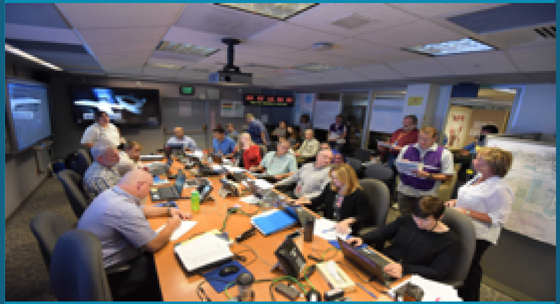
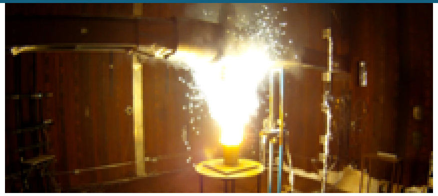
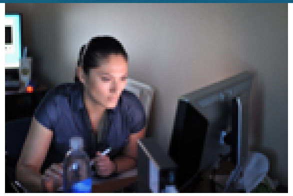
SAND2020-13239PE

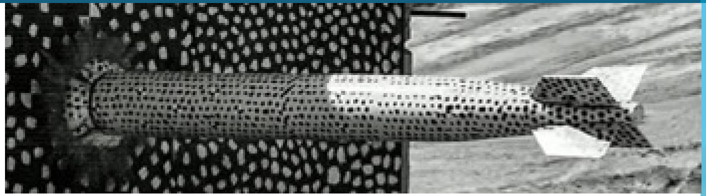
Sandia National Laboratories

Solar Thermochemical Hydrogen Production on Layered Perovskite $BaX_{0.25}Mn_{0.75}O_3$ (X = Ce, Nb, Pr)









14th Annual Postdoctoral Technical Showcase

December 9th and 10th, 2020

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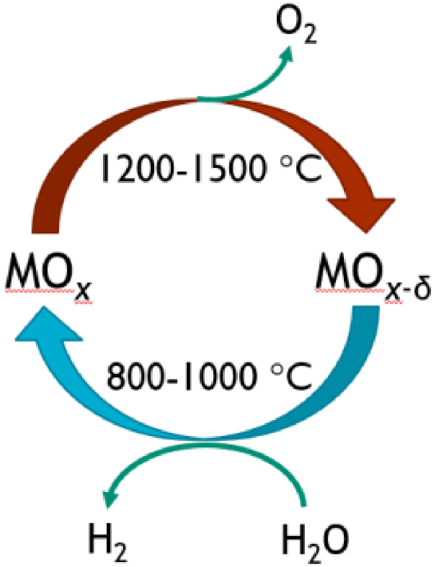
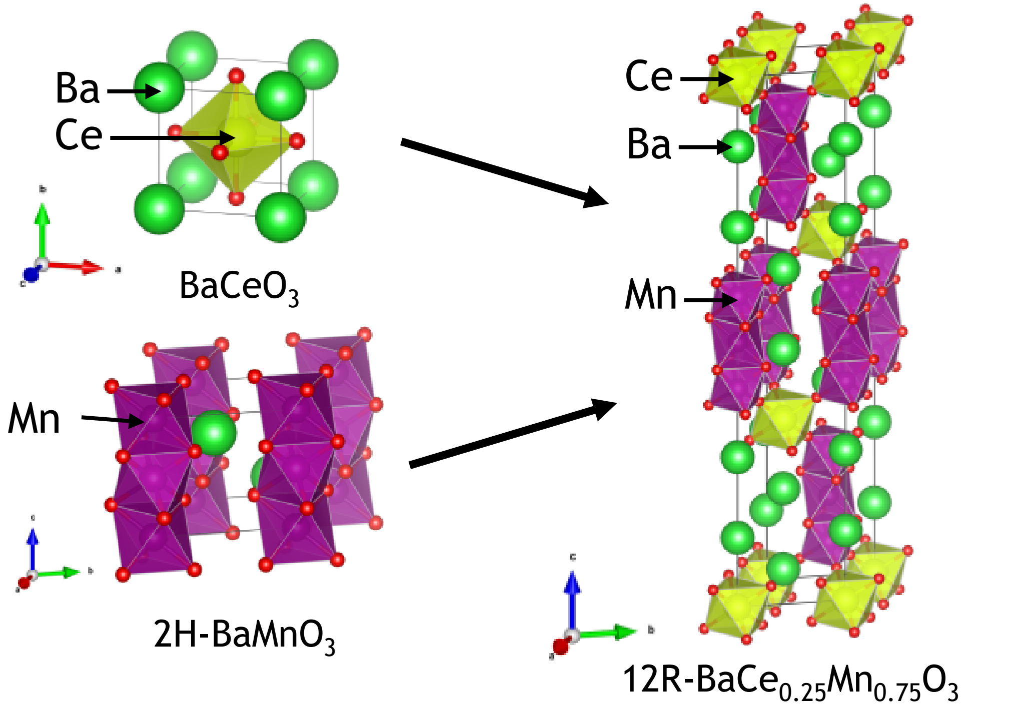
SAND2020-

Introduction

Solar Thermochemical Hydrogen Production (STCH)





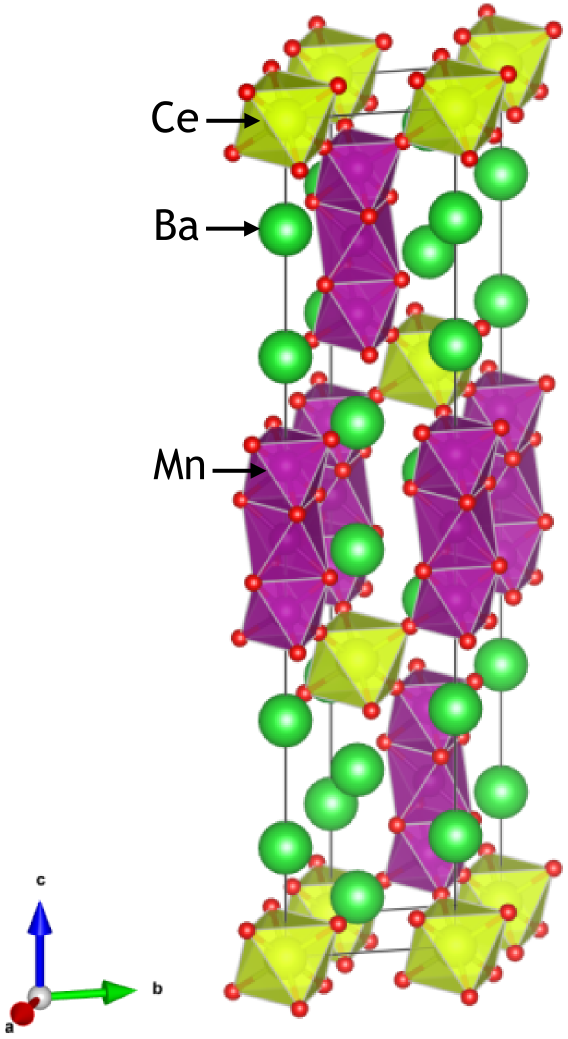
Non-water Splitters → Water Splitter

12R-BaCe$_{0.25}$Mn$_{0.75}$O$_3$ shows great water splitting behavior compared to CeO$_2$.

However, key aspects affecting the performance remain unknown.

Barcellos, D.R.; Sanders, M.D.; Tong, J.; McDaniel, A.H.; O'Hayre, R.P. *Energy Environ. Sci.* **2018**, *11*, 3256.
https://energy.sandia.gov/energy/renewable-energy/solar-energy/csp-2/nsttf/

Introduction



12R-$BaCe_{0.25}Mn_{0.75}O_3$ (BCM)

Goal:

- Examine substituting Ce with Nb and Pr to compare water splitting behaviors while maintaining the same structure.
- Understand key criteria/aspects for further development of STCH material.

Synthesis of $BaX_{0.25}Mn_{0.75}O_3$ (X = Ce, Nb, Pr):

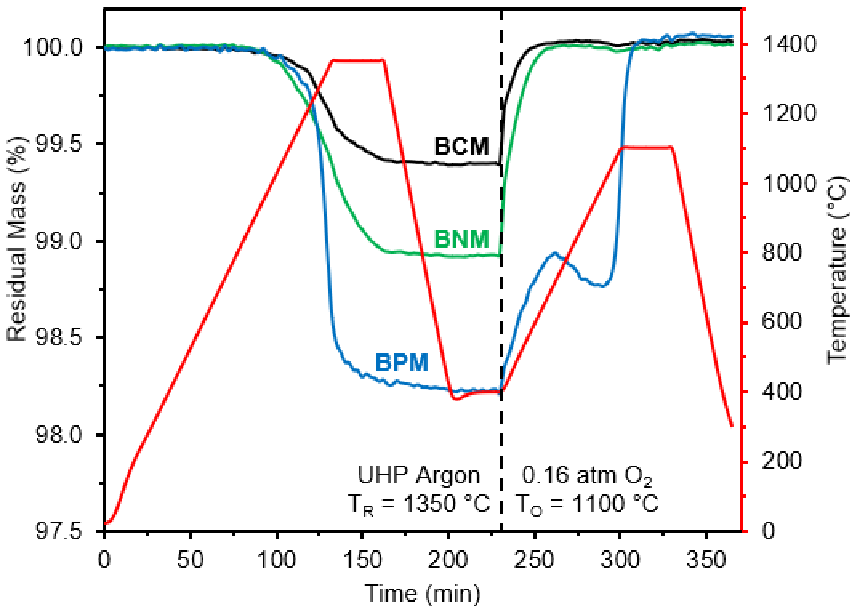
- Sol-gel based Pechini method reacting metal nitrate salts and sintering in air.
- All materials crystallize in the same 12R polytype structure with minimum impurity phases.

Barcellos, D.R.; Sanders, M.D.; Tong, J.; McDaniel, A.H.; O'Hayre, R.P. *Energy Environ. Sci.* **2018**, *11*, 3256.
https://energy.sandia.gov/energy/renewable-energy/solar-energy/csp-2/nsttf/

Redox and Water Splitting Behavior

Redox Behavior

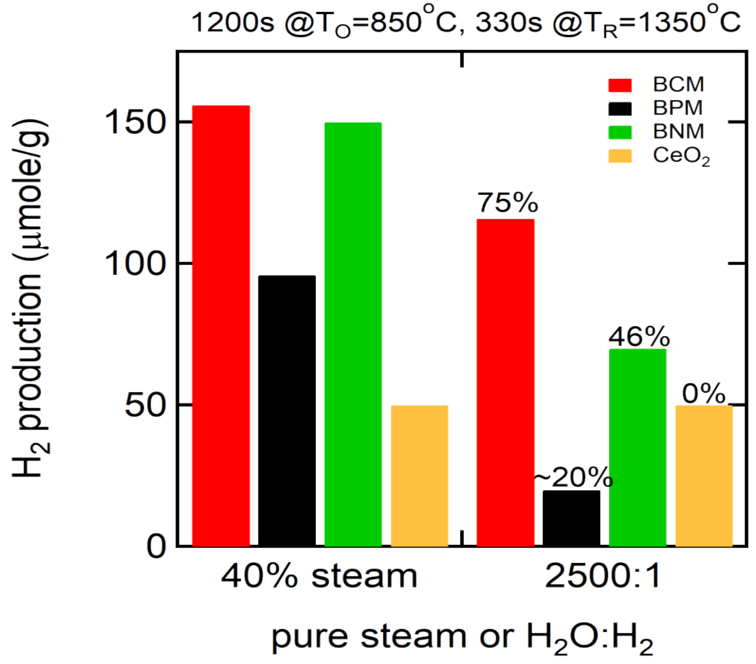
T_R = 1350 °C and T_o = 1100 °C



Thermogravimetric Analysis (TGA)

- Different mass losses under reduction.
- All three materials return to starting mass, and show reproducible behavior.

Water Splitting Behavior

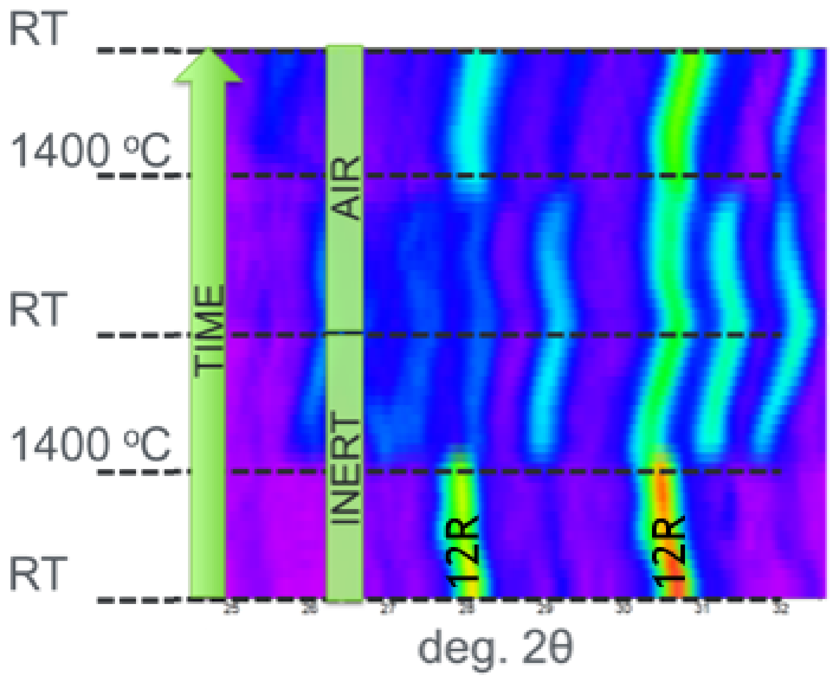


Stagnation Flow Reactor Results

- Different water splitting behaviors
  H_2 production: BCM ~ BNM > BPM
- Performance under pure steam vs. H_2O:H_2 shows BCM to be best.

XRD Phase Analysis Under Operating Conditions

High temperature XRD (HT-XRD) patterns collected from RT to 1400 °C under He and air.
Investigation of phase stability at different temperatures and atmospheres.



BPM HT-XRD Results

BCM and BNM

- Starting phase remains the major phase under operating conditions.

BPM

- BPM decomposes to form multiple phases when reduced, and reforms after oxidation.
- BPM's water splitting behavior can be from phase changes.

Summary/Acknowledgment

Two new water splitting materials, $BaNb_{0.25}Mn_{0.75}O_3$ and $BaPr_{0.25}Mn_{0.75}O_3$, were discovered.

Water Splitting Behavior

- BCM and BNM have similar production with steam.
- BCM still shows superior performance with lower pO_2.

Different Structural Behavior of BXM (HT-XRD)

- BCM and BNM mainly remain stable, but BPM decomposes when reduced.

Additional characterization methods are being used to investigate the difference in performance.

HydroGEN Advanced Water Splitting Materials

Funding

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

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