New Metal Oxides for Efficient Hydrogen Production via Solar Water Splitting

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June 8, 2016

Project ID #
PD118

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

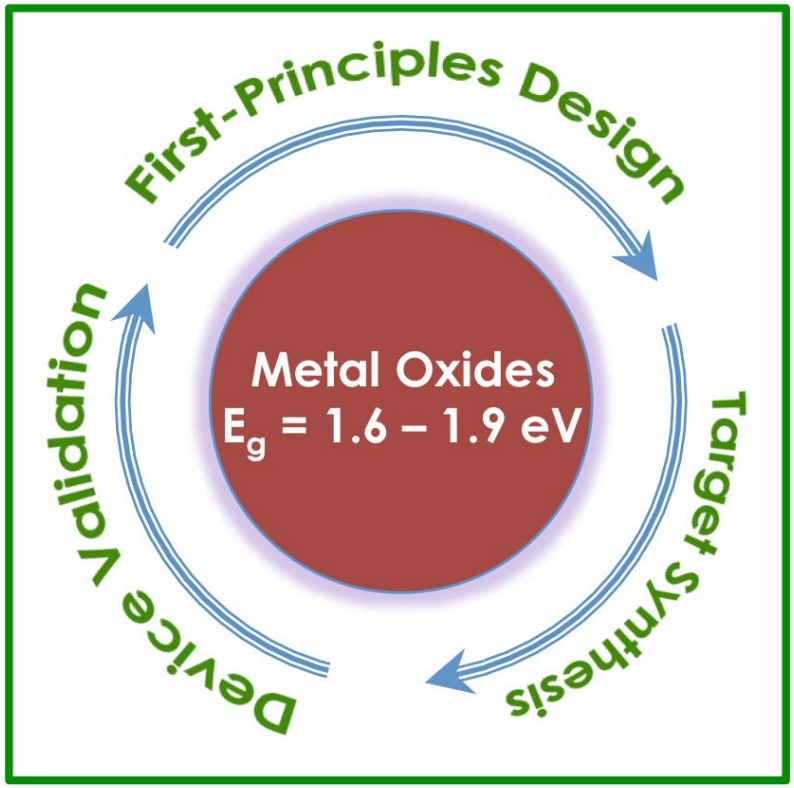
- National Renewable Energy Laboratory

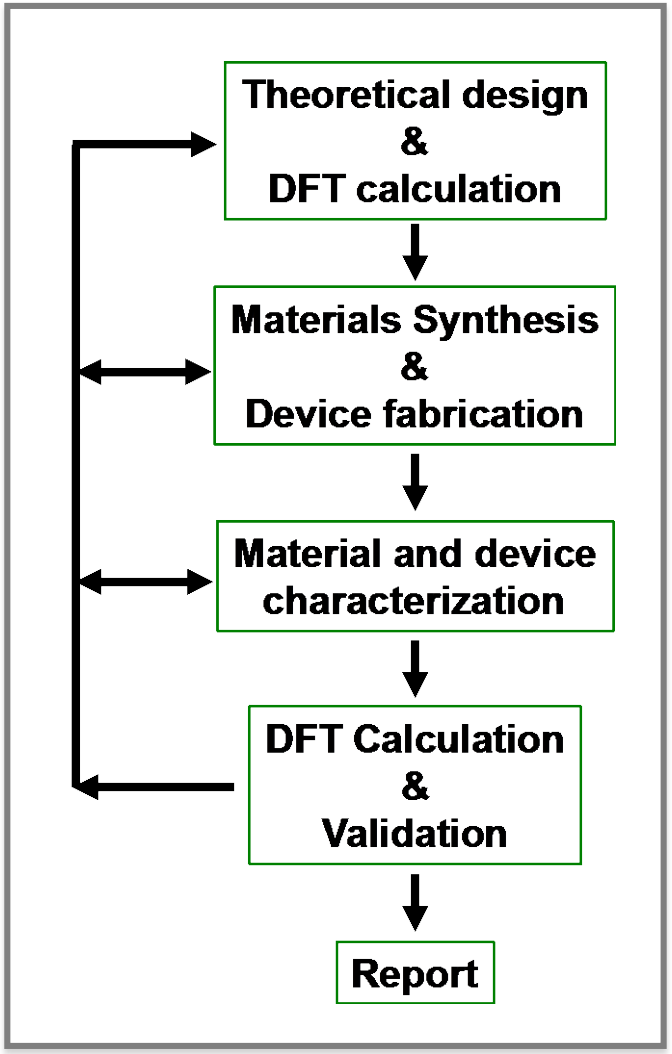
Relevance

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

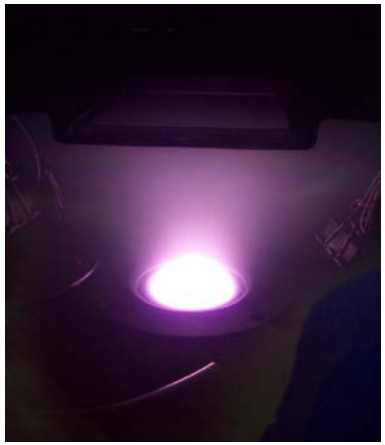

First-Principles Design
Target Synthesis
Device Validation
Metal Oxides
E_g = 1.6 – 1.9 eV

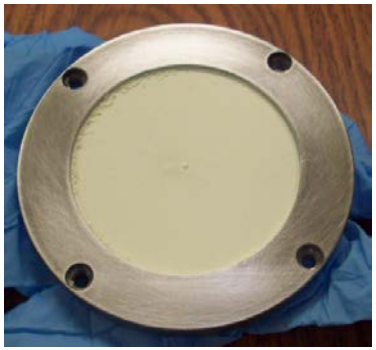

Theoretical design & DFT calculation
Materials Synthesis & Device fabrication
Material and device characterization
DFT Calculation & Validation
Report

Accomplishments and Progress

BBNO thin films grown on FTO/glass substrate by RF sputtering

Target



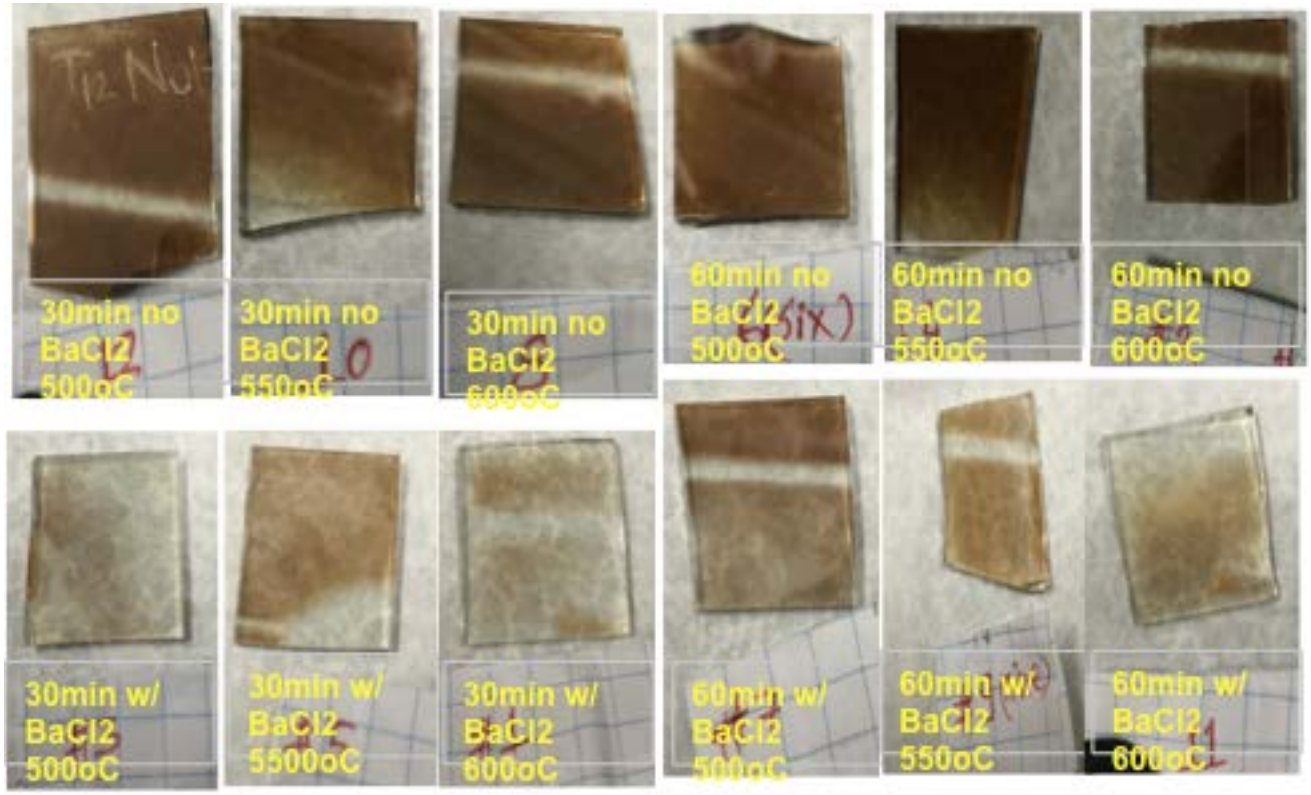


Before annealing

After annealing

Accomplishments and Progress

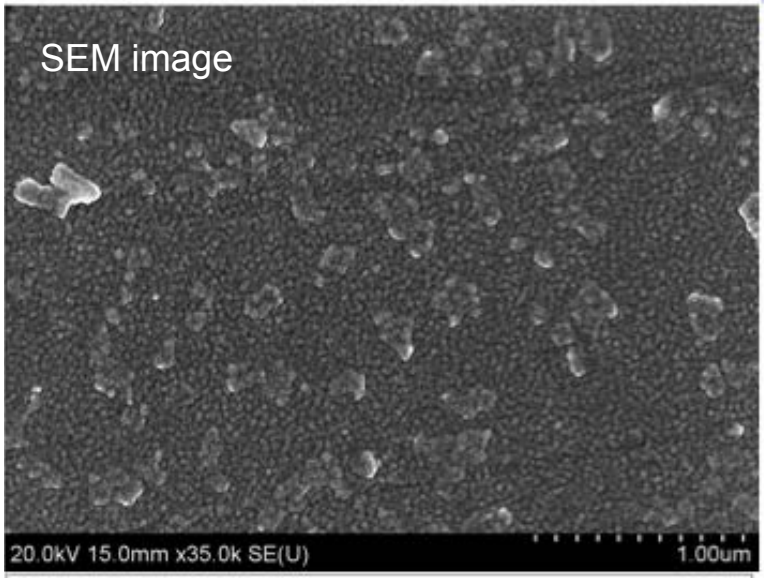
BBNO thin films grown on FTO/glass substrates by RF sputtering

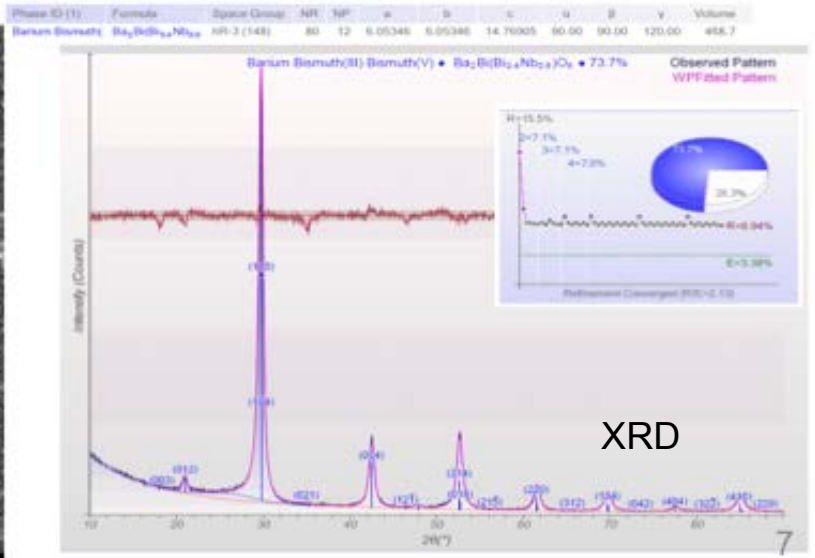


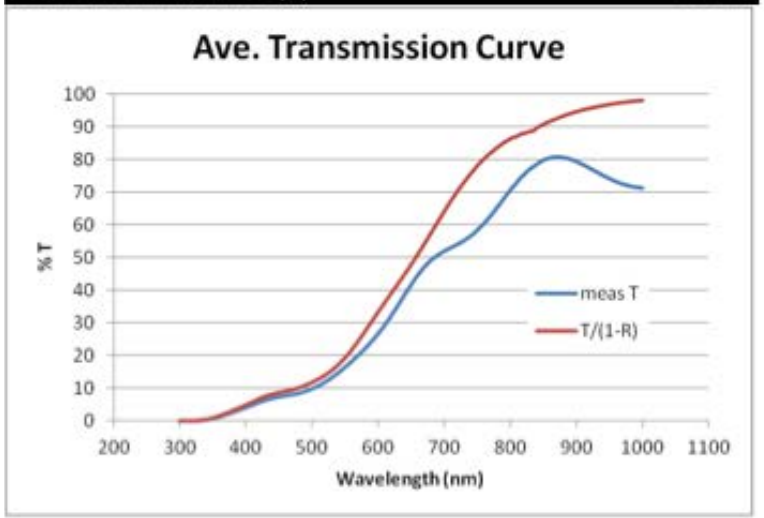
Samples w/o $BaCl_2$ appear same
Samples with $BaCl_2$ show loss of color

Accomplishments and Progress

BBNO thin films grown on FTO/glass substrates by RF sputtering







Room temp deposited
- 30min 500°C air anneal

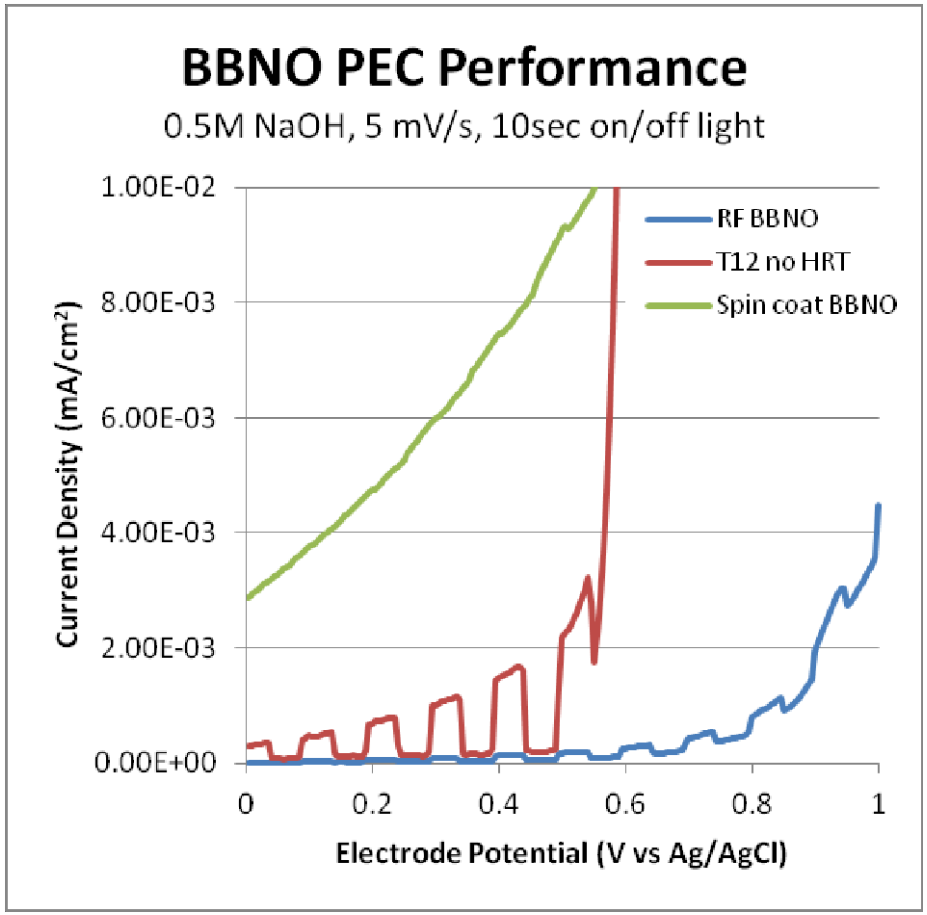
Direct bandgap:
- Approx. 2.05 eV

Single phase confirmed by XRD
- Rhombohedral (R-3)
- Perovskite structure

R_{sheet}: ~ 1.5×10^9 Ω/□

Accomplishments and Progress

BBNO thin films grown on FTO/glass substrates by RF sputtering

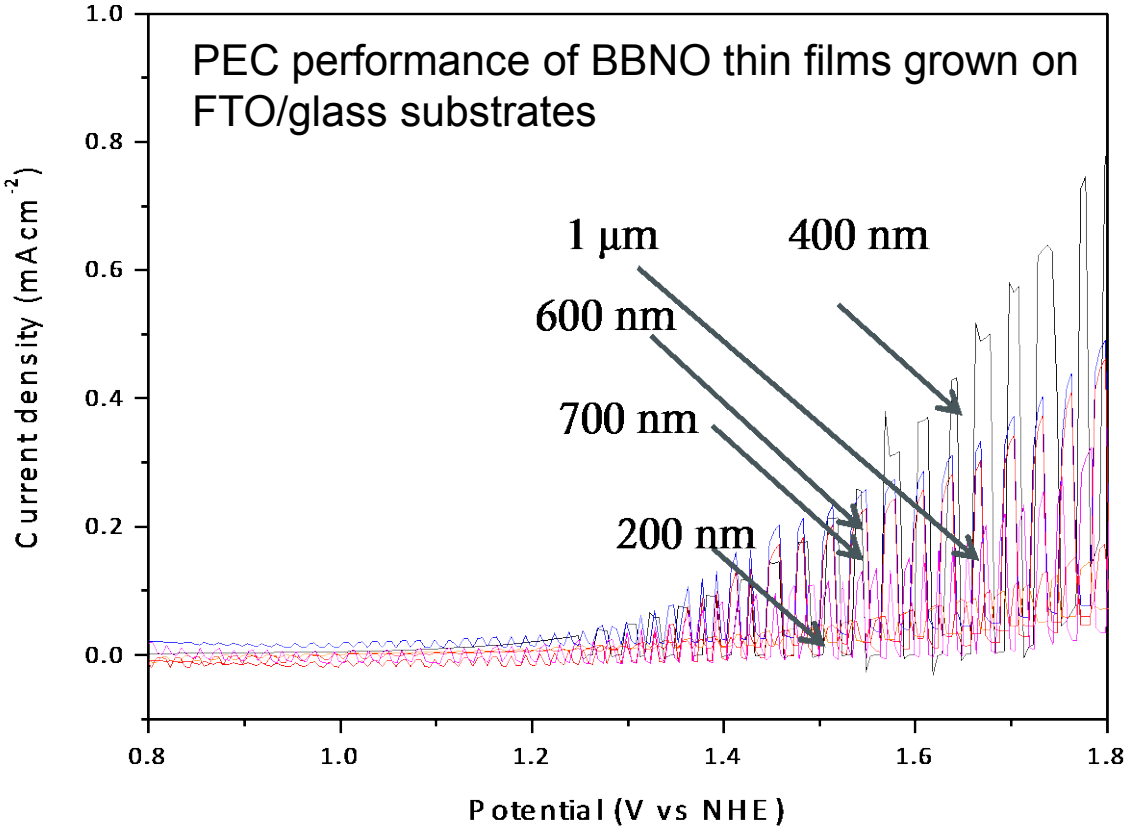


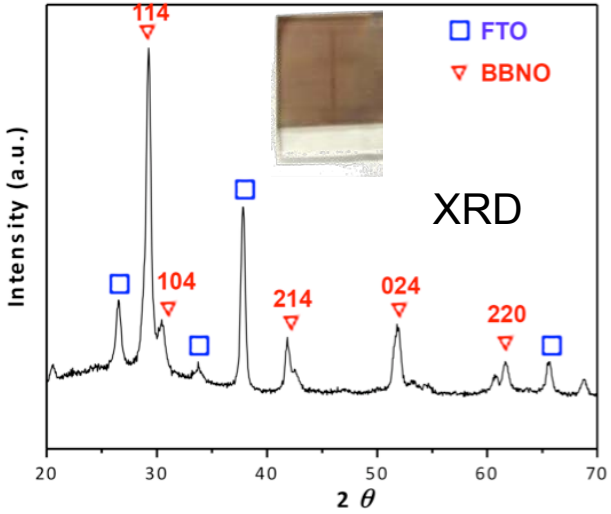
- Thin film synthesis
  - RF sputtered “Hasitha” system
  - Room temp, 240min, 50W, 10mTorr, 30 sccm Ar
  - ~ 200nm thick film
- PEC testing using 300W Xe light source
  - 1M NaOH (first, all electrodes)
  - 1M Na_2SO_3 & 0.5M KH_2PO_3 (referred to as “SS/PP”)

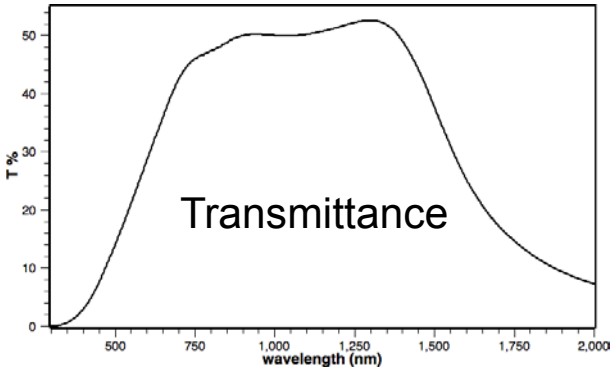
Accomplishments and Progress

BBNO thin films on FTO/substrates grown by Sol-gel method

Acetylacetone as chelating reagent
Ethyl glycol as solution
Spin-coating



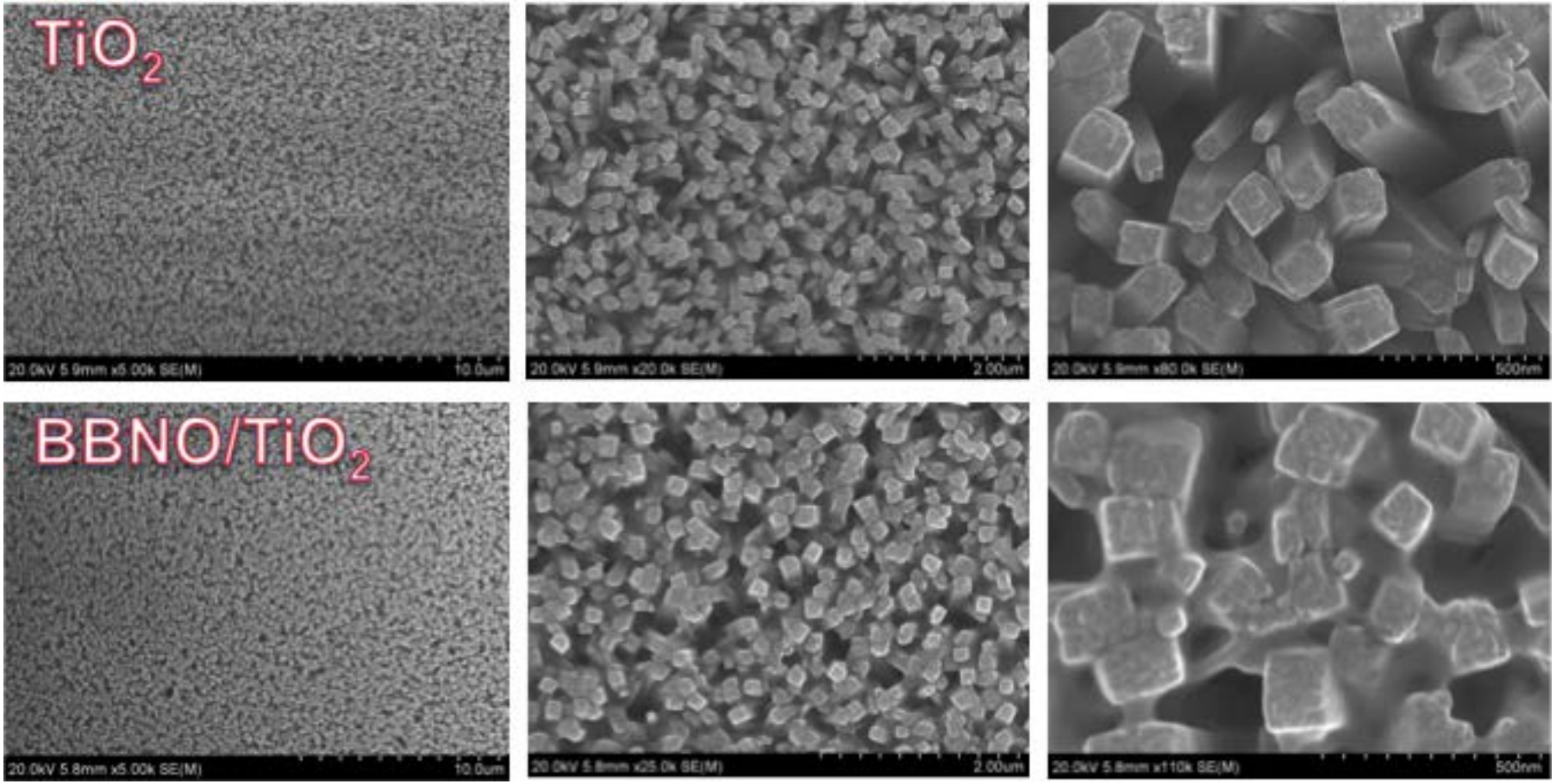




Accomplishments and Progress

BBNO thin films grown on TiO_2 nanowire arrays

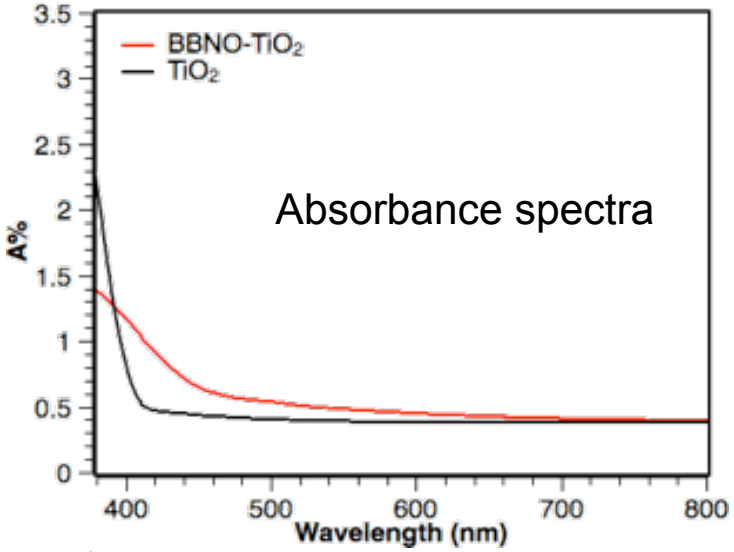
1) band position engineering; 2) high surface areas; 3) promote charge transfer

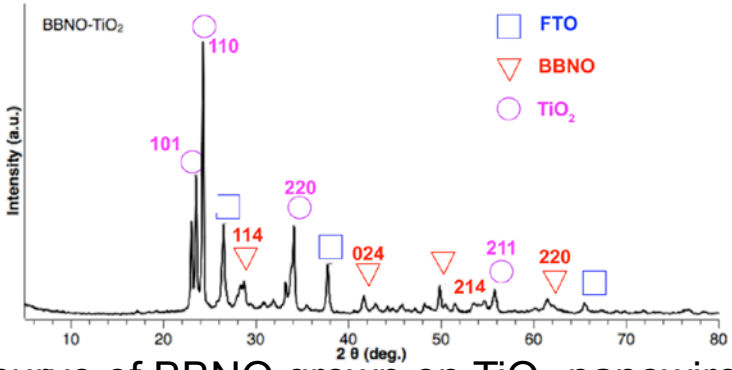


Accomplishments and Progress

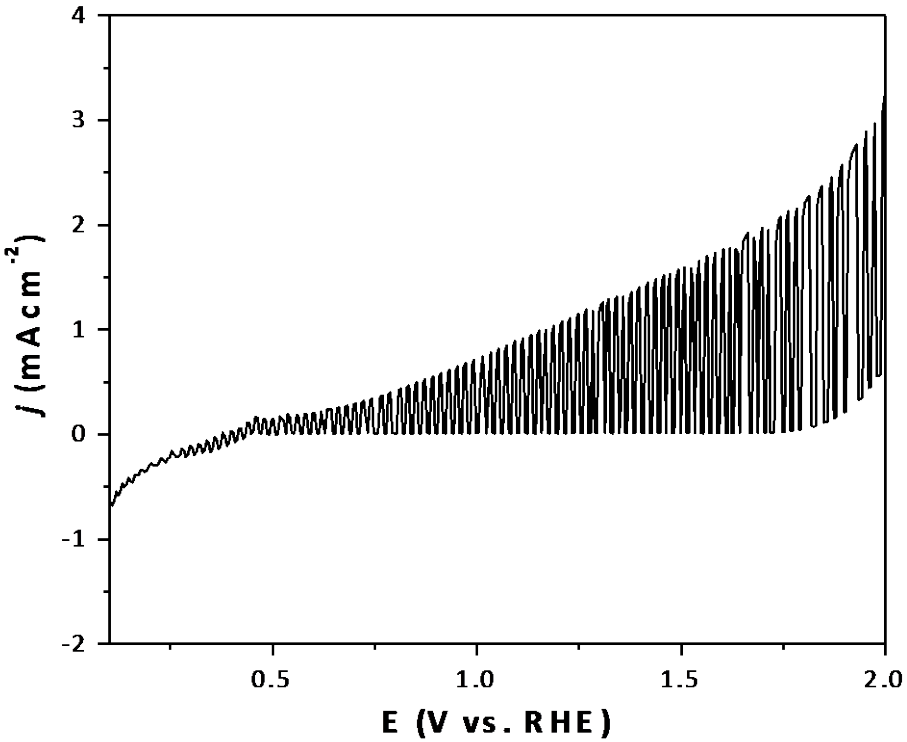
BBNO thin films grown on TiO_2 nanowire arrays

- Enhanced light absorption by TiO_2 nanowire arrays
- Improved PEC performance





XRD curve of BBNO grown on TiO_2 nanowire arrays

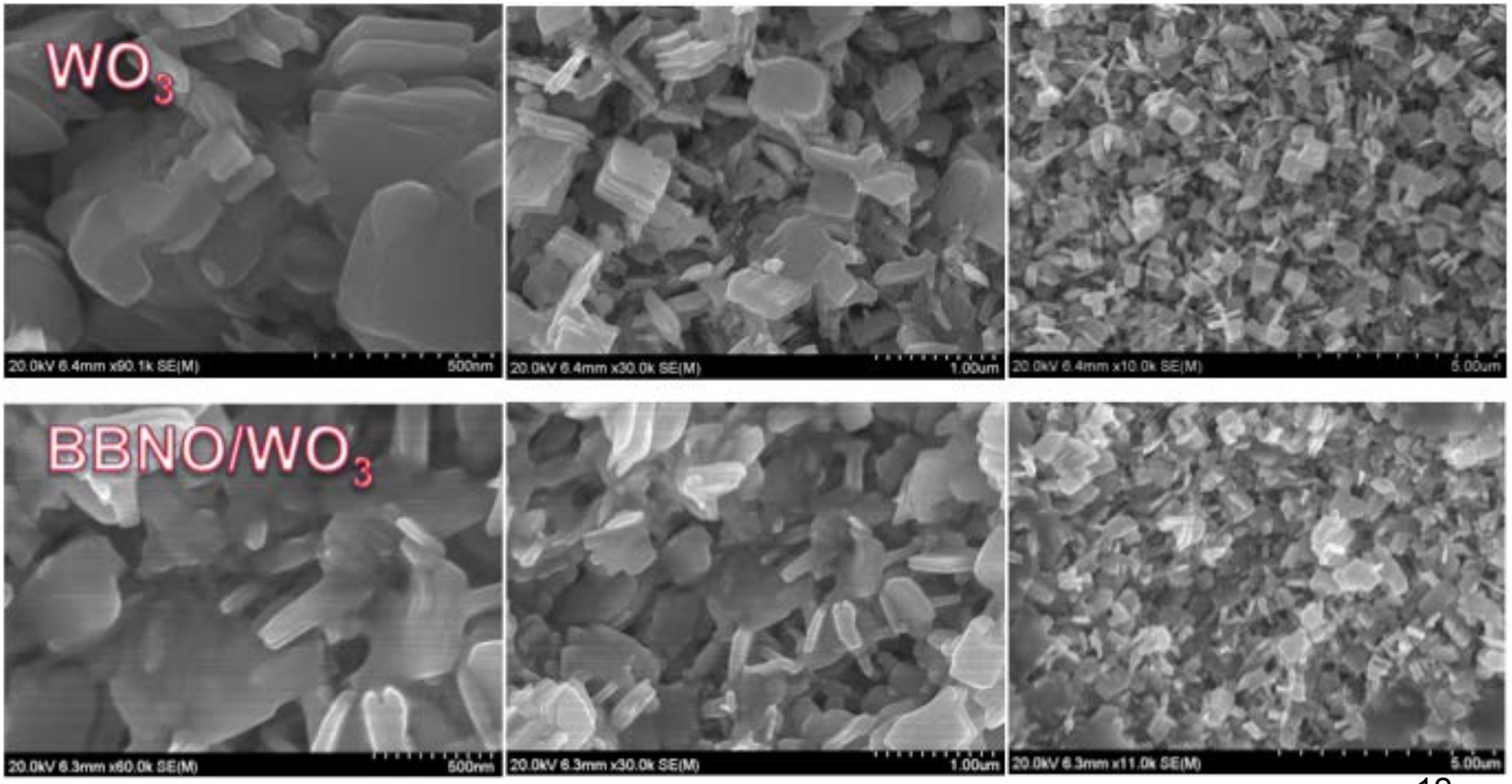


PEC performance of BBNO grown on TiO_2 nanowire arrays

Accomplishments and Progress

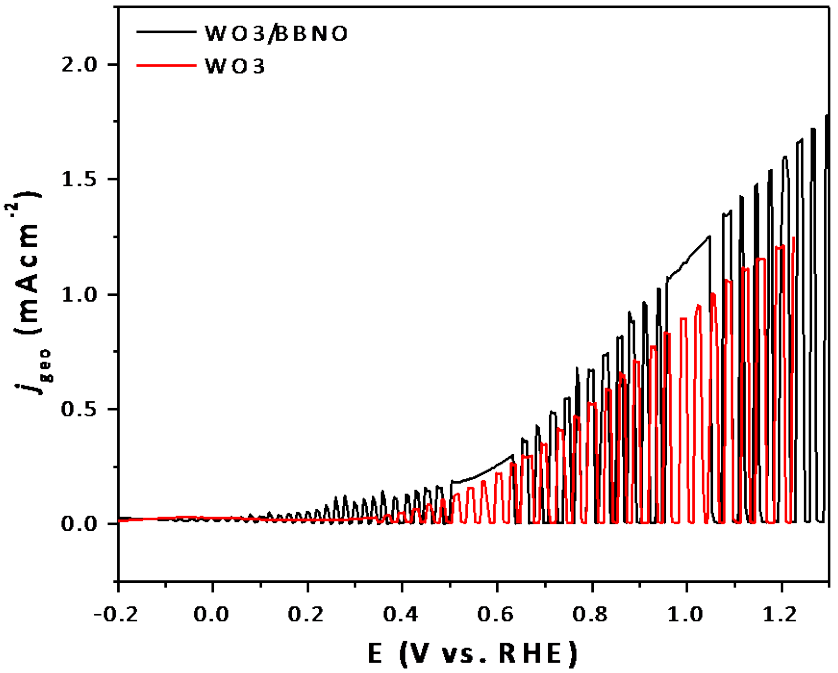
BBNO thin films grown on WO_3 nanosheets

1) 2-D materials; 2) band position engineering- lower conductive band

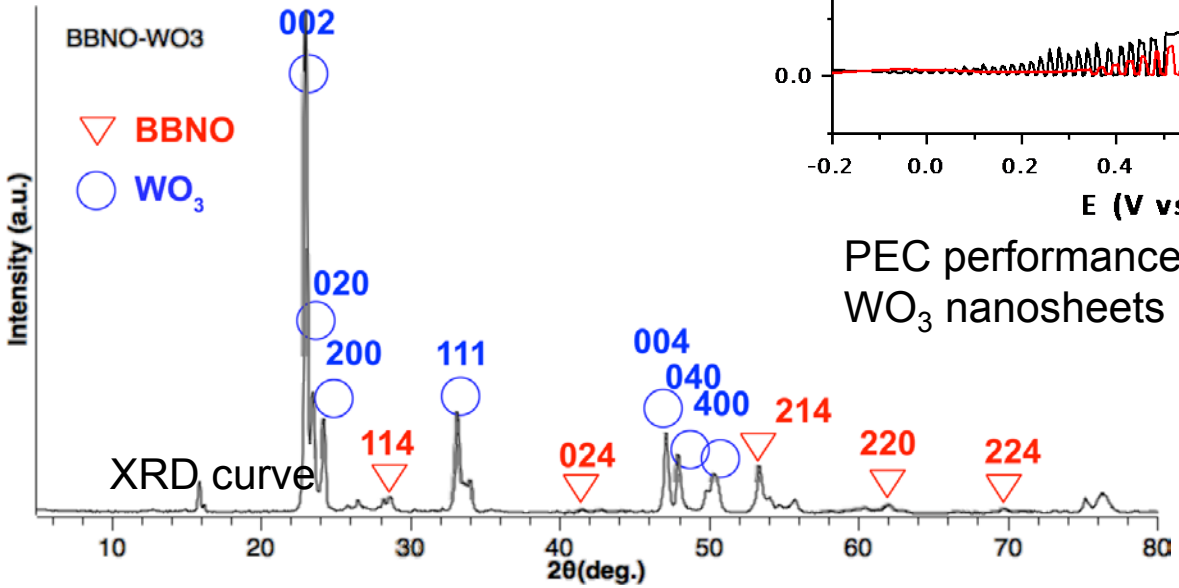


Accomplishments and Progress

BBNO thin films grown on WO_3 nanosheets



PEC performance of BBNO grown on WO_3 nanosheets



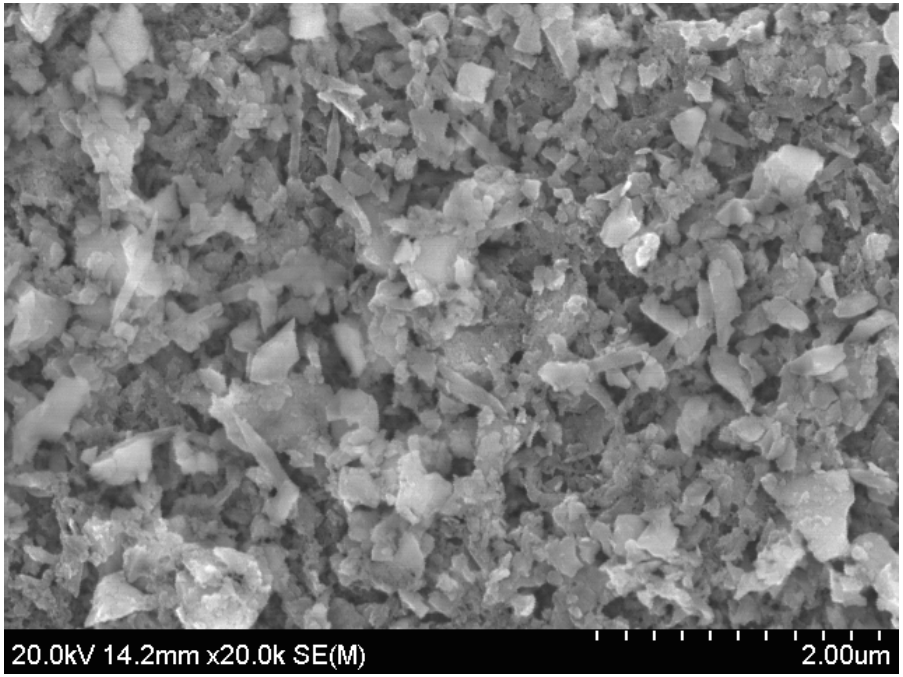
XRD curve of BBNO grown on WO_3 nanosheets

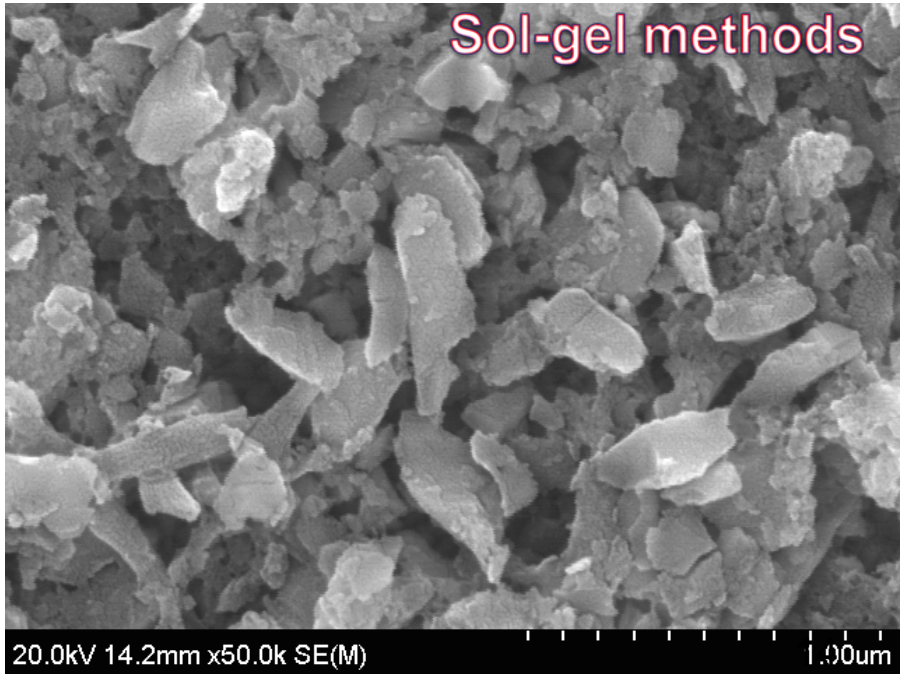
Accomplishments and Progress

BBNO nanopowders

BBNO size reduction:

1) Enhance surface areas to improve electrolyte contact
2) Exploring the facet orientation effects
3) Photocatalytic water splitting using both conductive and valence bands

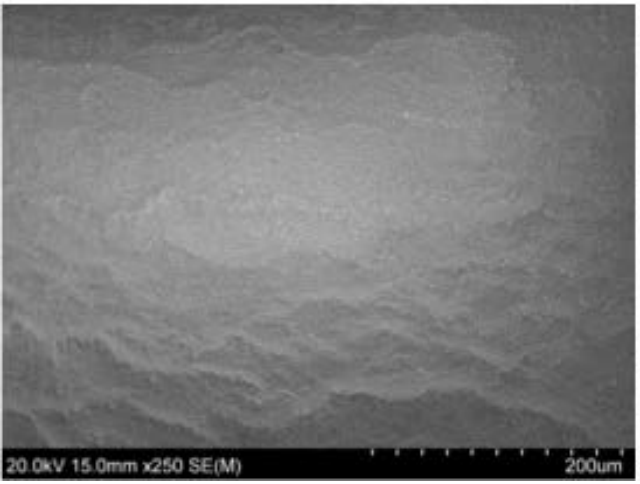


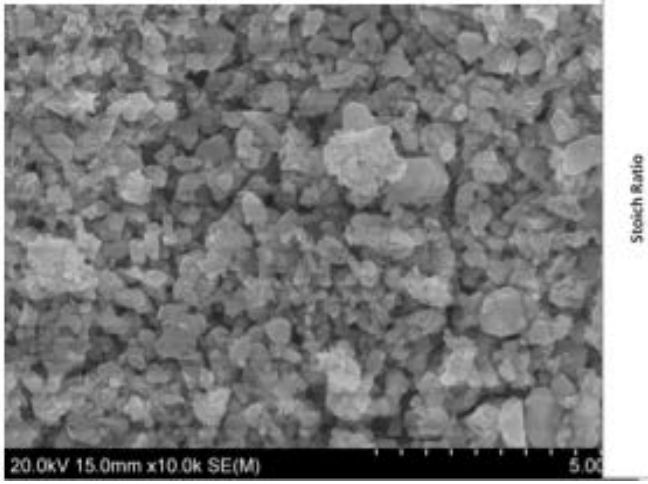


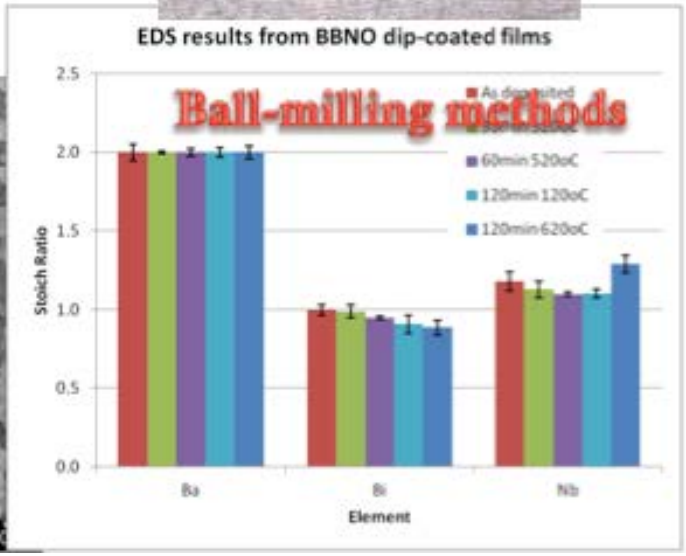
Accomplishments and Progress

BBNO nanopowders

Ball milled for total 11.5 hours
- 300 rpm
- 20-30mL acetone
- Agate jar & balls
  - 100x 6mm diameter
  - 16x 10mm diameter
- Reversed directions (CW, CCW) every few hours
- Diluted final suspension to ~60mL with acetone



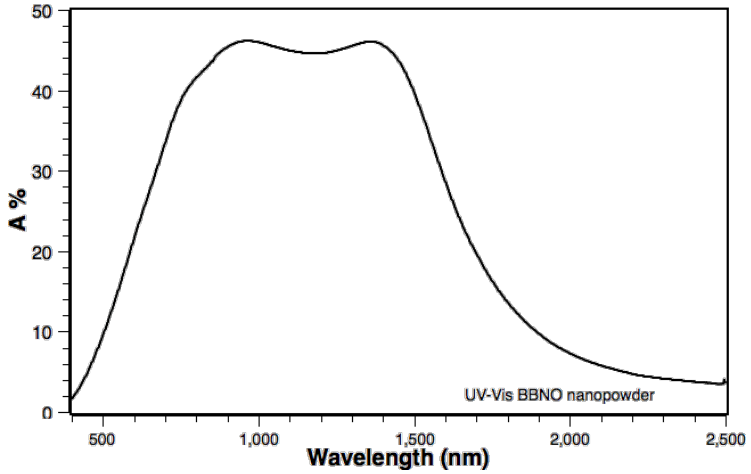




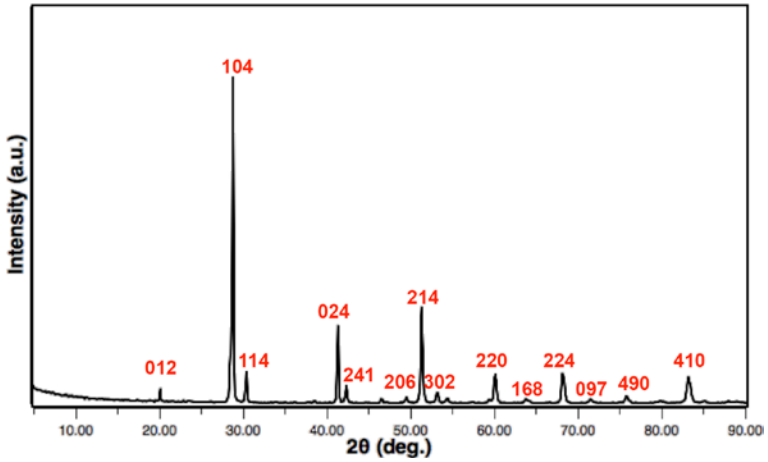
- Film surface mostly smooth with visible “wrinkles” – not cracks

Accomplishments and Progress

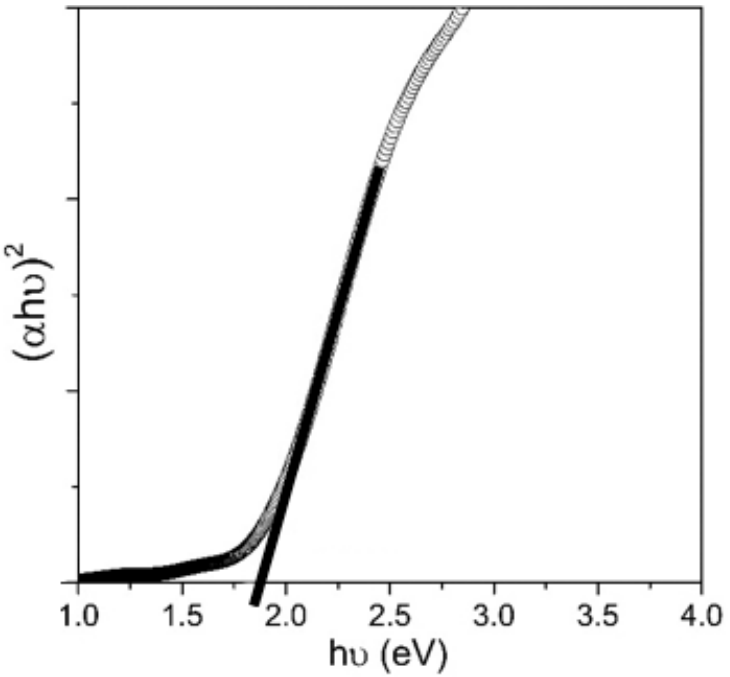
BBNO nanopowders



Absorbance of a BBNO nanopwoder film



XRD curve of a BBNO nanopwoder film



Absorbance of a BBNO nanopwoder film

Well crystallized double perovskite structure, Band-gap: 1.8 eV

Reviewers Comments

N/A

Collaborations

Todd Deutsch
National Renewable Energy Laboratory

Remaining Challenges

- BBNO thin films are too resistive.
- Charge transfer is not efficient
- Photocurrents are not high

Proposed Future Work

- Continue to explore nanostructures to facilitate charge transfer.
- Apply catalysts for oxygen evolution reaction
- Test slurry configurations
- Try to dope BBNO thin films.

Technology Transfer Activities

- N/A

Summary

- BBNO thin films were deposited on 1D TiO_2 nanowires and WO_3 nanosheets to improve photocurrents.
- BBNO nanoparticles were prepared.
- The optical properties of BBNO prepared by RF sputtering and spin-coating methods were studied