Advancing Solar Thermochemical Water Splitting R&D

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Albuquerque, NM, USA

Dr. Ellen B. Stechel,
Arizona State University
Tempe, AZ, USA (Moderator)

Structure of this Panel

- Moderator introduces context for the panel
- Panelists present opening remarks from their unique perspective
- Moderator asks some follow-up questions to the panelists
- Audience Q&A
- Time permitting – closing remarks from each panelist

Ellen B. Stechel, Arizona State University

- Co-Director, ASU LightWorks® campus wide initiative in Energy and Sustainability
- Professor of Practice, School of Molecular Sciences
- Works on thermochemical energy storage, thermochemical water & CO_2 splitting, and renewable ammonia

- **Co-PI on Benchmarking and Protocols Project in the DOE Energy Material Network HydroGEN Advanced Water Splitting Material consortium (Nel Hydrogen, ASU, CalTech, & PNNL)**
- PI on a Solar Thermochemical Hydrogen Production Project: Materials Discovery (with Princeton University)
- Principal Investigator of the ASU SETO Long Duration Storage Project (with Oregon State, Sandia, Siemens, & SwRI)
- Co-PI on Solar Thermochemical Ammonia Production (Sandia, ASU, Georgia Institute of Technology)

Benchmarking Advanced Water Splitting Technologies: Best Practices in Materials Characterization

In 2018 DOE awarded a project to a team that combined all advanced water splitting approaches and to focus on benchmarking, protocols, and roadmaps (Project ends Feb 2021) as part of the HydroGEN Advanced Water Splitting Materials Network

Proton OnSite, now **NEL Hydrogen** (**Dr. Kathy Ayers**) **Low temperature electrolysis** (LTE)

Pacific Northwest National Laboratory (**Dr. Olga Marina**) **High Temperature Electrolysis** (HTE)

California Institute of Technology (**Prof. CX Xiang**) **Photo-(electro)-chemical** (PEC)

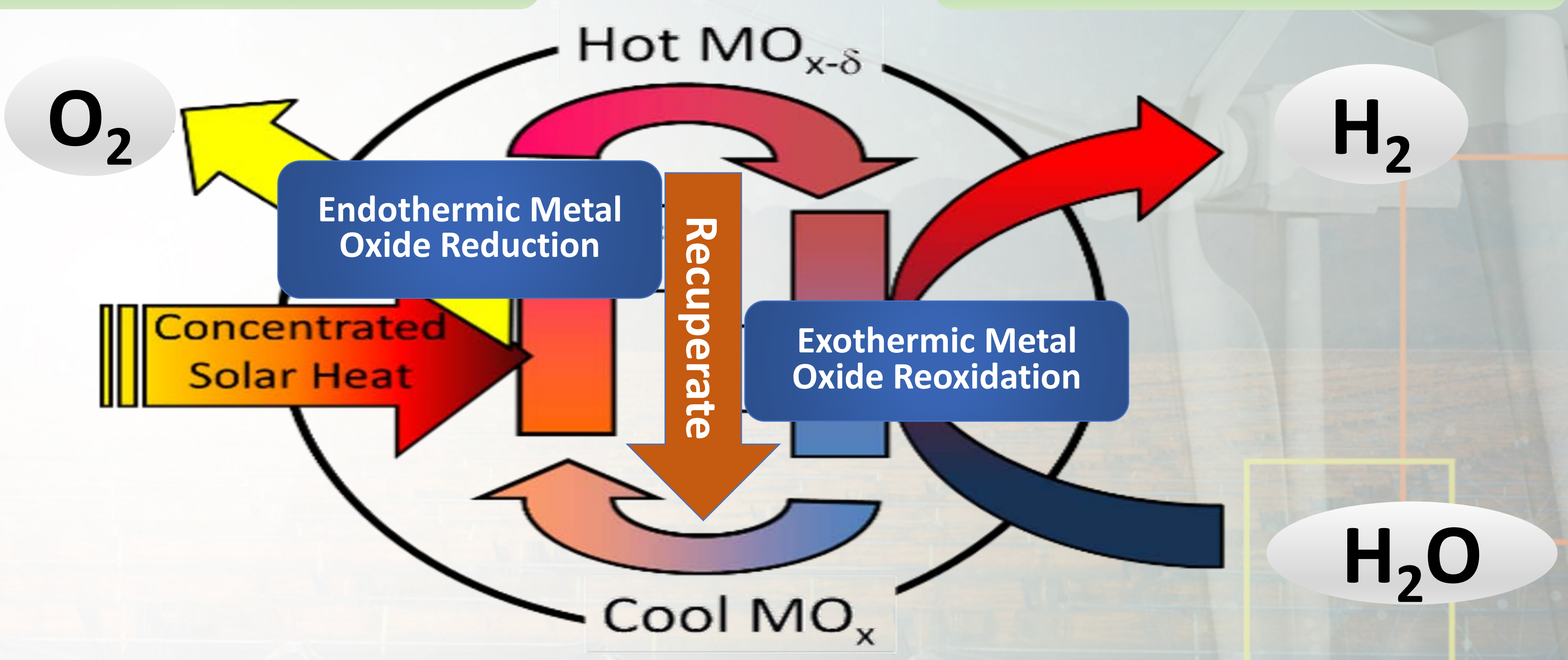
Arizona State University (**Prof. Ellen B Stechel**) **Solar Thermochemical** (STCH)

H_2 Technology Consulting LLC (**Dr. Karl Gross**) Hydrogen Storage

Solar Thermochemical Water Splitting: Two Step Metal Oxide Cycle

Energy in > 1300°C
Oxygen out

Oxygen in, Energy out < 1100°C



Anthony McDaniel, Sandia National Laboratories

- Principal Member of the Technical Staff
- Deputy Director for DOE's HydroGEN Advanced Water Splitting Materials Consortium
- Developing technologies for energy storage and conversion based on water and carbon dioxide gas splitting and high temperature electrochemistry

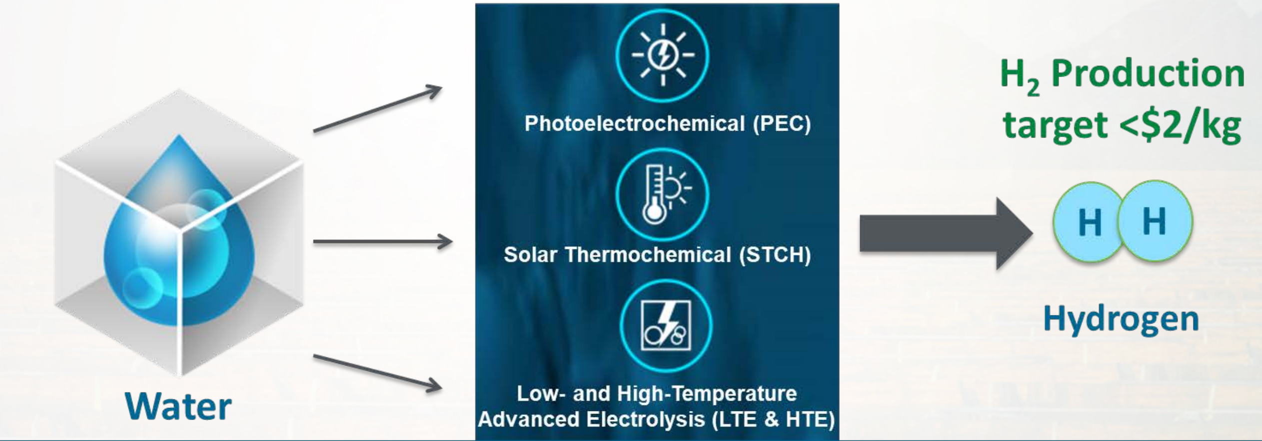
Experience at Sandia National Laboratories

- Thermochemistry and electrochemistry of advanced functional materials that include complex oxides used in water and carbon dioxide gas splitting and solid oxide fuel cell electrodes. Developed novel synchrotron-based X-ray diagnostic platforms for operando studies of surface electrochemistry and thermochemistry to probe material behavior in relevant, high-temperature functioning environments.
- Served as PI, co-PI, and Project Manager on competitively awarded multidisciplinary, multinational R&D efforts totaling more than $20M. Lead a team comprised of five US Universities and the German Aerospace Center (DLR) to develop materials for solar thermochemical water splitting, and to design and build a 5kWth-scaled demonstration of Sandia's particle bed reactor technology.
- Deputy Director for HydroGEN (https://www.h2awsm.org), which is a multimillion dollar consortium funded by the US Department of Energy that brings together six US National Laboratories and is tasked to develop advanced water splitting materials and platforms for solar fuel production.

HydroGEN
Advanced Water-Splitting Materials (AWSM)

AWSM Consortium Six Core Labs: NREL, Berkeley Lab, Sandia National Laboratories, INL (Idaho National Laboratory), Lawrence Livermore National Laboratory, SRNL

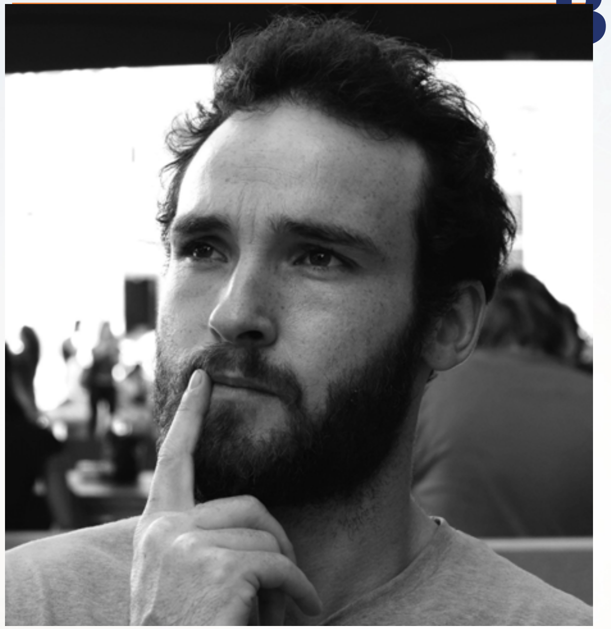
Accelerating R&D of innovative materials critical to advanced water splitting technologies for clean, sustainable, and low cost H_2 production, including:



HydroGEN consortium supports early stage R&D in H_2 production

National Innovation Ecosystem

Brendan Bulfin, ETH Zurich



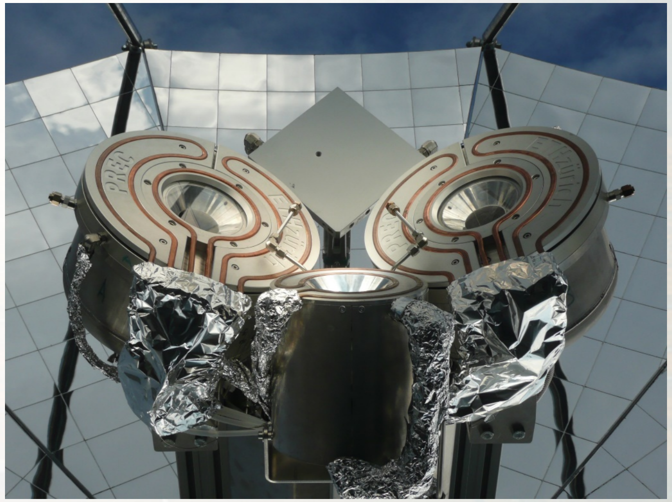
- Lecturer and research Scientist at ETH Zurich's Department of Mechanical and Process Engineering
- Research on redox materials and chemical process engineering.

- Leading SFERA–III workpackage on solar fuel production technologies, 2019 - present.
- Lecturer of Fuels Synthesis Engineering, a masters level course at ETHZ covering conventional and emerging technologies for the production of fuels, 2018-present
- Project leader and research Scientist at the German Aerospace Center's Institute of solar research, 2015-2017
- Ph.D. in Physics from Trinity College Dublin 2015

SFERA-III – EU's Horizon 2020 Research Infrastructure Programme
Solar Facilities for the European Research Area (14 RIs)

Solar fuels work package

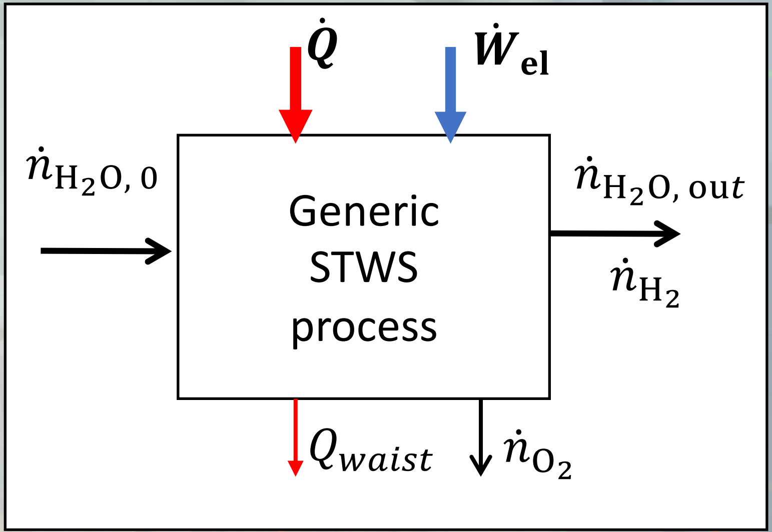
- Benchmarking techniques and protocols for materials and reactor performance.
- **Materials** – STWS we plan to align/adopt protocols from the HydroGEN project.
- **Reactors** – Figures of merit for benchmarking solar reactors



SFERA
Solar Facilities for the European Research Area

Reactor benchmarking

Whenever possible follow the methods established in classical chemical reactor engineering [1]. Reactor performance relates reactor size and complexity to production rates and total feedstock supply. It is crucial for assessing the economics of a process.



Process efficiency: $$\eta = \frac{\dot{n}_{H_2} \mathrm{HHV}_{H_2}}{\dot{Q}+\dot{W}} \quad \text{or} \quad \frac{\mathrm{HHV}_{H_2} \int \dot{n}_{H_2} \mathrm{d}t}{\int \dot{Q}+\dot{W}\, \mathrm{d}t}$$

Feedstock conversion: $$X_{H_2O} = \frac{\dot{n}_{H_2O,0} - \dot{n}_{H_2O,out}}{\dot{n}_{H_2O,0}}$$

A reactors performance equation then relates X and $\dot{n}_{H_2O,0}$ to the reactor volume V and process conditions T, p.

$$\text{output} = f(\text{input}, \text{reactor}, T, p)$$

[1] Octave Levenspiel, Chemical Reaction Engineering, 3rd Edition, Wiley

Andrea Ambrosini, Sandia National Laboratories

- Principal Member of R&D Staff, Concentrating Solar Technologies Dept.
- Exploration and development of functional oxide and nitride materials for renewable energy applications, particularly in the field of CSP

Projects:

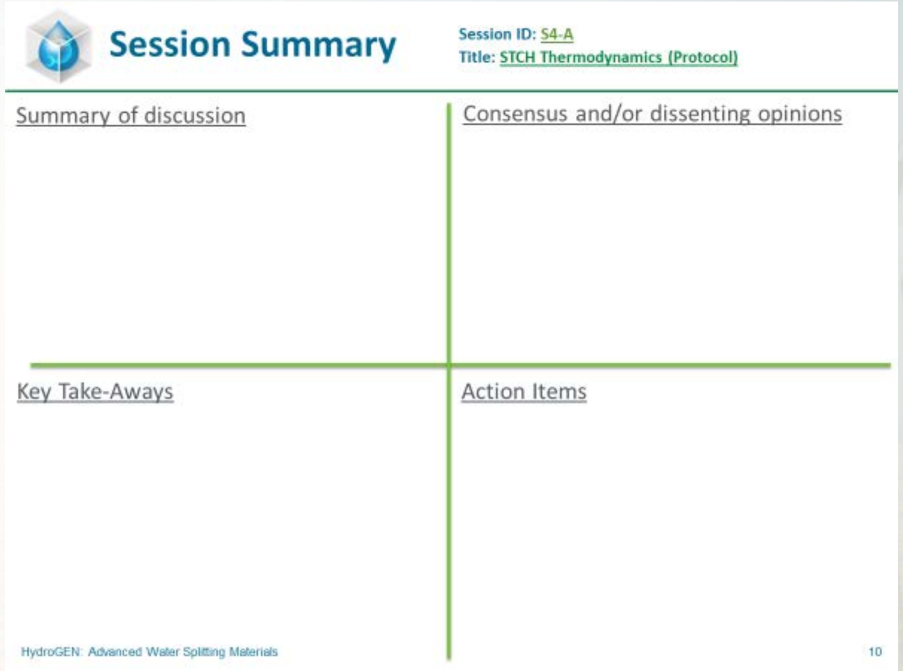
- PI on government- and industry-funded, international projects including:
  - Solar Thermal Ammonia Production
  - High-Performance RedOx Metal Oxides for Thermochemical Energy Storage
  - High-T Solar Selective Coating Development for Power Tower Receivers
- Co-PI/Materials Lead:
  - Long Duration Storage (w/ ASU)
  - Sunshine2Petrol (Sandia)
  - TGA Benchmarking (Benchmarking & Protocol, HydroGEN AWSM)

Experience

- Synthesis and characterization of novel materials for solar thermochemical fuel and chemical production, solar receiver coatings, and thermochemical energy storage
- 30+ peer-reviewed publications, 7 patents (4 pending)
- PhD Inorganic Chemistry (Northwestern University)

Developing a testing protocol and benchmarks for solar thermochemical water splitting materials

- Methods of testing, analyzing, and reporting on new materials for TCWS becoming increasingly varied
- A common set of benchmarks and protocols to assess performance necessary to compare “apples to apples”
- Workshops sponsored by HydroGEN AWSM Benchmark Project to gain input and buy-in from the STCH community to draft protocols and define benchmarks



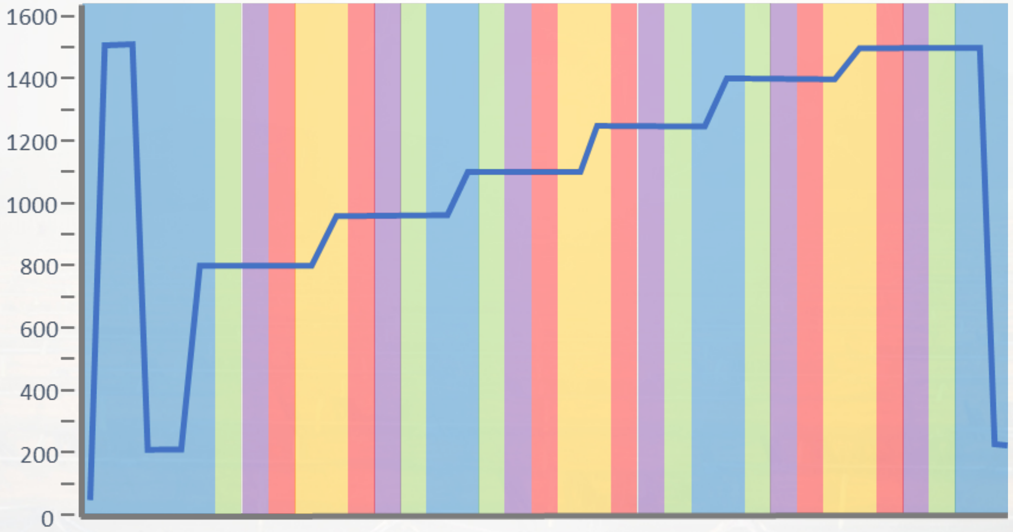
Topics

- Metrics (units and operating boundaries)
- Standards beyond the state-of-the-art ceria
- Characterize thermodynamics
- Characterize kinetics
- Efficiency calculations
- Durability
- Role and challenges for materials discovery using Density Functional Theory

Example: Thermodynamics via Thermogravimetric Analysis (TGA)

Proposed Protocol: variable T (blue line) and pO2 (colored columns) TGA screen

- All systems should run standard(s) to qualify system
- Care should be taken to properly measure pO_2 in order to ensure accuracy of δ
- At each step (T/pO_2) the sample must come to equilibrium, i.e., weight loss must stabilize, before advancing to the next step
- Break-in cycle to eliminate any surface adsorbed species and ensure materials are equilibrated under a common set of conditions
  - Sample mass at this temperature and pO_2 is considered to be the starting point of the analysis, where it is assumed that $\delta=0$



Discussion Points

- Can you use other methods than TGA?
- Separate protocol for pO_2 vs T and water splitting?
- How low pO_2 do we need to hit?
- How reasonable is it to consistently achieve super-low pO_2?
- How do we establish standard protocol for achieving?
  - Round Robin?
- Standard sample mass/form?

Thank you!

Drs. Anthony McDaniel; Brendan Bulfin; and Andrea Ambrosini

Follow-up Questions

Thank you!

Drs. Anthony McDaniel; Brendan Bulfin; and Andrea Ambrosini

Questions and Discussions

Thank you!

To the Audience, the Panelists, the Organizers, and ASME Staff

We are going to end this session and have a short break; the next sessions start at 2:00PM. **That is Eastern Time Zone**

Please go to the Conference Home Page and select which session you wish to join.

We will see you soon!