

New Metal Oxides for Efficient Hydrogen Production via Solar Water Splitting

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Project ID #
PD118

Overview

Timeline

- Start date: 9/2014
- Project end date: 8/2017
- Percent complete: 25%

Budget

- Total project funding
\$740,000
- Funding received in FY14
\$240,000
- Funding for FY15
\$250,000

Barriers

- Barriers addressed
 - Y. Materials efficiency
 - Z. Materials durability
 - AB. Materials synthesis

Partners

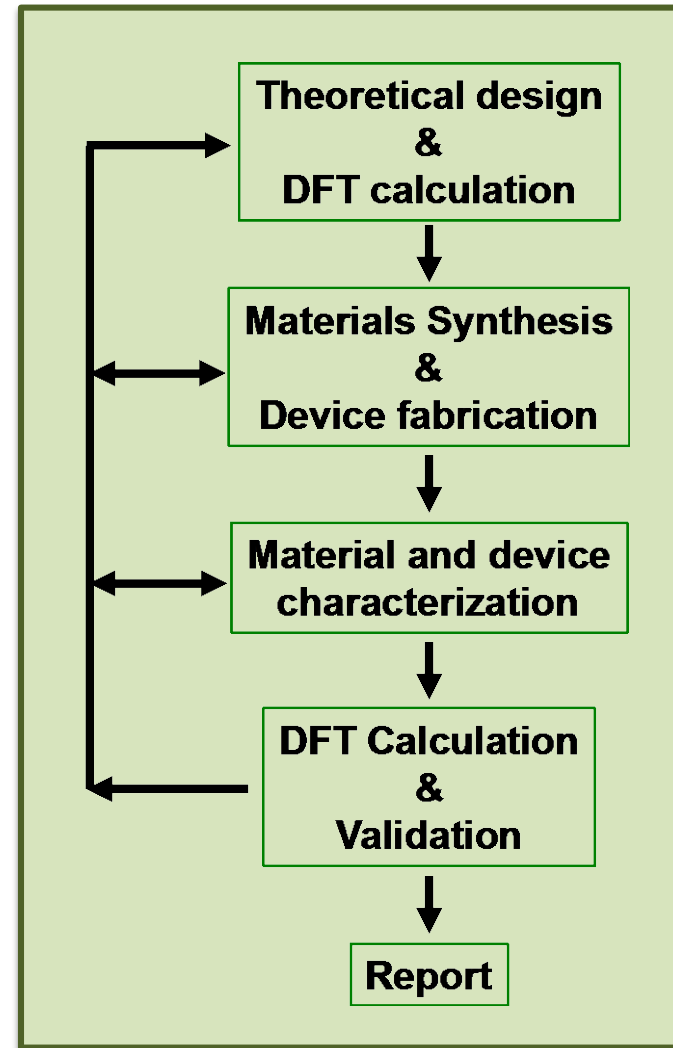
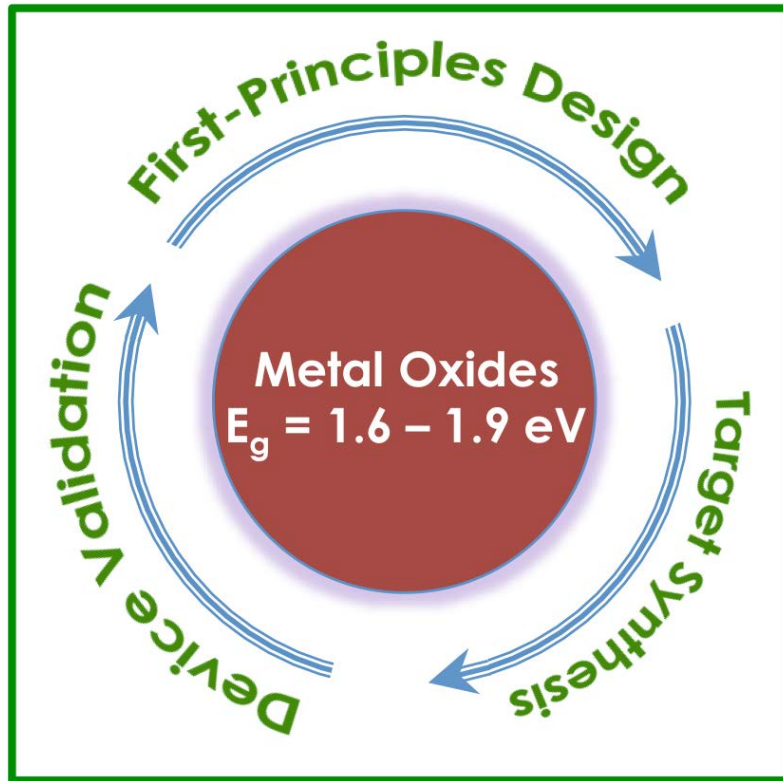
- National Renewable Energy Laboratory

Relevance

Project Objectives

- Design new metal oxides for PEC hydrogen production
- Develop approaches for synthesizing designed metal oxides
- Examine PEC properties of new metal oxides
- Education and outreach

Approach



Approach/Milestone

Milestone 1. Designing of new metal oxides

- 1.1 Develop design principles
- 1.2 Density-functional theory calculation

Milestone 2. Synthesis of new metal oxides

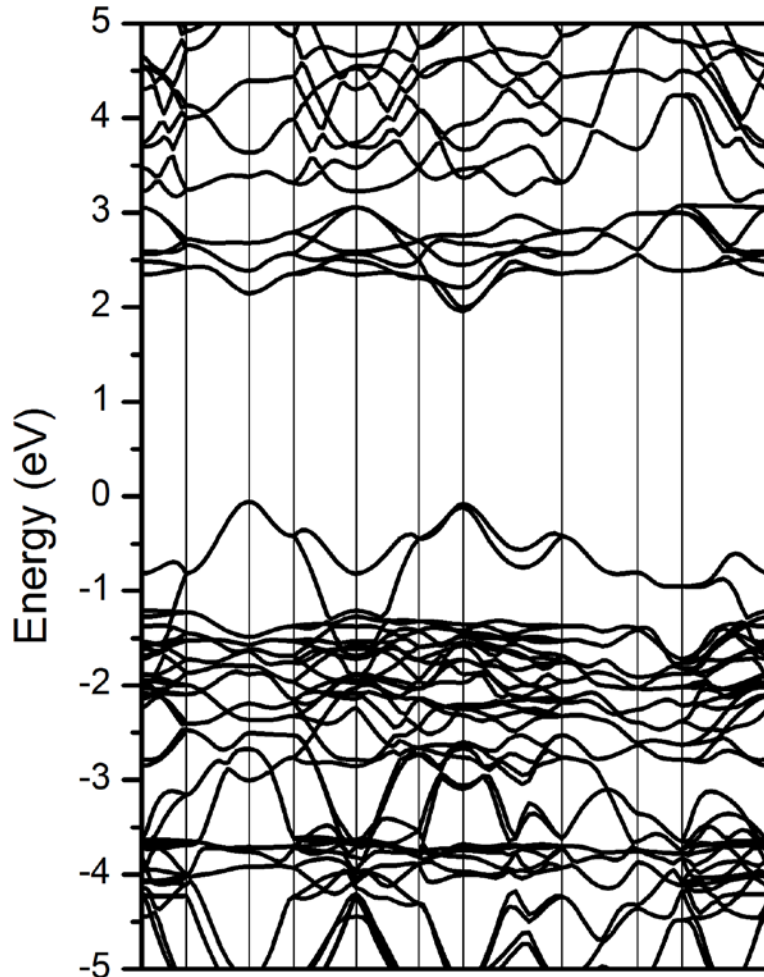
- 1.1 Synthesis bulk material
- 1.2 Synthesis of thin films

Milestone 3. PEC performance of new metal oxides

- 1.1 PEC measurement of small cells
- 1.2 Develop overall PEC systems

Accomplishments and Progress

1. Designing of new metal oxides

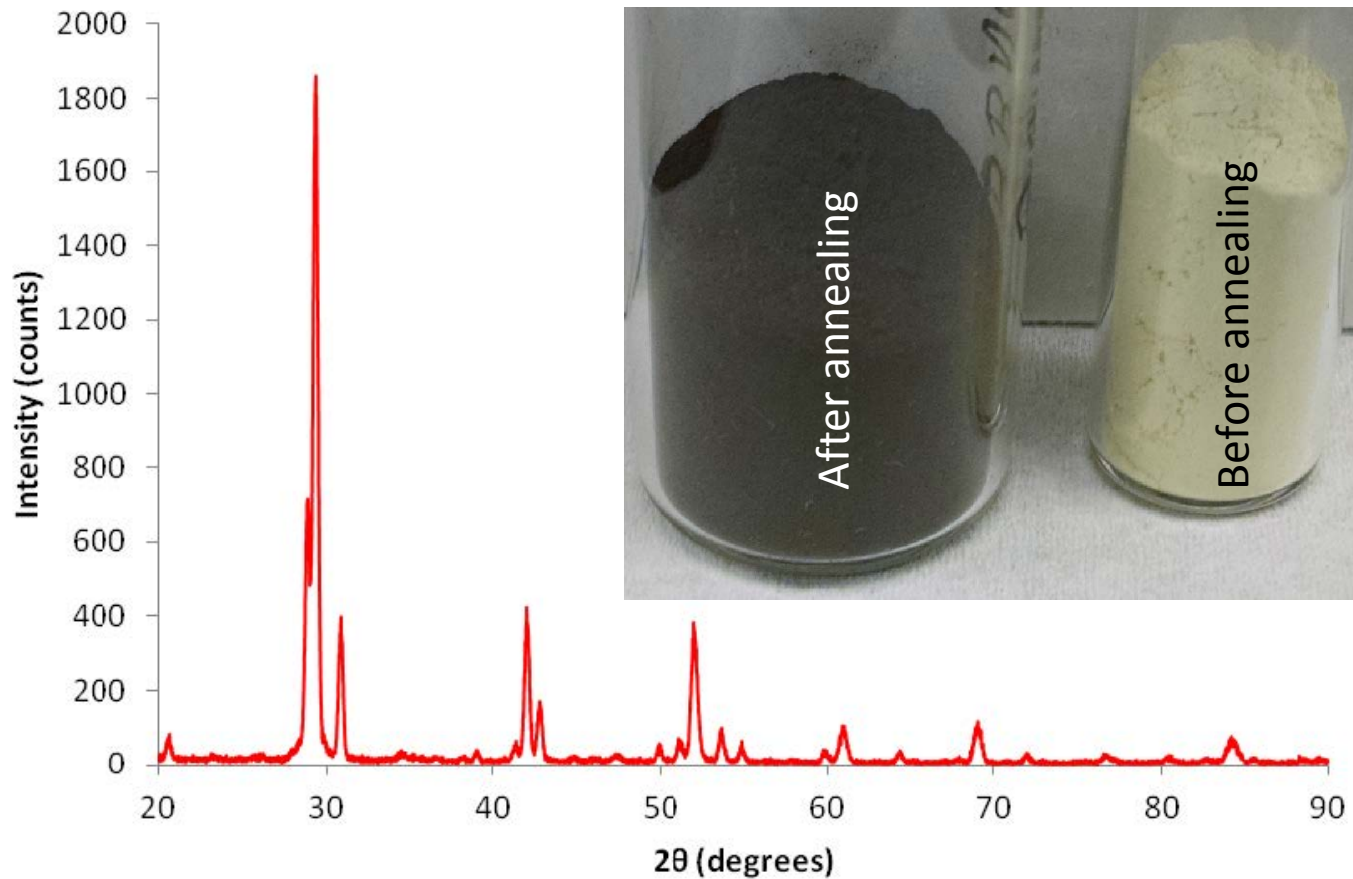


Calculated DFT band structure of B₂NO

Band gap: ~2.0 eV

Accomplishments and Progress (cont.)

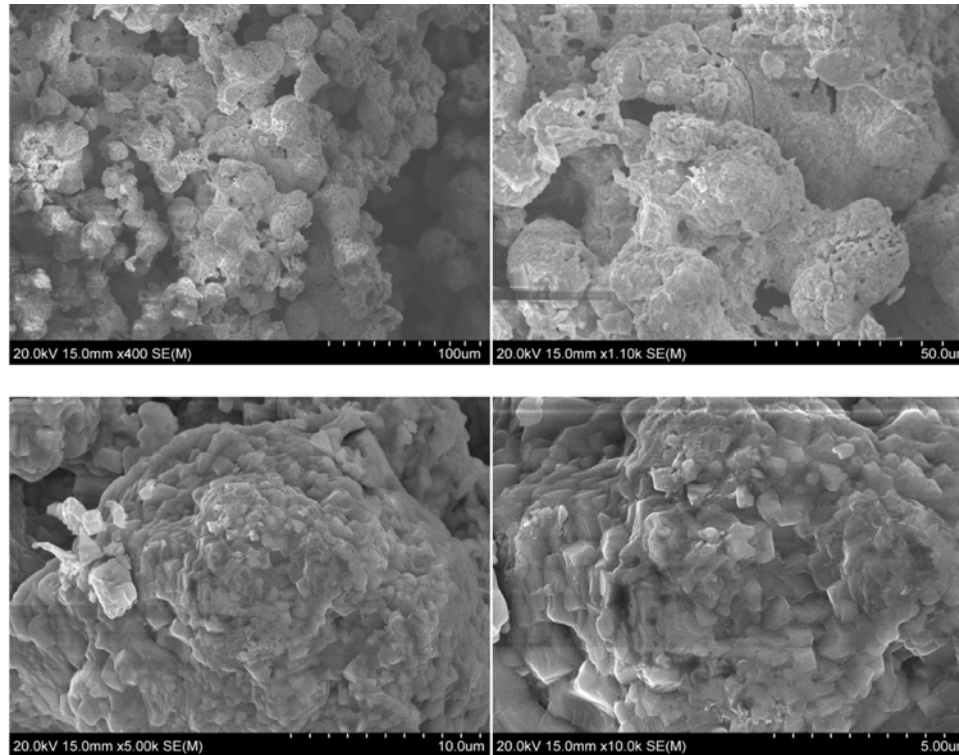
2. Synthesis of new metal oxides-bulk materials



XRD curve from annealed B₂NO powder

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-bulk materials

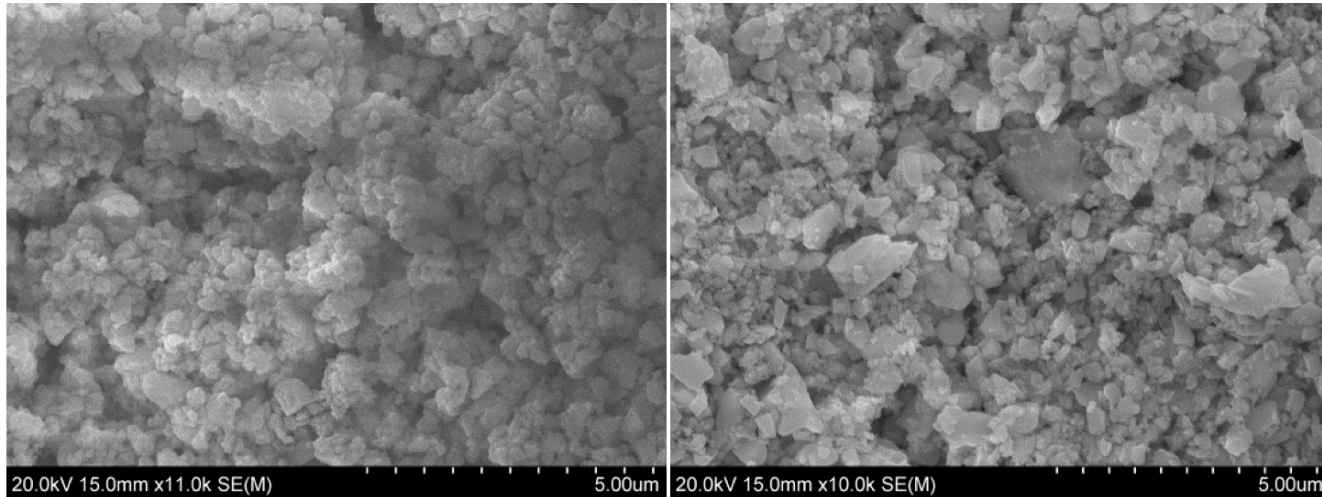


SEM images of the annealed B₂NO powder at various magnifications

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

(Spin & Dip Coating)

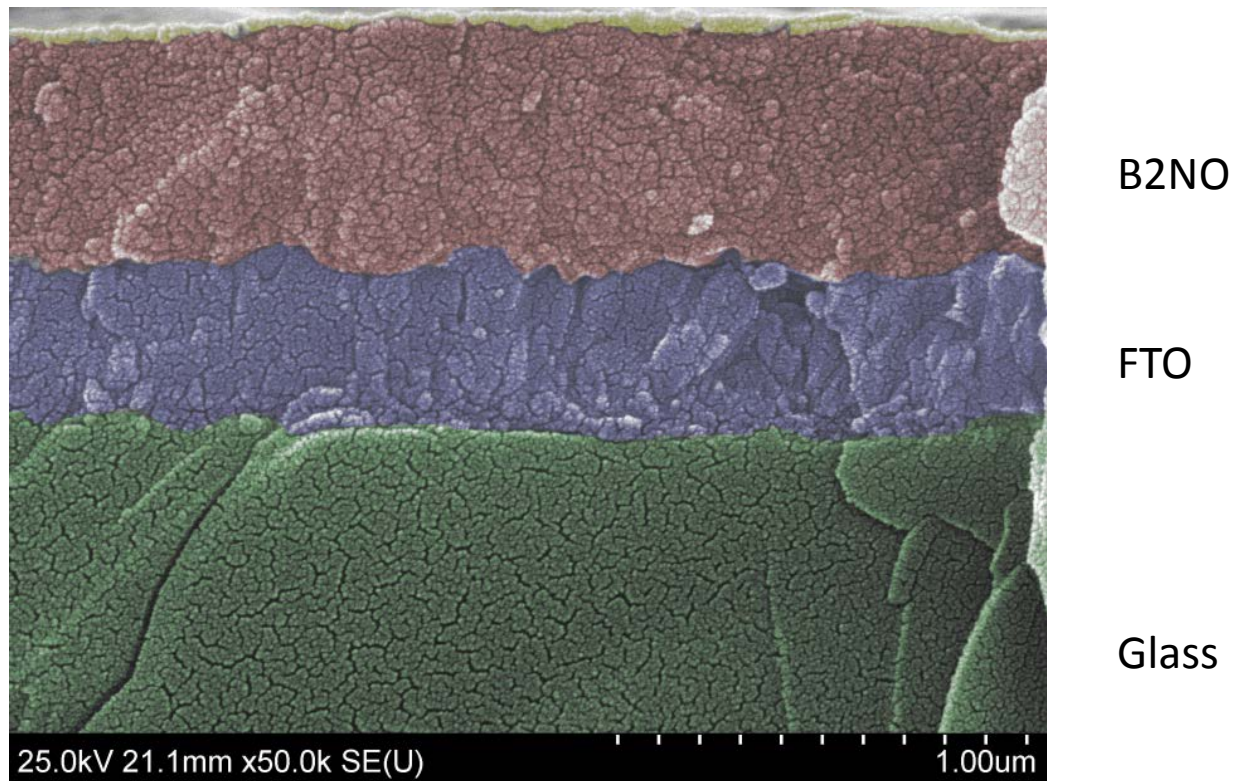


Plane view images of spin coated (left) and dip coated (right) films

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

(RF sputtering)

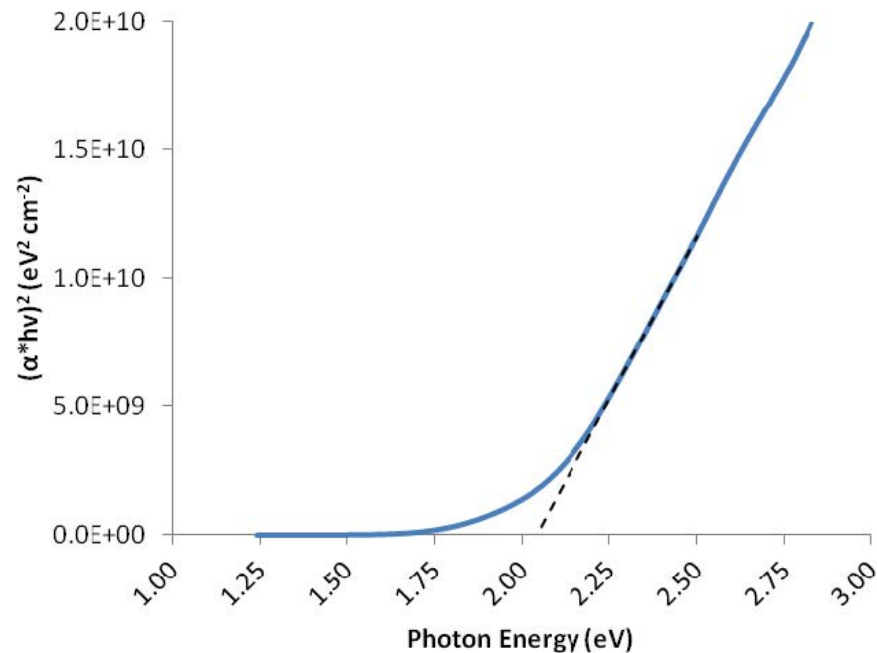


Cross sectional SEM image of a RF sputtered film

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

(RF sputtering)

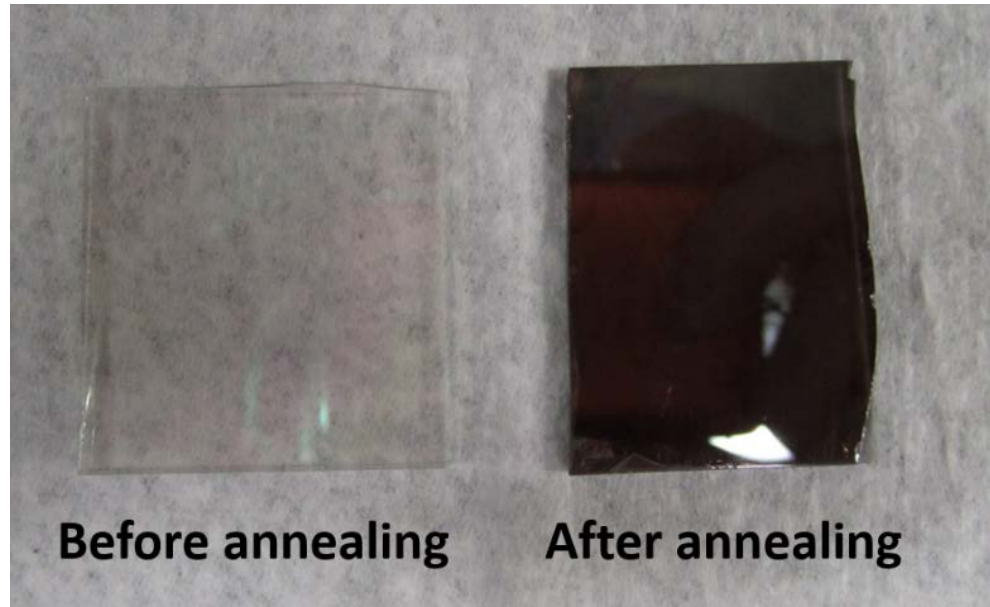


Direct band gap estimation from Tauc plot

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

(Spin-coating)

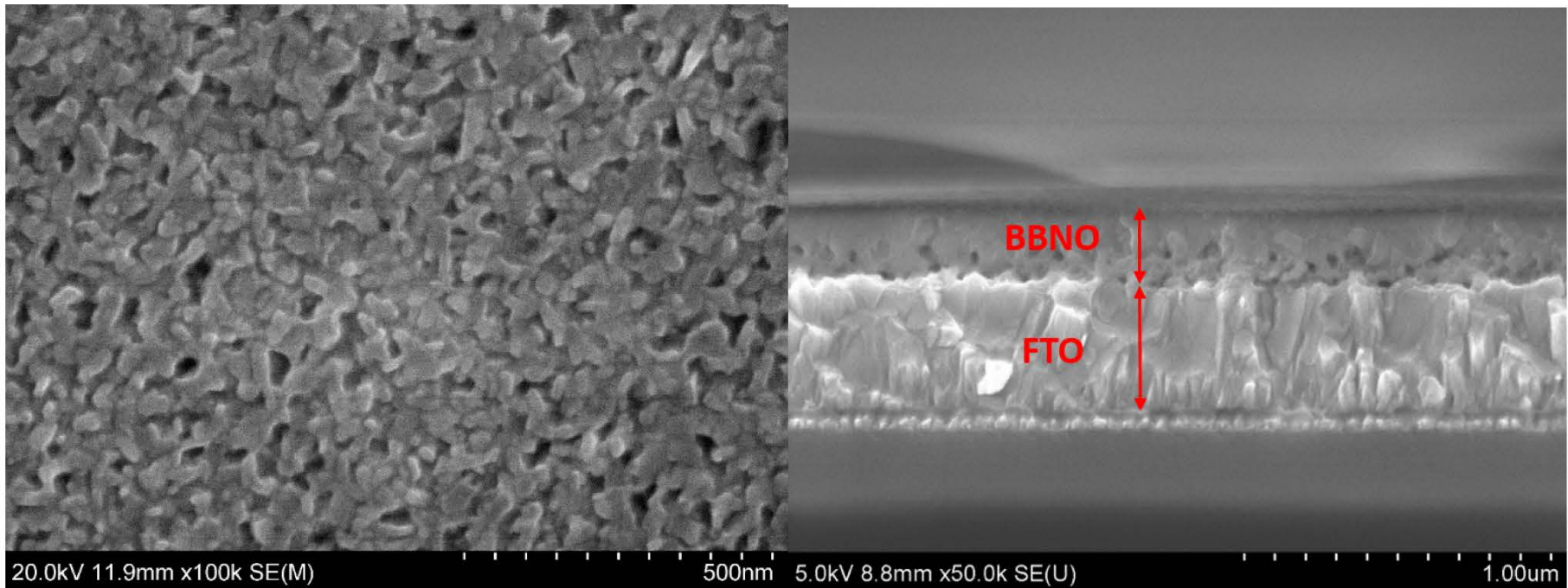


Solution process

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

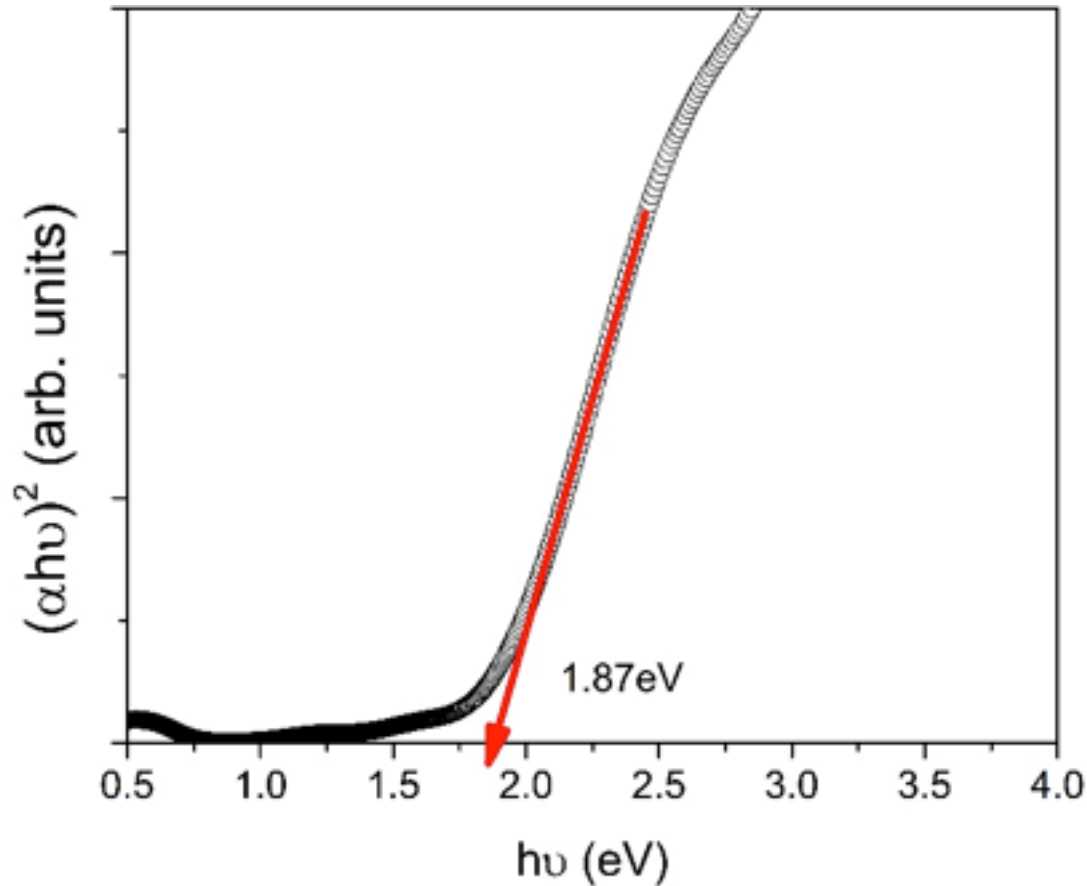
(Spin-coating)



Plan-view and cross-sectional SEM images of an annealed film

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

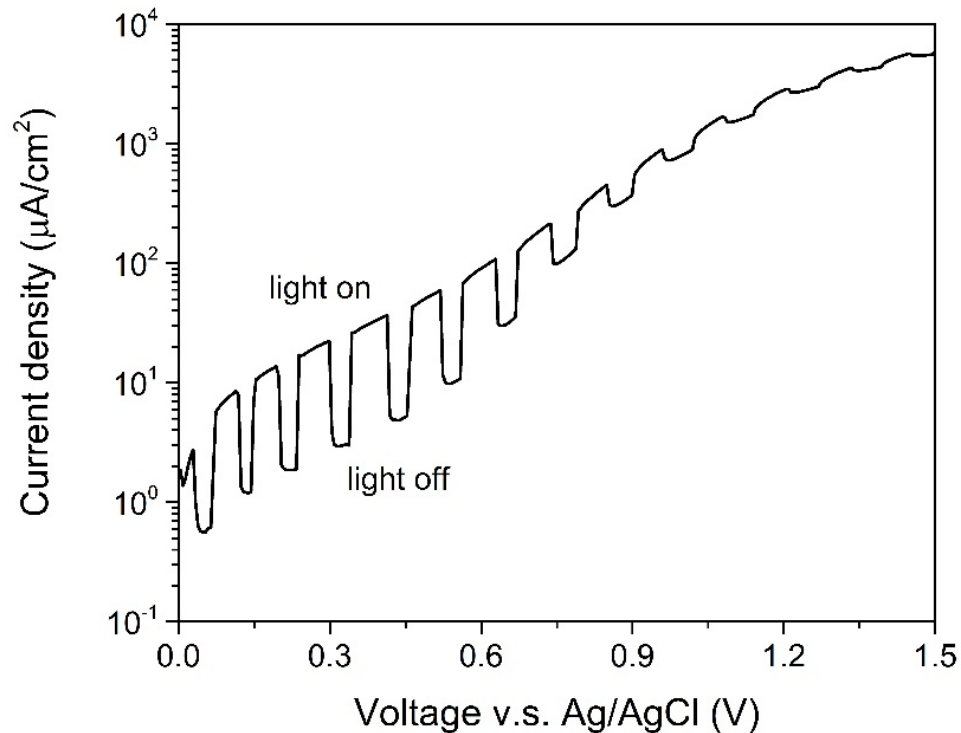


Direct band gap estimation from Tauc plot

Accomplishments and Progress (cont.)

3. PEC performance of new metal oxide films

(Spin-coating)



Preliminary result of J-V curve of a B2NO metal oxide film

Reviewers Comments

N/A

Collaborations

N/A

Remaining Challenges and Barriers

- The quality of synthesized B₂NO metal oxide thin films is low
- The initial PEC performance of metal oxides is low
- New metal oxides are needed

Proposed Future Work

- Synthesis of high quality B2NO metal oxide thin films
- Synthesis of nanostructured metal oxide thin films
- Synthesis of catalysts for O₂ and H₂ evolutions
- Improve PEC performance of metal oxides
- Design new metal oxides

Technology Transfer Activities

- Plan to file a patent on the new metal oxide

Summary

- A new metal oxide has been designed for PEC hydrogen production via solar water splitting
- DFT calculations show suitable band gap and effective masses
- Bulk materials were synthesized and XRD data were obtained.
- Thin films were synthesized by both solution and sputtering methods.
- The band gap of the new metal oxide was measured
- Initial PEC response was obtained