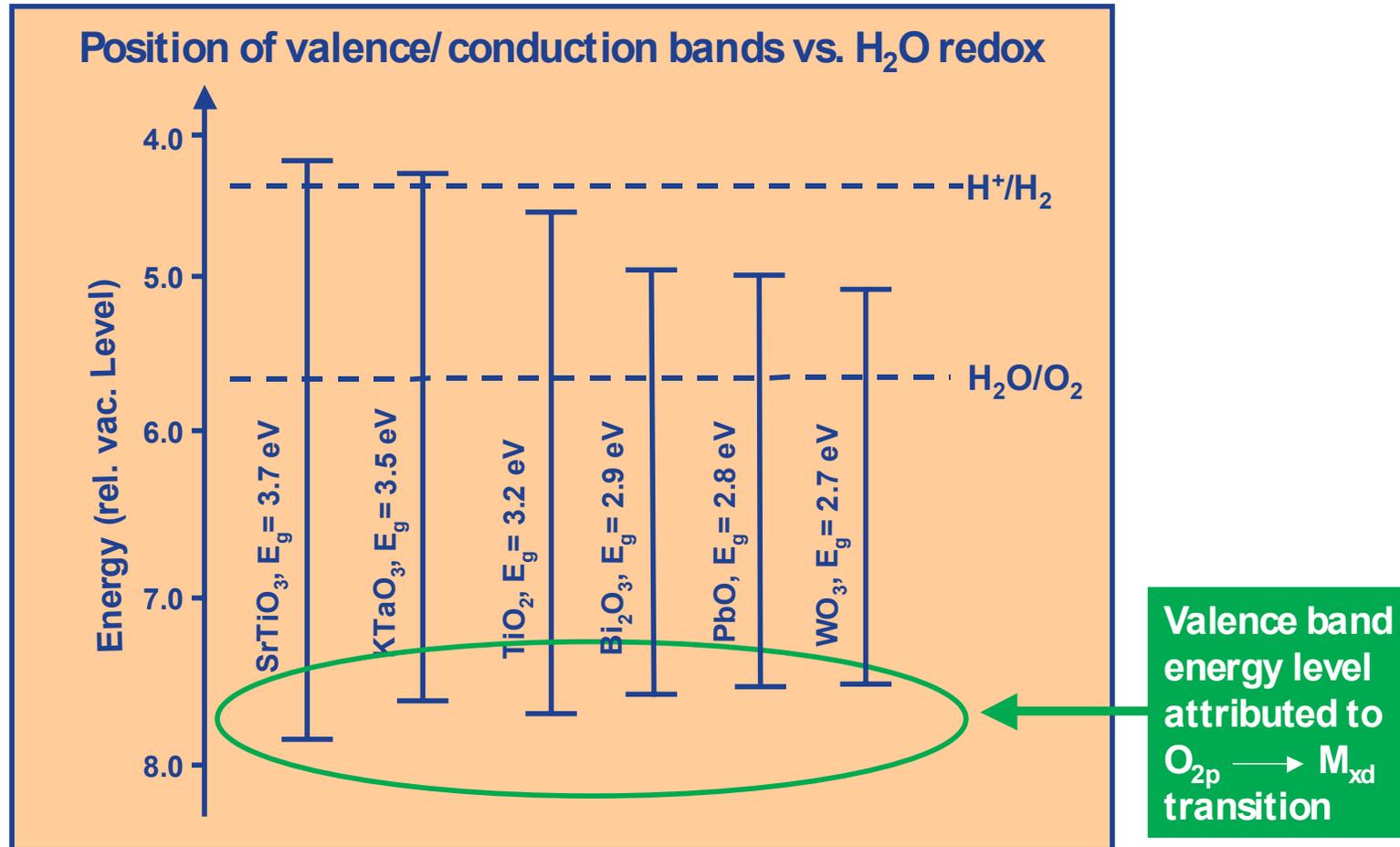
# Concept

## Advantages:

- reduced cost
- greater materials flexibility
- $H_2$  formed separately from  $O_2$

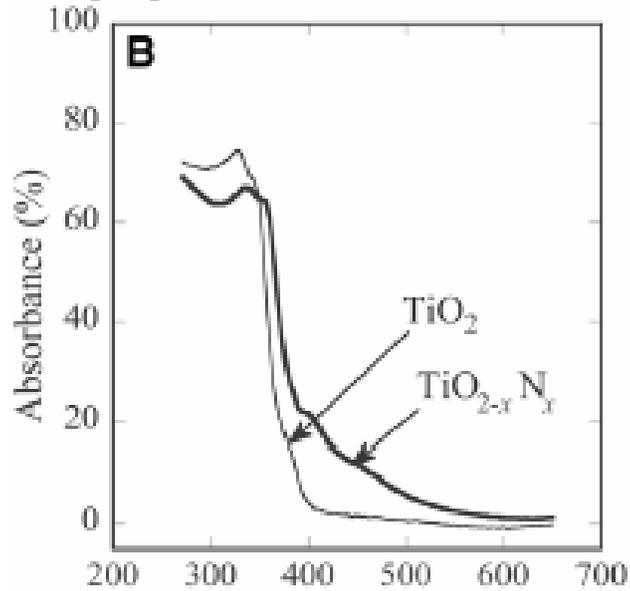


# Approach

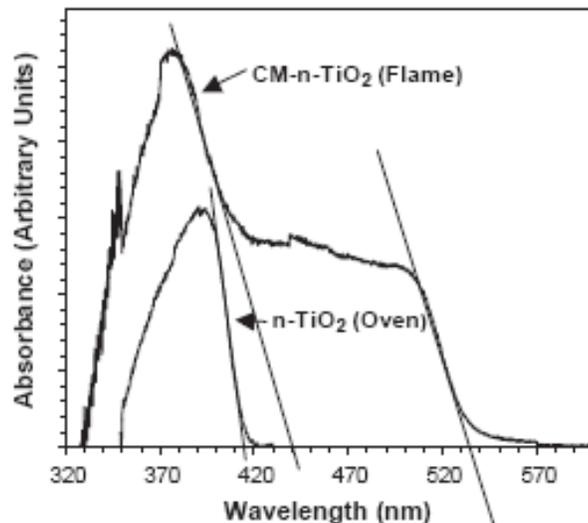


- Solar efficiency of oxides limited by VB position
- Anionic substitution offers potential of reducing VB energy level

# Approach



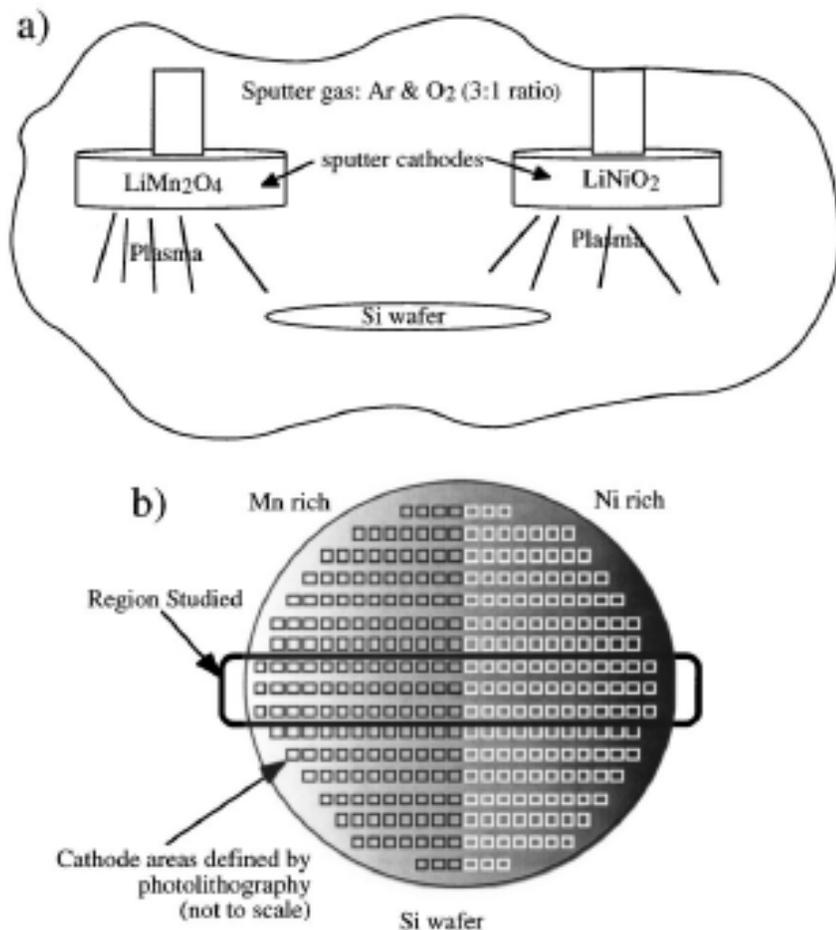
Asahi et.al., *Science*, **293** (2001) 269-271



Kung et.al., *Science*, **297** (2002) 2243-2245

- Anionic doping of  $\text{TiO}_2$  shown to reduce overall band-gap
- Conduction band effects not reported
- $\text{TiO}_{2-x}\text{N}_x$  and  $\text{TiO}_{2-x}\text{C}_x$  not optimized
- Other systems (e.g.  $\text{SrTiO}_3$ ,  $\text{KTaO}_3$  not reported
- Long-term stability unknown

# Approach

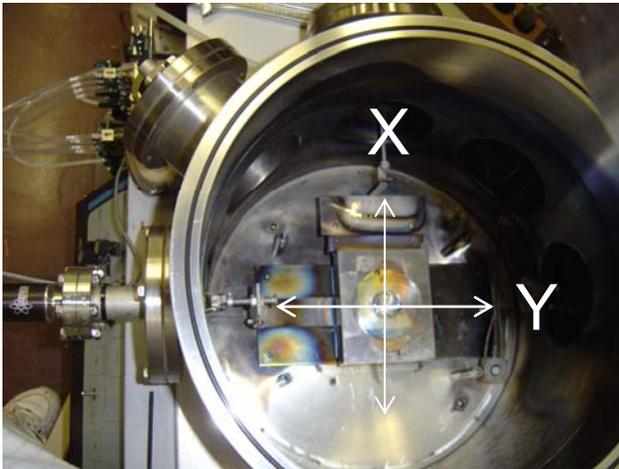


- HTS demonstrated as useful technique to measure effects of compositional perturbation
- HTS coupled with reactive sputtering deposition to optimize concentration of nitrogen/carbon substitution

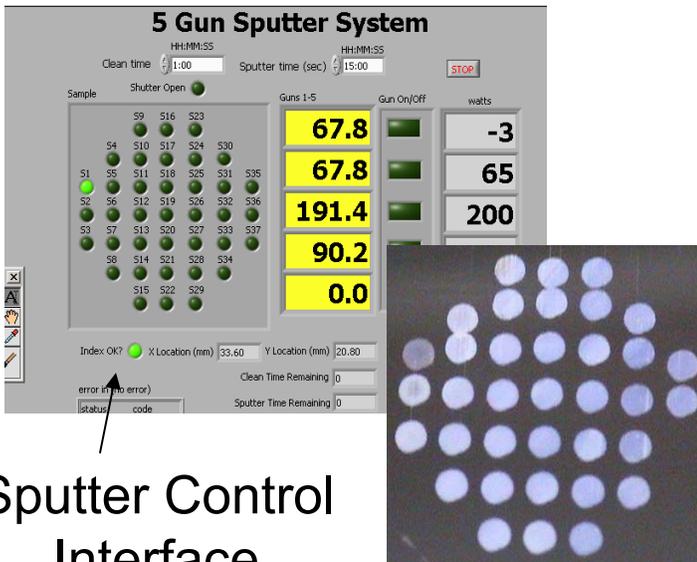
*Journal of The Electrochemical Society*, 150 (12) A1676-A1683 (2003)

# Technical Progress

Compositional optimization by HTS:



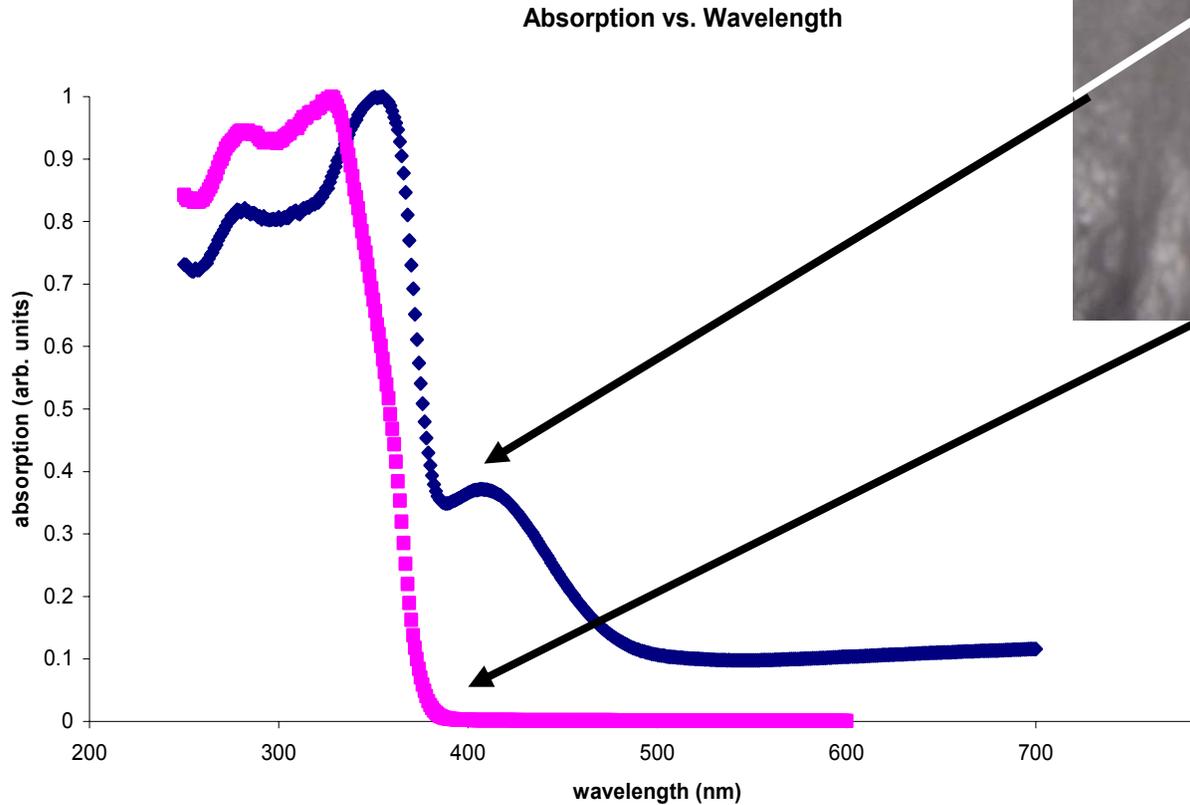
- X-Y stage allows 48 samples to be sputtered sequentially
- Each sample can be sputtered at different N/Ar flow ratio varying from 0 to 20 vol%.
- Electronic circuitry fabricated directly on top of each sample
- Direct photoelectrochemical measurement.



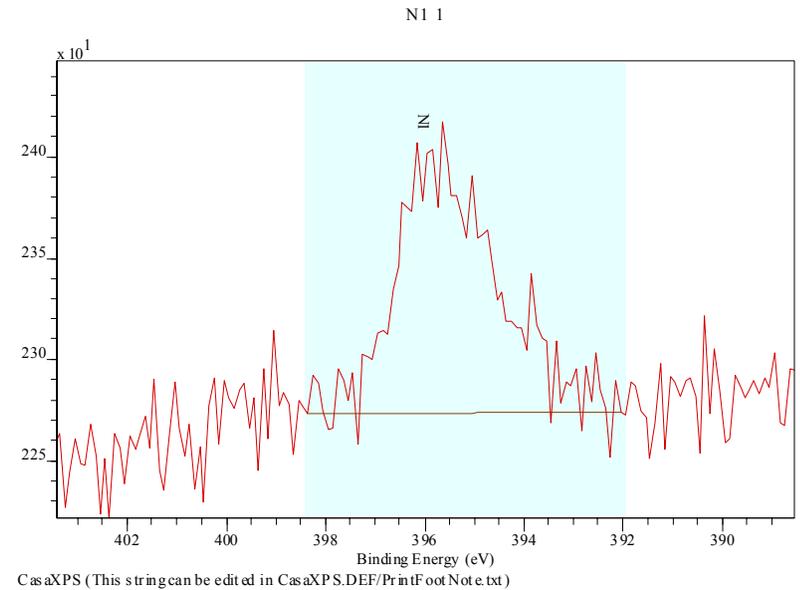
Sputter Control Interface

# Technical Progress

Valence band modification:

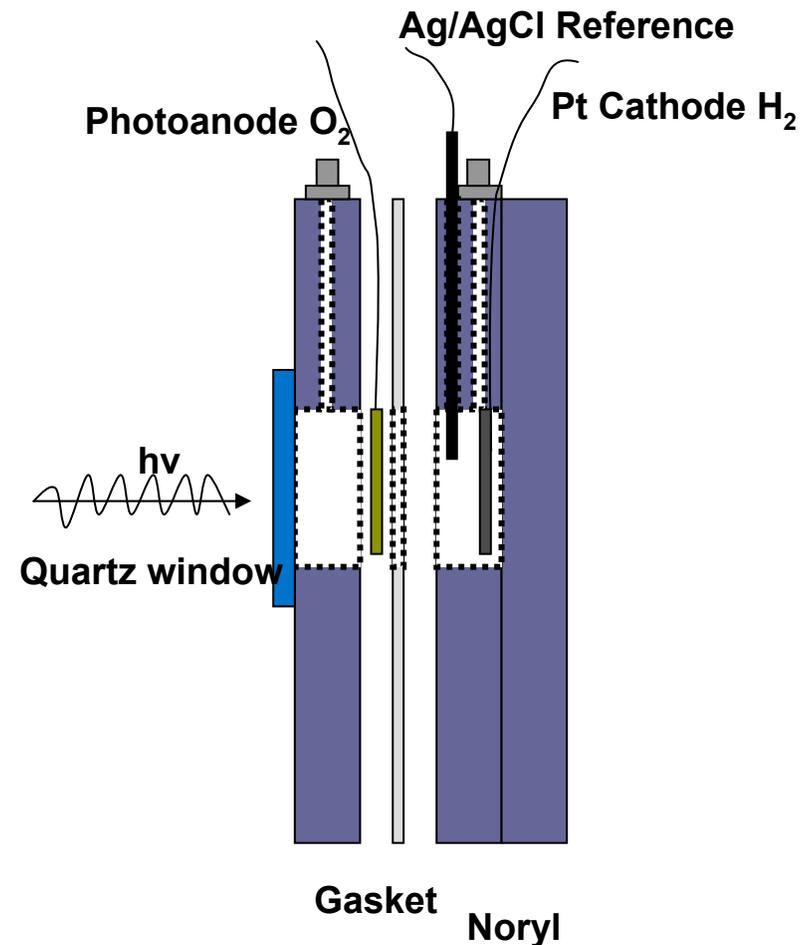
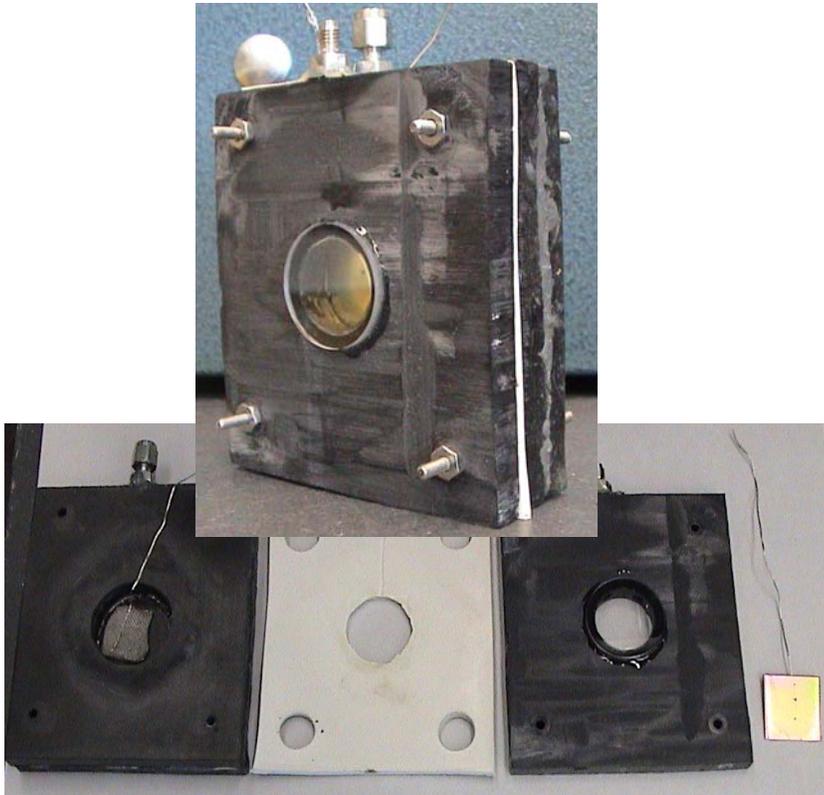


• Nitrogen substitution leads to absorbance state at lower energy



# Technical Progress

Photoelectrochemical cell:



- Modular
- Split-cell, membrane cell, particulate capability
- Upgradeable

# Future Work

- High throughput screening:
  - 48 sample thin-film array with individually-addressable cells for dopant optimization
  - nitrogen, carbon doping of oxides
- Powder optimization:
  - Optimization of powder morphology for incorporation into membranes
  - Bulk synthesis of powders identified in HTS
  - VB, CB measurements by UPS
- Membrane development:
  - Processing optimization
  - Characterization / optimization of surface morphology
  - Membrane-based photoelectrochemical testing