New Metal Oxides for Efficient Hydrogen Production via Solar Water Splitting

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Project ID #
PD118

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Overview

Timeline

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

Barriers

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

Budget

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

Partners

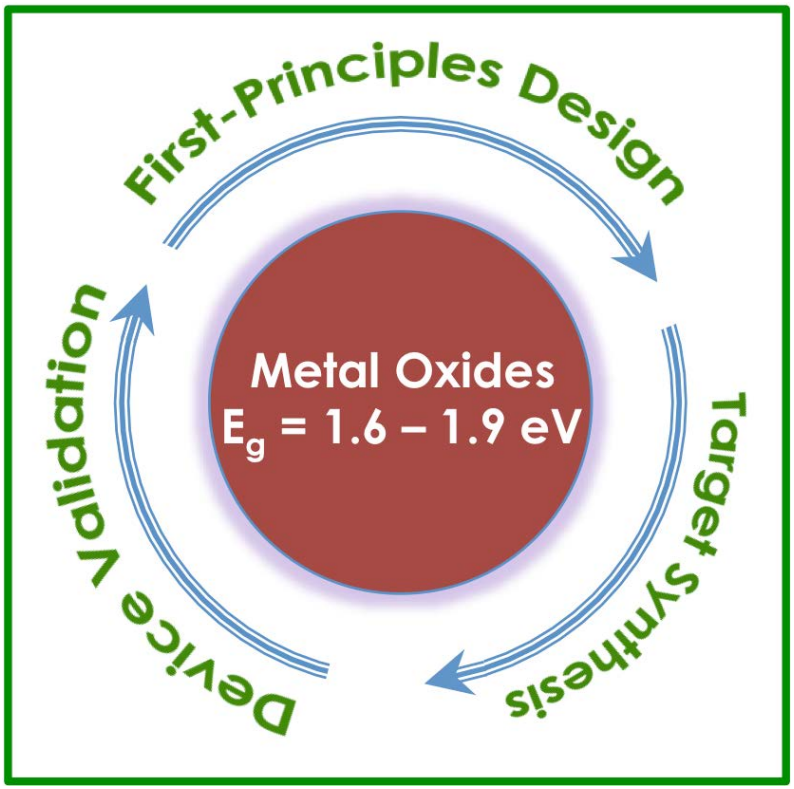
- National Renewable Energy Laboratory

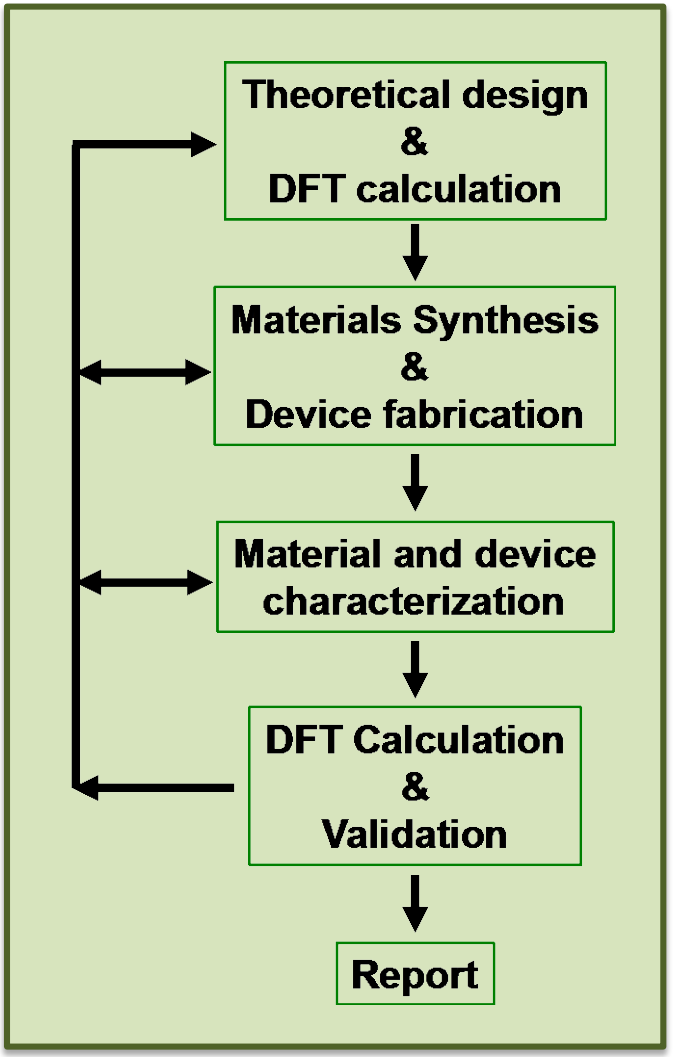
Relevance

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


First-Principles Design
Target Synthesis
Device Validation
Metal Oxides
E_g = 1.6 – 1.9 eV


Theoretical design & DFT calculation
Materials Synthesis & Device fabrication
Material and device characterization
DFT Calculation & Validation
Report

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

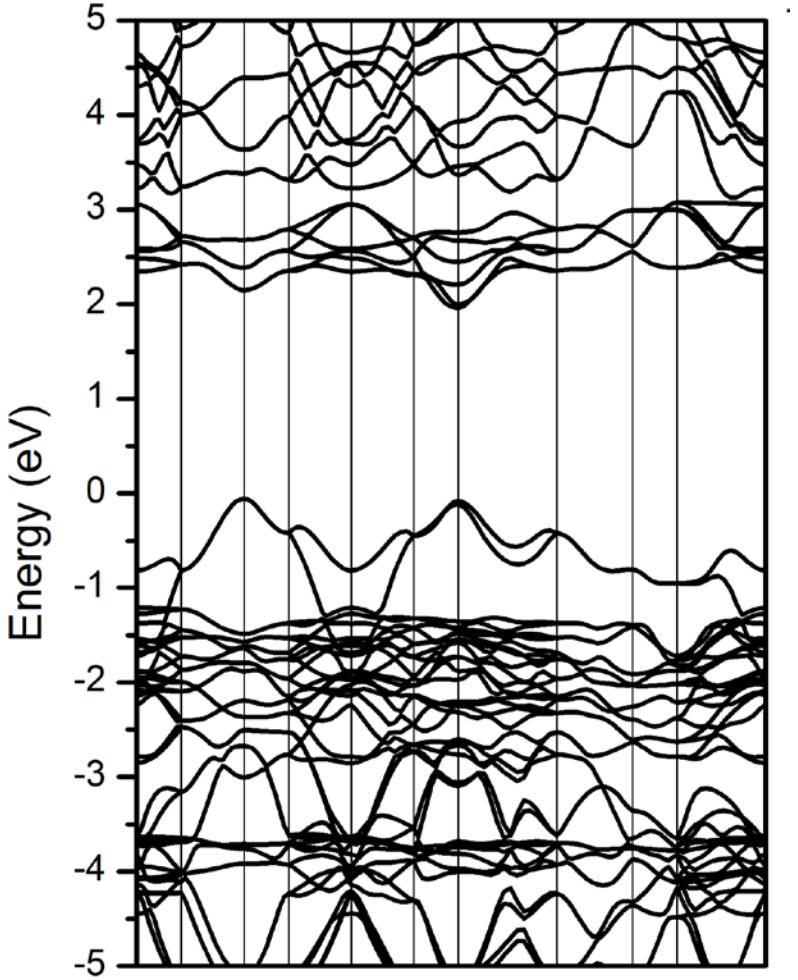
Milestone 3. PEC performance of new metal oxides

1.1 PEC measurement of small cells

1.2 Develop overall PEC systems

Accomplishments and Progress

1. Designing of new metal oxides

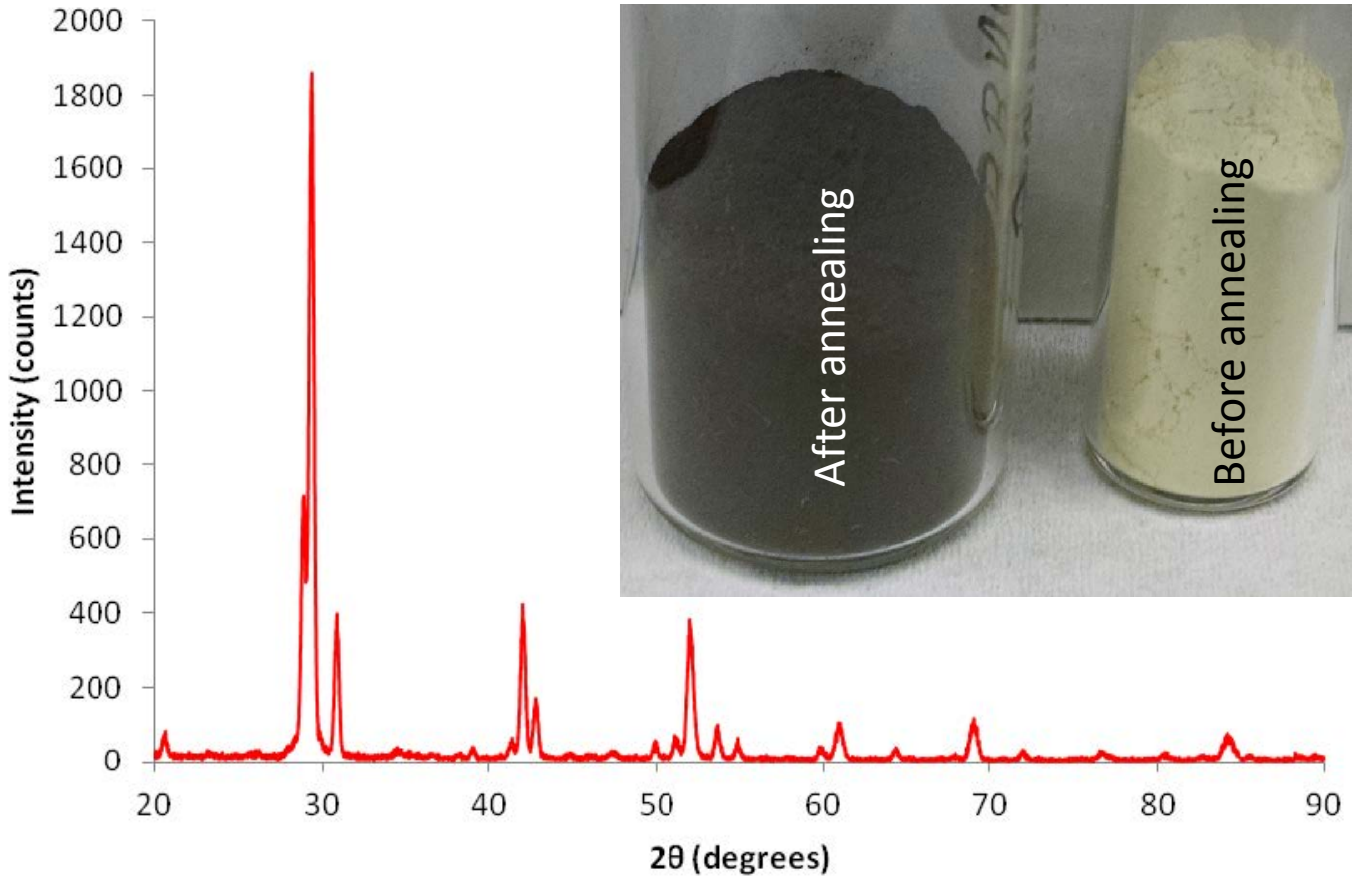


Calculated DFT band structure of B2NO

Band gap: ~2.0 eV

Accomplishments and Progress (cont.)

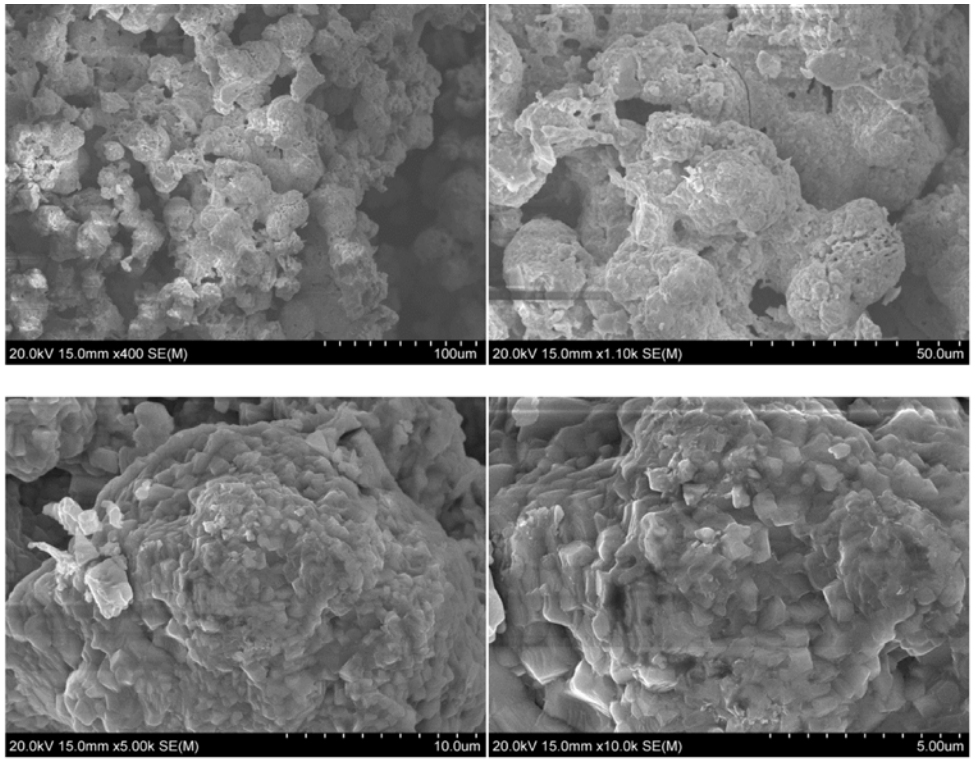
2. Synthesis of new metal oxides-bulk materials



XRD curve from annealed B2NO powder

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-bulk materials

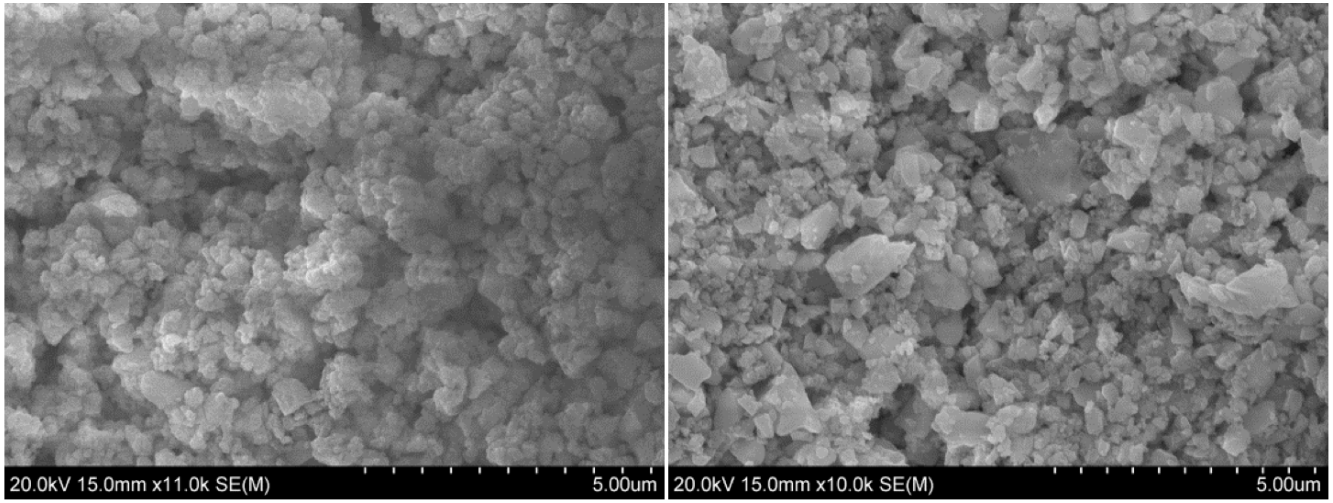


SEM images of the annealed B2NO powder at various magnifications

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

(*Spin & Dip Coating*)

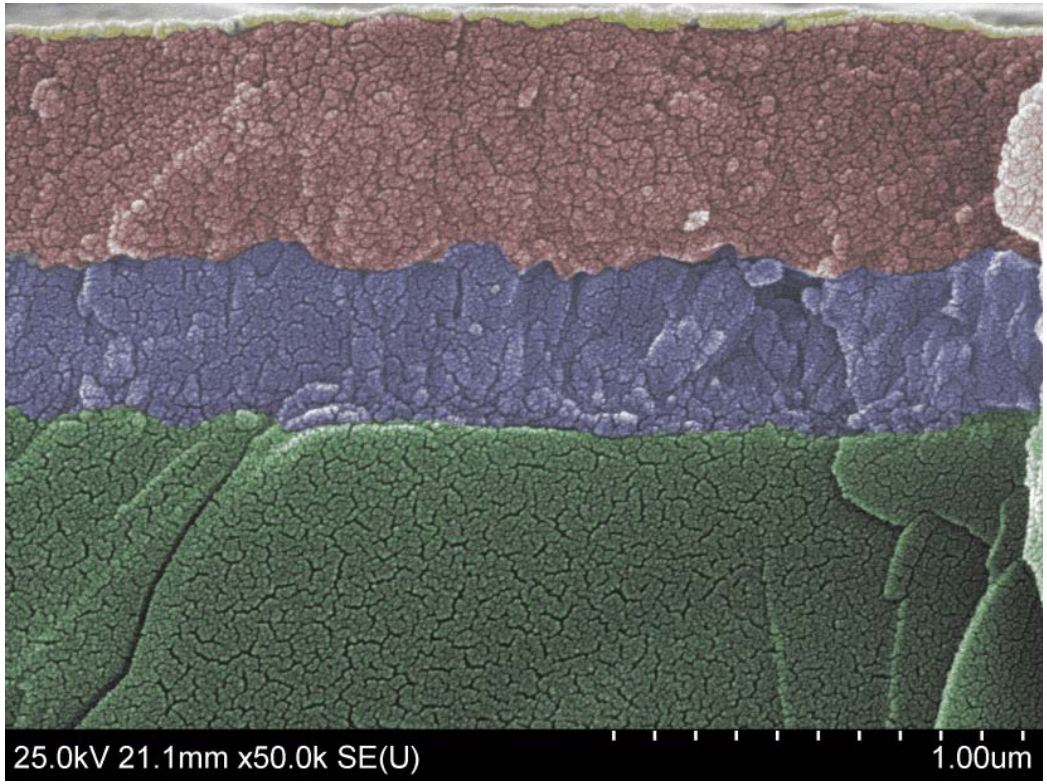


Plane view images of spin coated (left) and dip coated (right) films

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

(*RF sputtering*)



B2NO

FTO

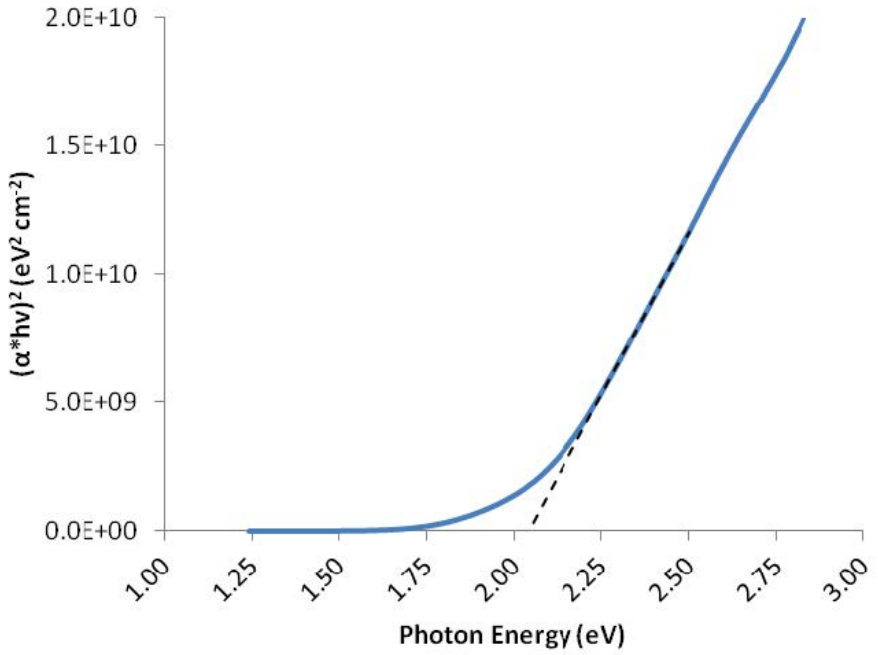
Glass

Cross sectional SEM image of a RF sputtered film

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

(*RF sputtering*)

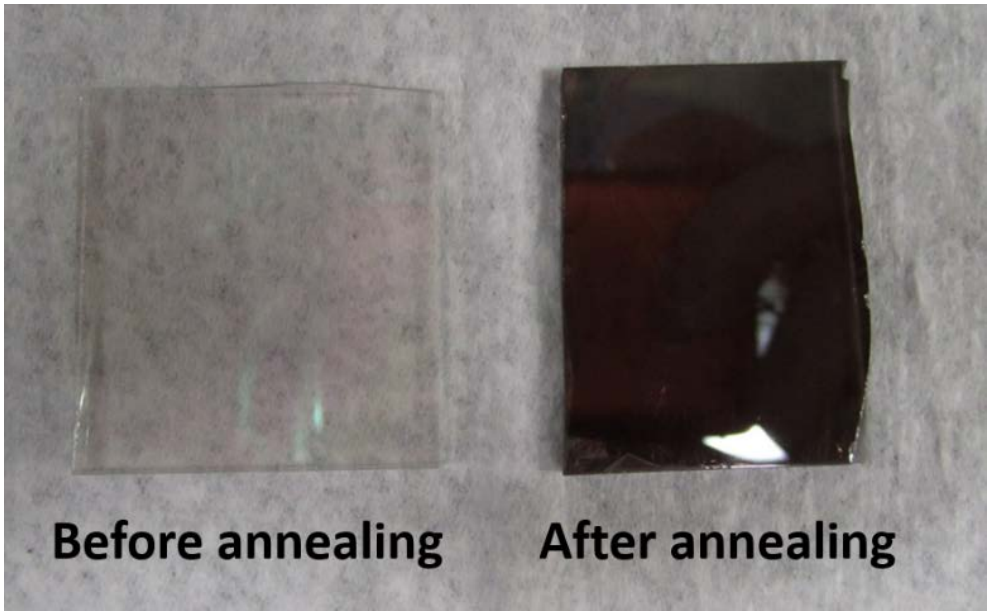


Direct band gap estimation from Tauc plot

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

(*Spin-coating*)

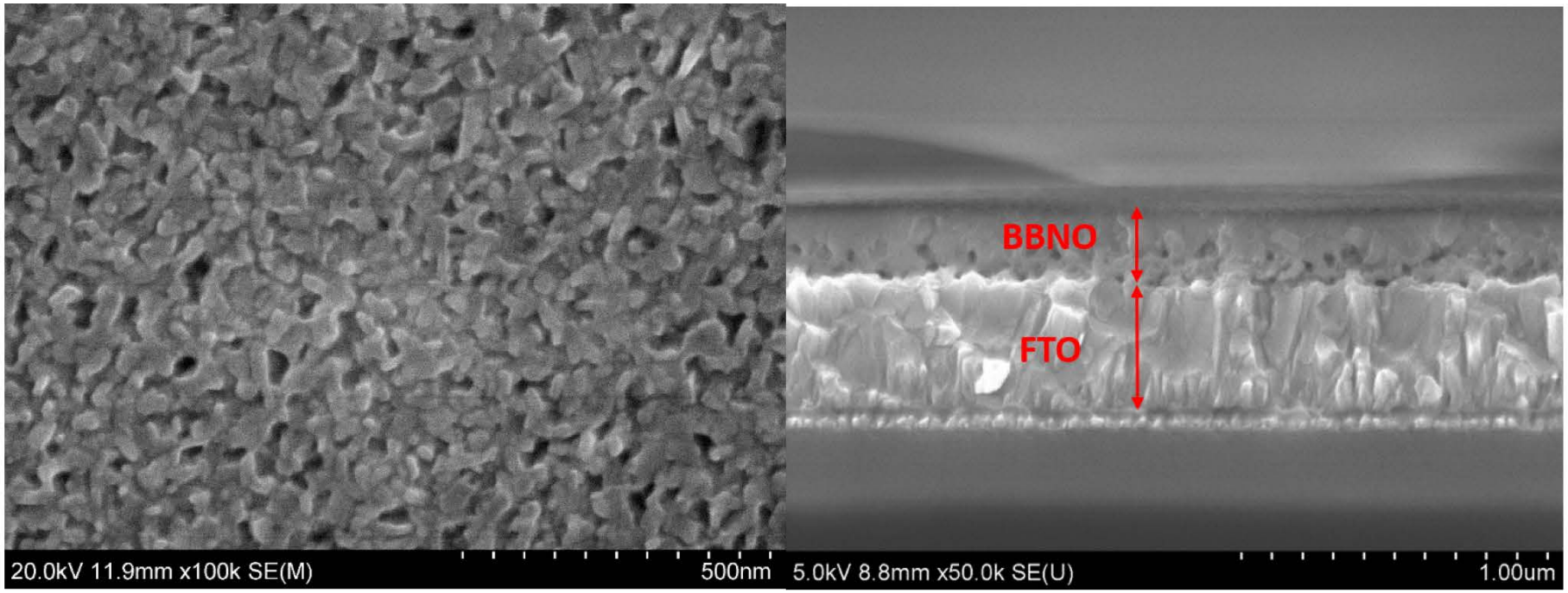


Solution process

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

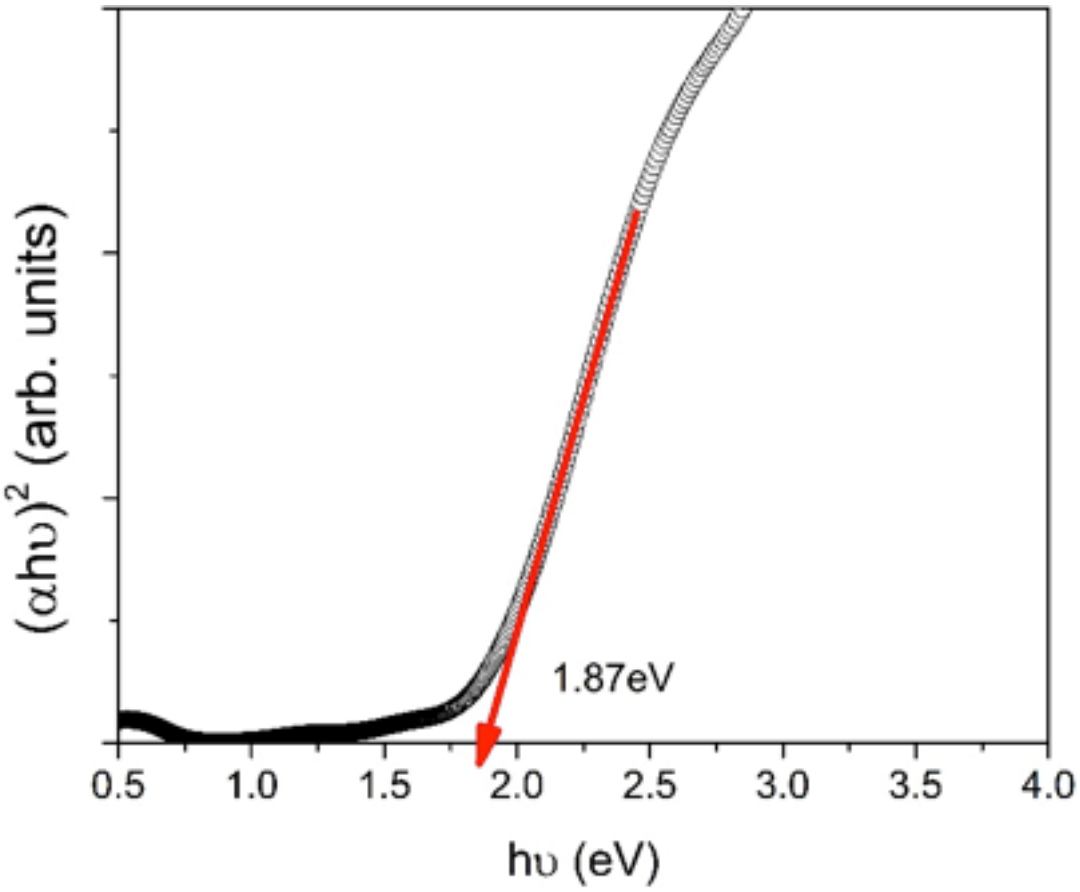
(*Spin-coating*)



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

Accomplishments and Progress (cont.)

2. Synthesis of new metal oxides-thin films

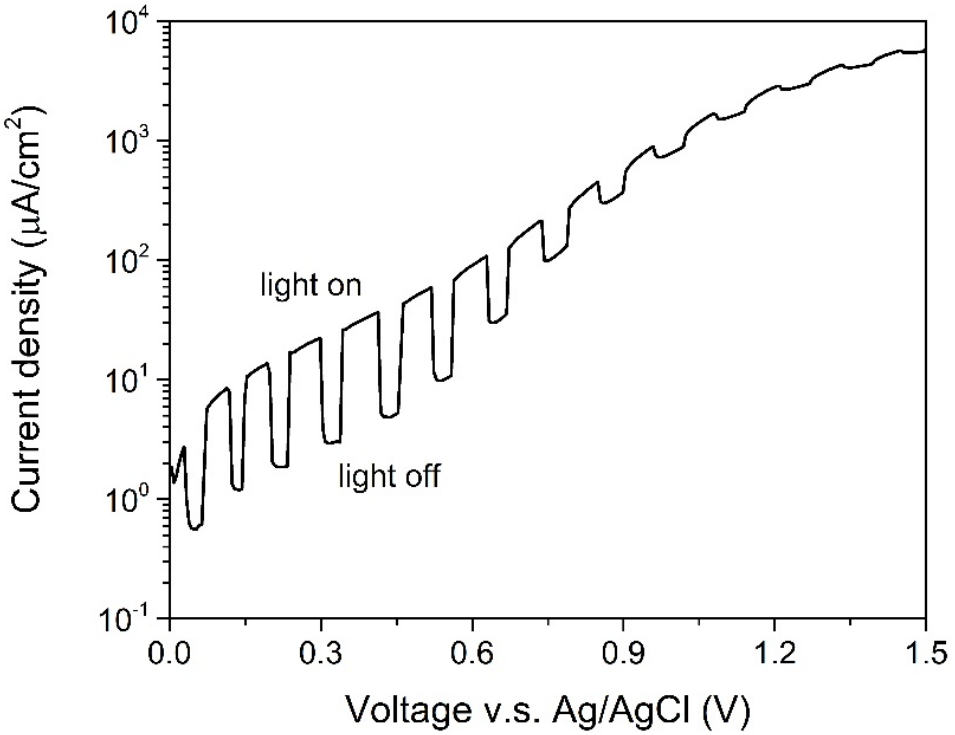


Direct band gap estimation from Tauc plot

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