Solar Water Splitting: Photocatalyst Materials Discovery and Systems Development

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GE Global Research
May 23, 2005

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

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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

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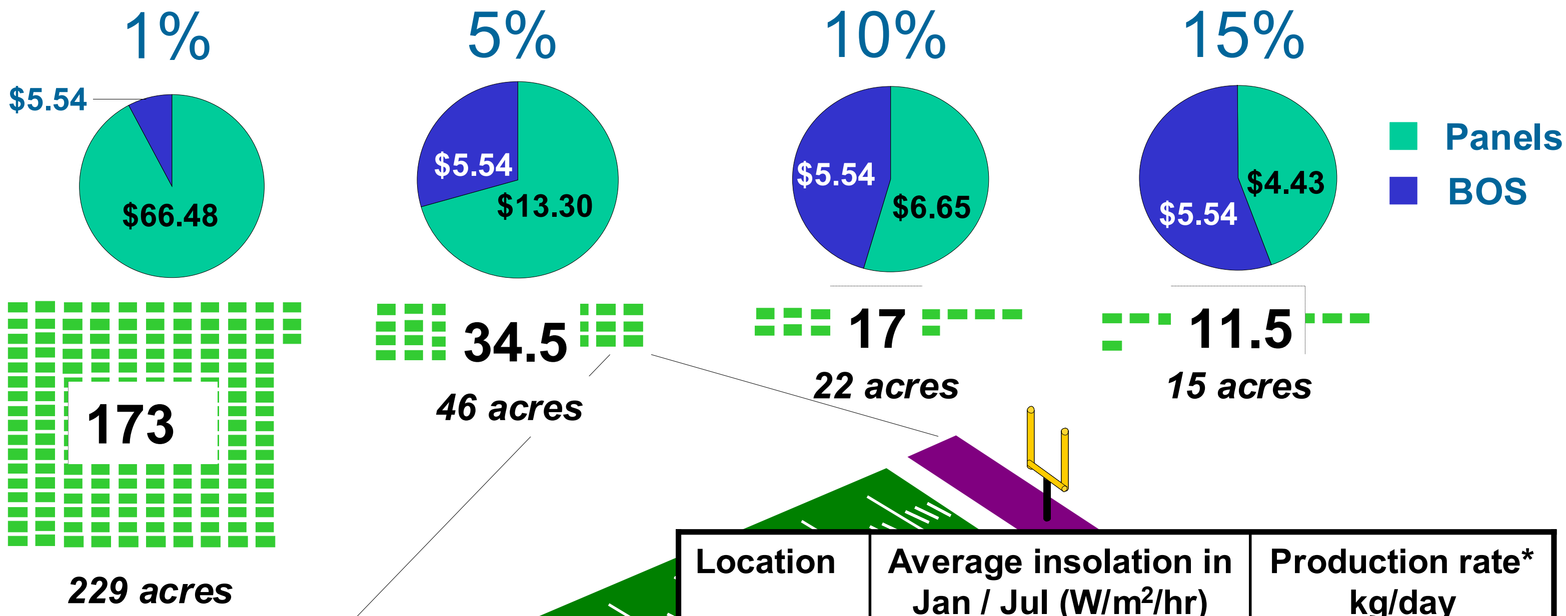
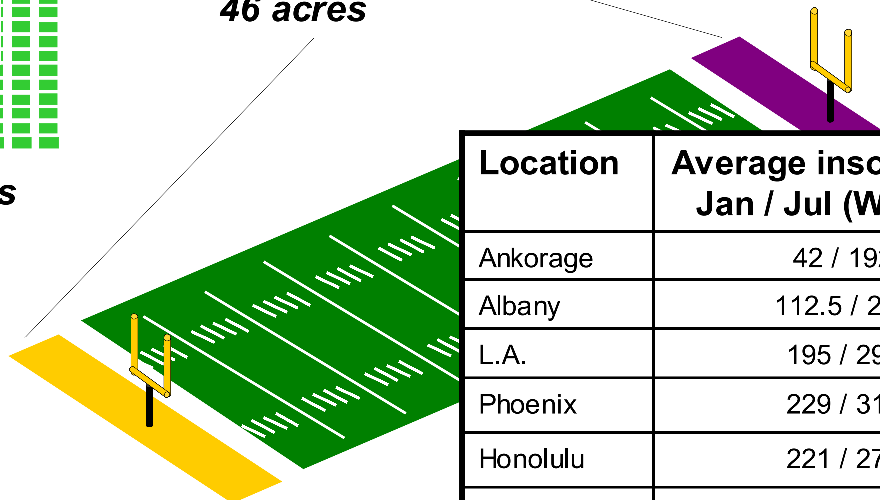
Background

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





Location	Average insolation in Jan / Jul ($W/m^2/hr$)	Production rate* kg/day
Ankorage	42 / 192	247.5 / 1132
Albany	112.5 / 254	634 / 1500
L.A.	195 / 296	1148 / 1748
Phoenix	229 / 317	1369 / 1898
Honolulu	221 / 275	1305 / 1620
Singapore	185 / 188	1091 / 1110

*assumes 10% efficiency

- System cost / efficiency critical technology drivers
- Performance regional

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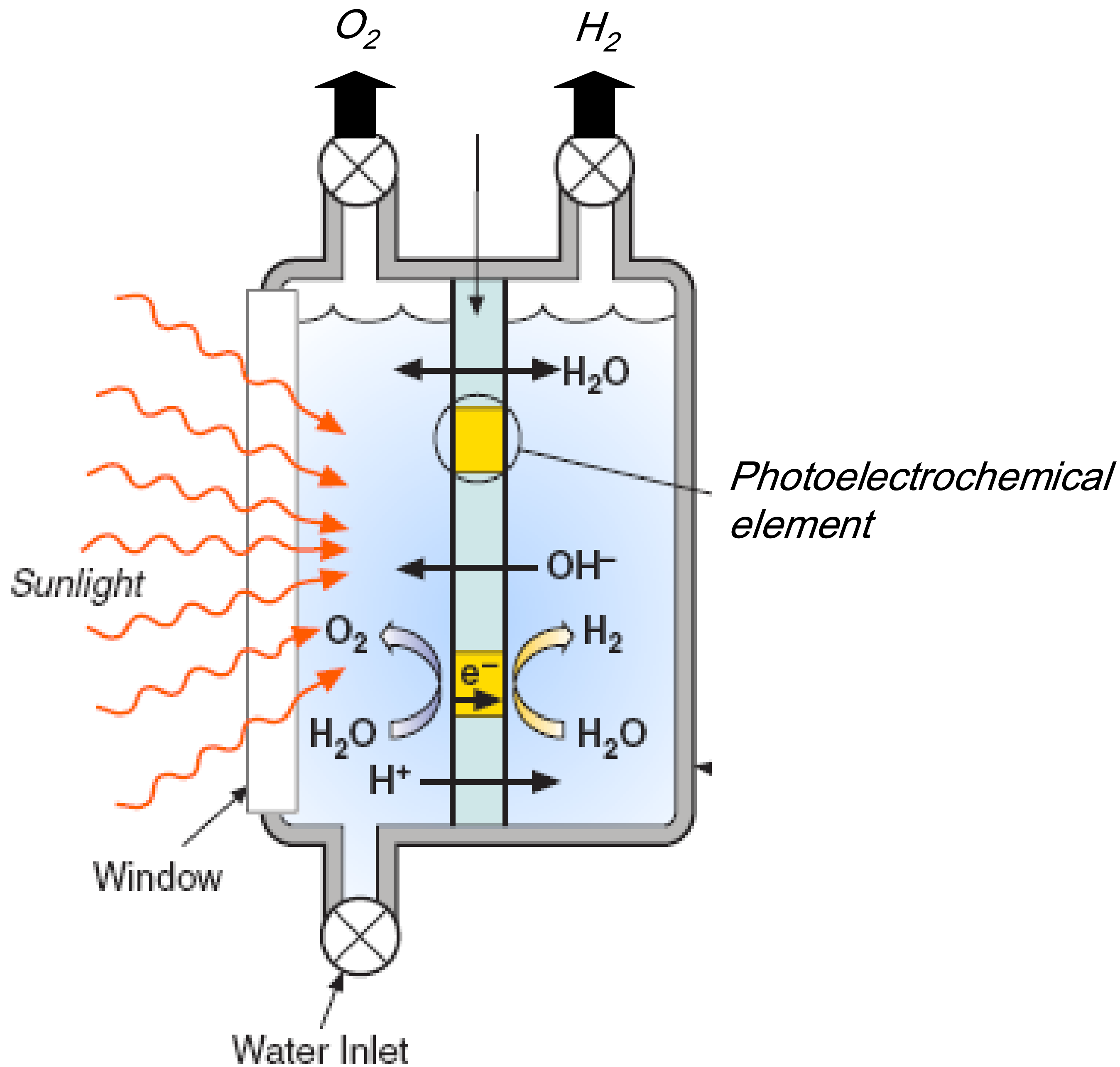
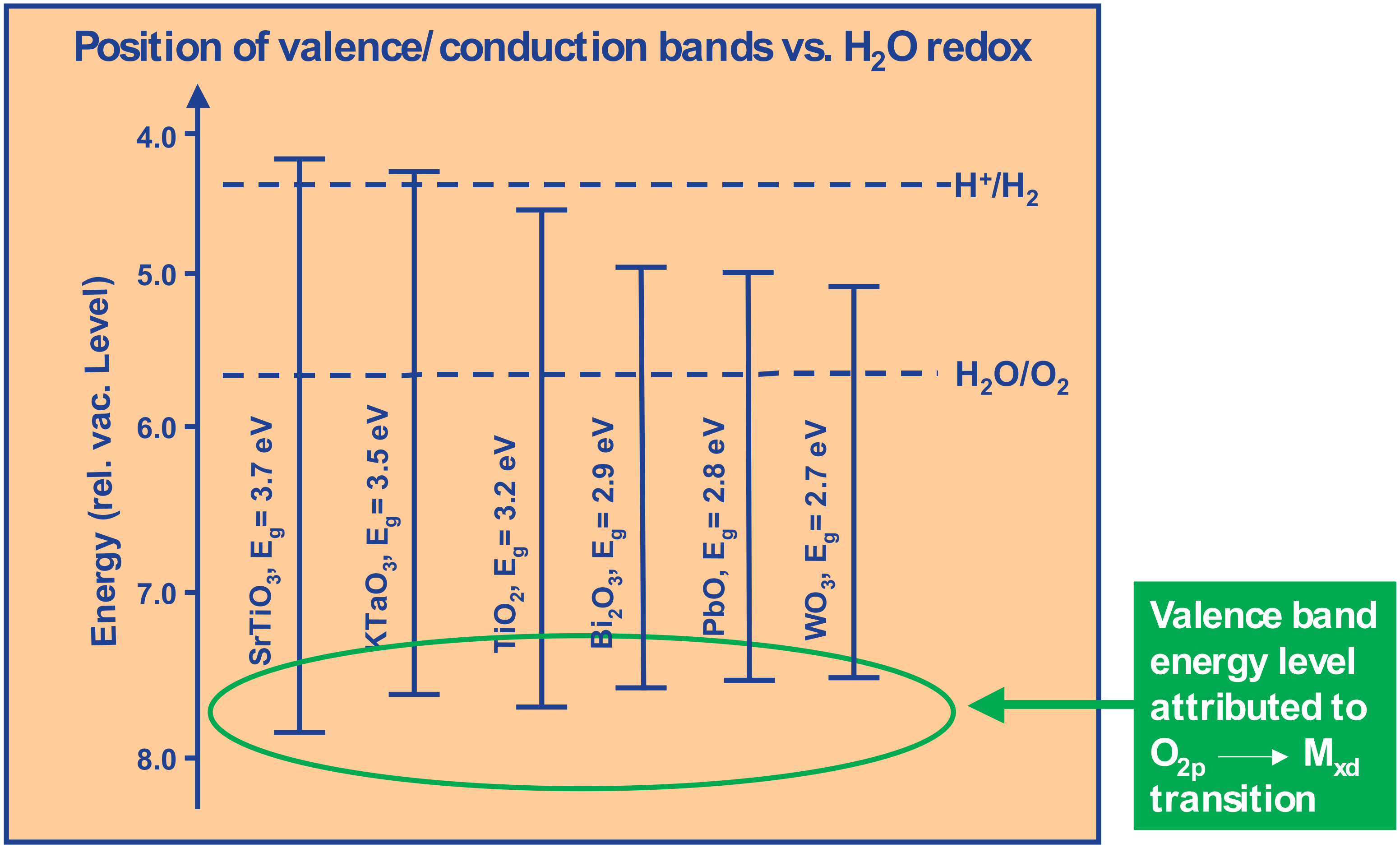
Concept



<u>Advantages</u>:
- 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

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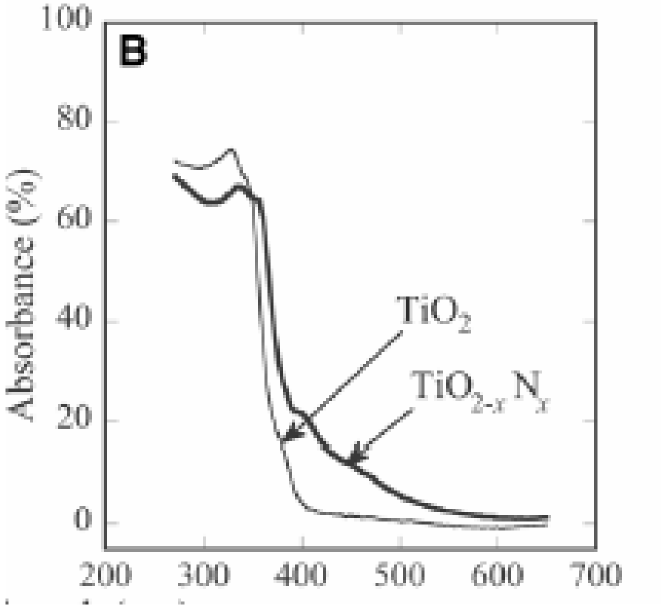
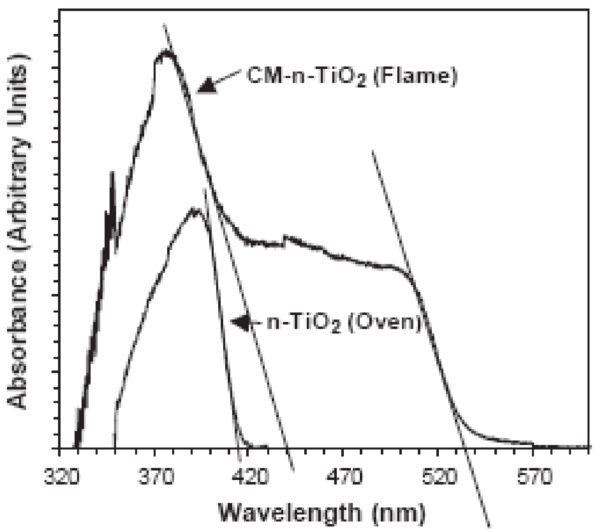
Approach



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



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

- Anionic doping of TiO_2 shown to reduce overall band-gap
- Conduction band effects not reported
- $TiO_{2-x}N_x$ and $TiO_{2-x}C_x$ not optimized
- Other systems (e.g. $SrTiO_3$, $KTaO_3$ not reported
- Long-term stability unknown

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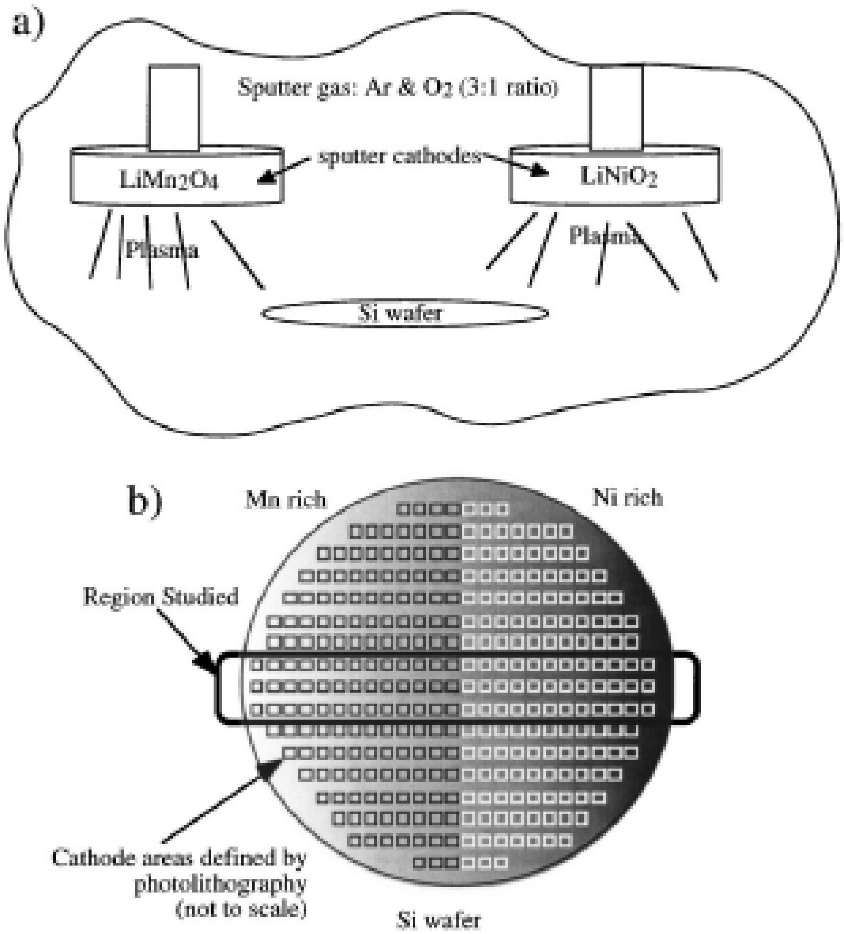
Approach



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

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

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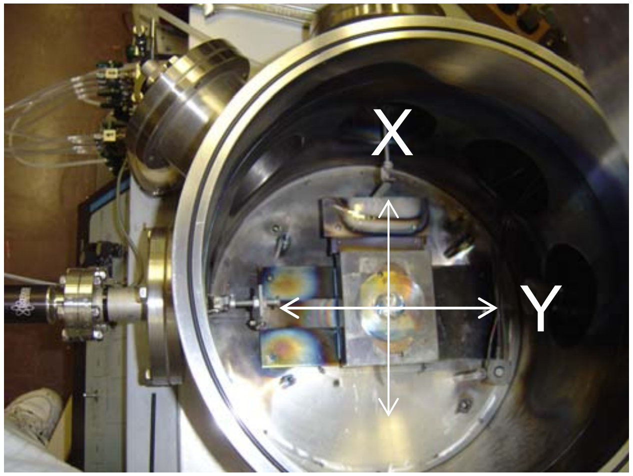
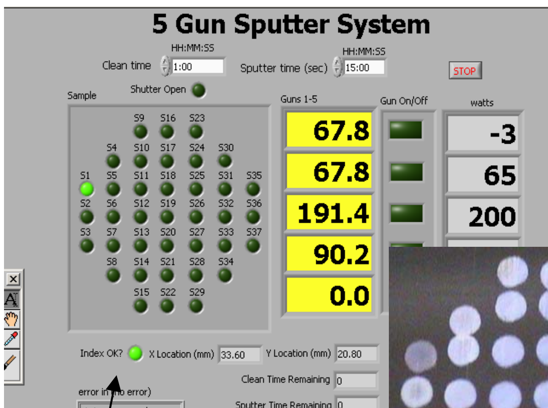
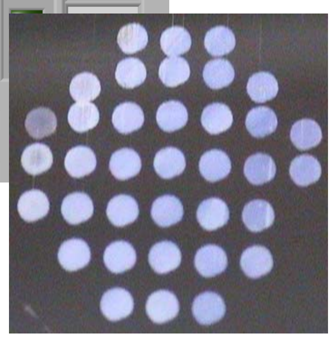
Technical Progress

Compositional optimization by HTS:







Sputter Control Interface

- 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.

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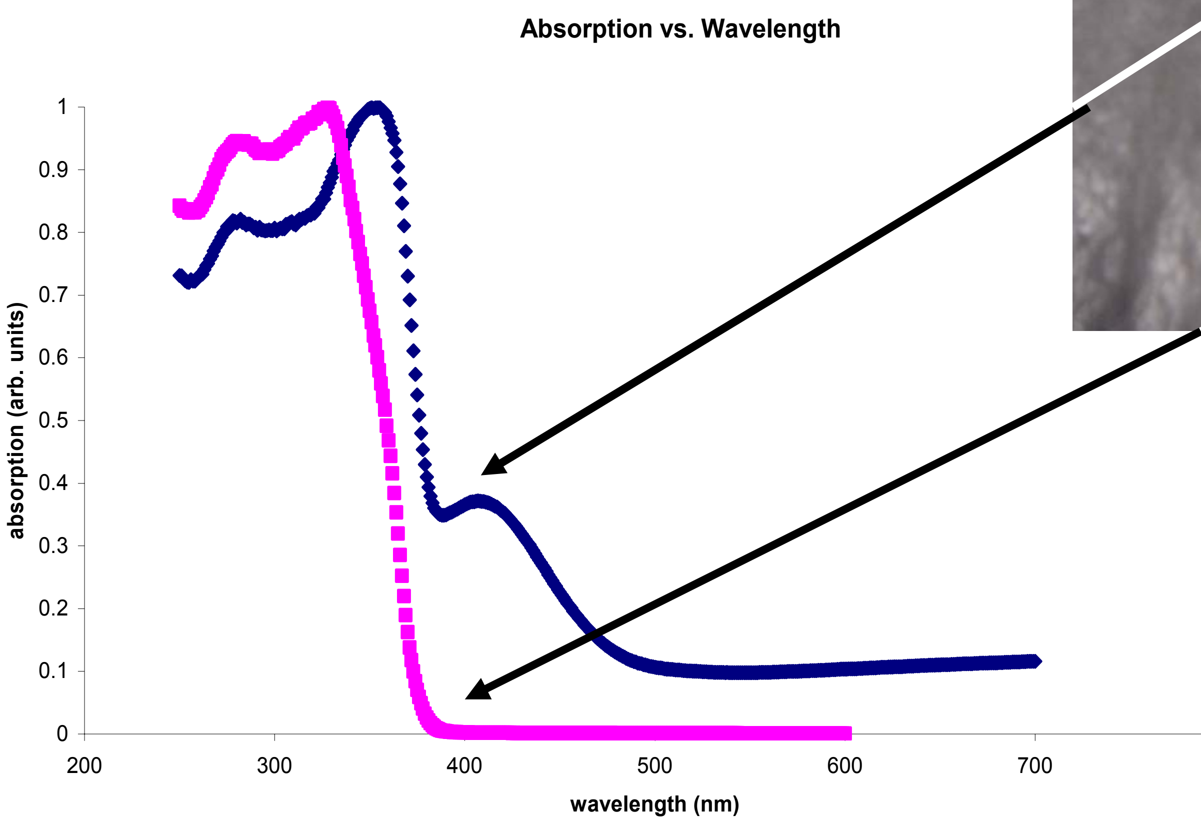
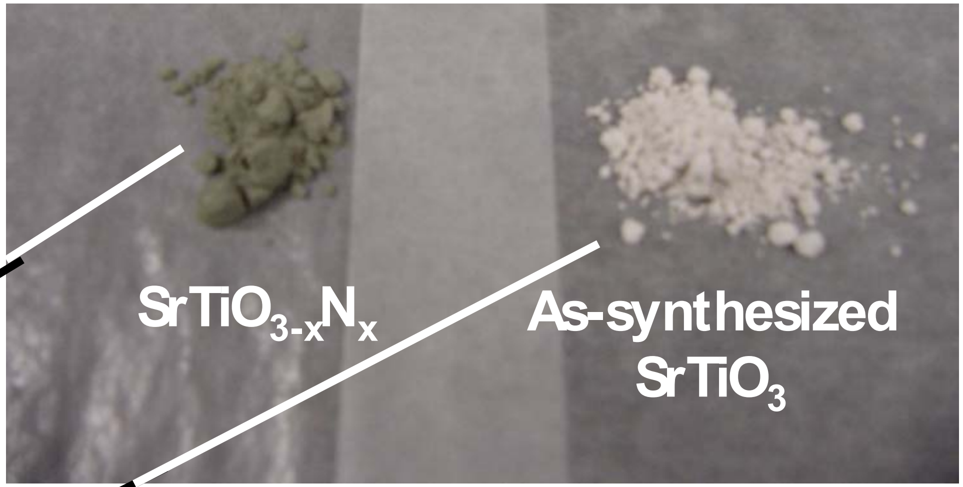
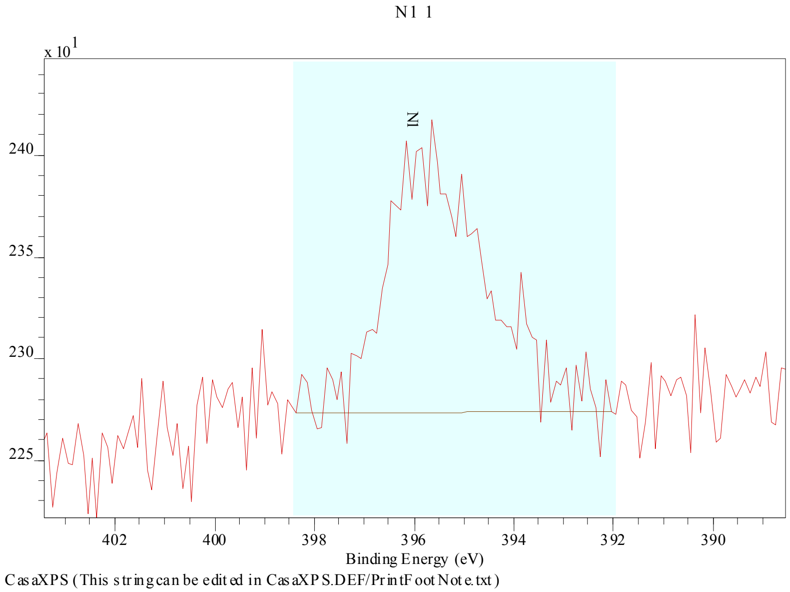
Technical Progress

Valence band modification:



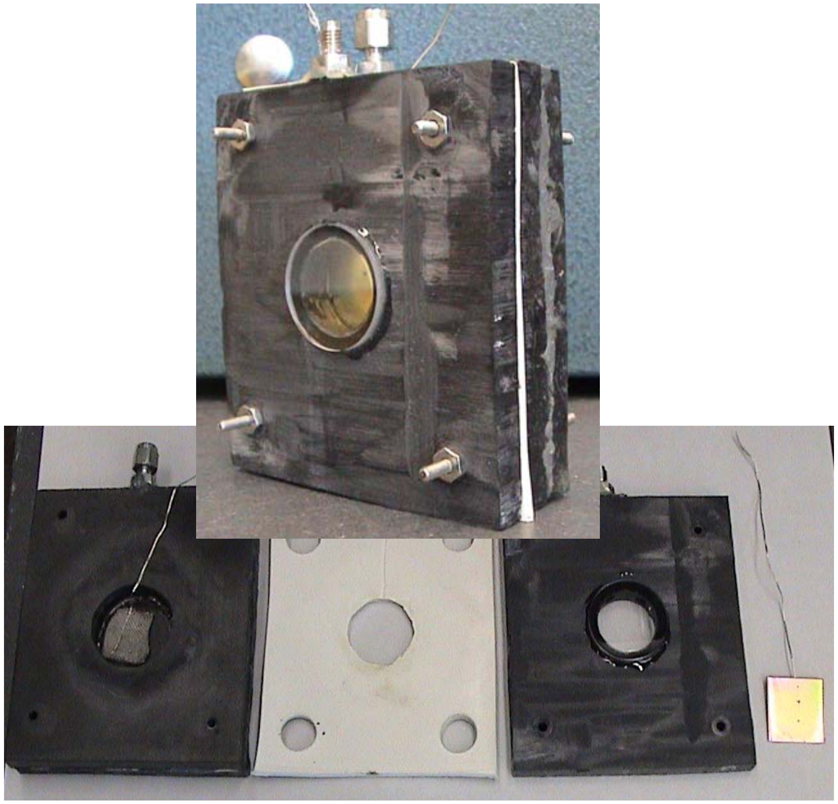


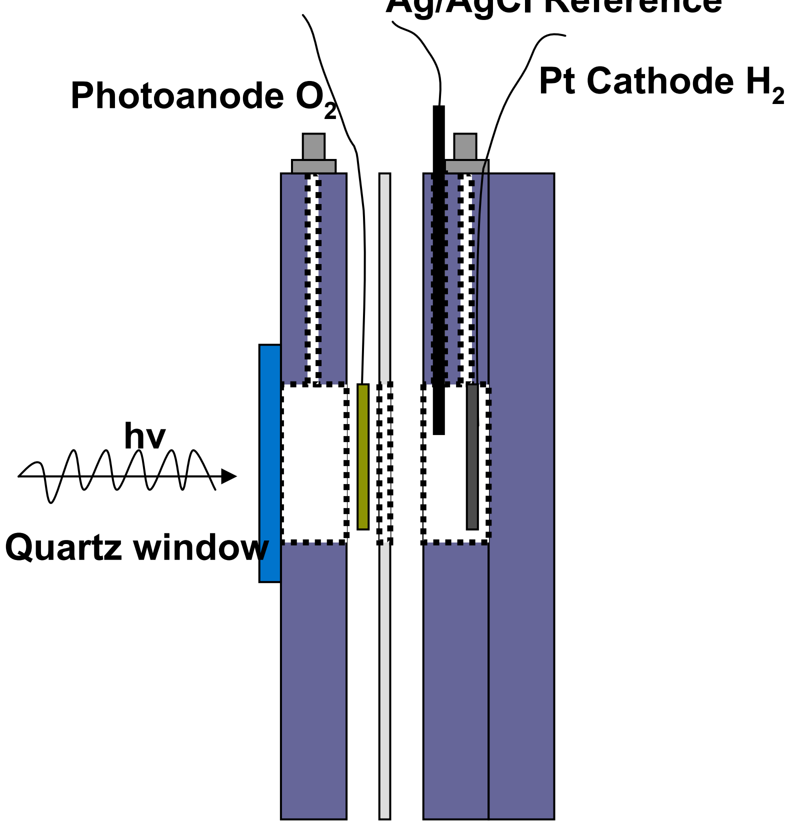


- Nitrogen substitution leads to absorbance state at lower energy

Technical Progress

Photoelectrochemical cell:





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

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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