HydroGEN
Advanced Water Splitting Materials

Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Breakout Session Summaries
Solar Thermochemical Hydrogen (STCH)

March 2 – 4, 2021

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Session Summary

Session ID: 2021 STCH-1 (Jonathan Scheffe Session Lead)

Title: STCH Kinetics (Protocol)

Summary of discussion

A summary and updates since 2019 was presented

Discussion centered around finalizing experimental specifics of the protocol such as operating temperature, particle size, gas concentration and reactant gas species

There was good agreement and consensus among the attendees and clear action items going forward

Consensus and/or dissenting opinions

- Two particle size ranges rather than one is preferable.
- Ddurability testing dependent on durability protocol but need to account for burn in -- Effect of cycle number will also be borne out in statistical analysis
- Chemical and thermal reduction methods are fine to assess oxidation kinetics
- Divide characterization prior to kinetic testing into two categories, necessary and recommended. E.g., XRD, an estimate of surface area (whether BET, image based, etc.) and bulk composition necessary, whereas BET, SEM, PSD recommended
- pO_2 controlled via O_2 mixes or H_2/H_2O ratios - consensus
- Pure steam should be used during oxidation rather than H_2O/H_2 mixture – consensus
- At least three temperatures with 50-100 K spacing – consensus
- Model based approaches to compliment experiments using method of McDaniel - consensus

Key Take-Aways

- Identifying perhaps two particle size distributions, e.g., small (1-10 μm and 10-100 μm) and large, may be important to help separate materials that may look good in one range and poor in another, like ferrites
- Durability testing will be outsourced to the Durability Protocol

Action Items

- Finalize protocol draft
  1. J. Scheffe – Experimental Procedure
  2. A. McDaniel – Model Based Analysis
- Finalize appropriate PSD's and initial characterization methods

Session Attendee List

Session ID: STCH-1
Title: STCH Kinetics (Protocol)

Name	Affiliation
Andrea Ambrosini	Sandia National Laboratories (SNL)
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Brendan Bulfin	EPFL, Switzerland
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Dylan McCord	University of Florida
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Hector De Santiago	Savanah River National Laboratory (SRNL)
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James Miller	Arizona State University
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Kangjae Lee	German Aerospace Center (DLR)

Session Attendee List

Session ID: STCH-1
Title: STCH Kinetics (Protocol)

Name	Affiliation
Kent Warren	University of Colorado Boulder (UC Boulder)
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Levi Irwin	DOE Contractor
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Ryan O'Hayre	Colorado School of Mines
Sai Gautam Gopalakrishnan	Indian Institute of Science
Shang Zhai	Stanford University
Stefan Brendelberger	German Aerospace Center (DLR)
Steven Wilson	Arizona State University
Tadashi Ogitsu	Lawrence Livermore National Laboratory (LLNL)
Waseer Mohamed	Columbia University
Wei Li	West Virginia University
Zach Bare	University of Colorado Boulder (UC Boulder)
Zhiwen Ma	National Renewable Energy Laboratory (NREL)

Session Summary

Session ID: 2021 STCH-2 (Anthony McDaniel Session Lead)

Title: STCH Technology Roadmap Discussion

Summary of discussion

Discussed the need for a roadmap, debated on specific topical R&D areas such as materials, reactors, and subsystems, but stopped short of formulating a plan for action

Discussion vacillated between setting endpoint performance targets for materials, reactors, and subsystems and then working backwards to look for "choke points" versus select a material, put it into a reactor, run it and work forwards by finding solutions to technology barriers as they become more evident in real operating conditions

Consensus and/or dissenting opinions

- Recognized that development of materials and reactors will likely continue along independent paths, which makes it difficult to evaluate progress.
- There is a need for a "universal" testing system for materials in real world operating conditions.
- Need an action plan for creating an community driven roadmap.

Key Take-Aways

- If this community does not develop a R&D roadmap, then somebody else will do it for us and we may not agree with that outcome
- It would be wise to learn and take lessons from other industries such as PV or automotive. The state of STCH was likened to 1950's PV (inefficient and expensive)
- Now is the time to select a material and develop a reactor around it. Uncertainty expressed about scale of this reactor due to cost and manageability (e.g., difficult to source 100kgs of materials, too much for labs to make, too small for industry to get interested)

Action Items

- Survey members of the community on whether there is interest in volunteering time to preparing a roadmap

Session Attendee List

Session ID: STCH-2
Title: STCH ROADMAP

Name	Affiliation
Andrea Ambrosini	Sandia National Laboratories (SNL)
Anthony McDaniel	**Sandia National Laboratories (SNL)**
Anyka Bergeson-Keller	Colorado School of Mines
Charles Musgrave	University of Colorado Boulder (UC Boulder)
Chris Muhich	Arizona State University
Dawei Zhang	University of California San Diego (UCSD)
Dylan McCord	University of Florida
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Session Attendee List

Session ID: STCH-2
Title: STCH ROADMAP

Name	Affiliation
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Katie Randolph	Department of Energy
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Zach Bare	University of Colorado Boulder (UC Boulder)
Zhiwen Ma	National Renewable Energy Laboratory

Session Summary

Session ID: 2021 STCH-3 (Andrea Ambrosini Session Lead)
Title: STCH Thermodynamics (Protocol)

Summary of discussion

- Details in the developing protocol were discussed in terms of suggested experimental parameters and methods
- Implementation of protocol
- Reference standard candidates were discussed
- Requirements for reporting data
- Time spent on low pO_2 issues

Consensus and/or dissenting opinions

- Participating labs must show that their TGA is well calibrated by showing that their data taken on a reference material matches each other within acceptable error bars (SNL, CSM, UF)
- Water splitting capability should be considered when determining reference standards
- Results should show reproducibility w/ error bars
- CEF may be a possible substitute for very low pO_2 measurements (have to first show capability to extrapolate)

Key Take-Aways

- Reaching very low pO_2 (< 1 ppm) is difficult for many labs
- Protocol for achieving low pO_2 by most labs should be identified and explained in detail
- Systems should be qualified by running standards
- Perovskite standard should be identified and exercised in addition to the existing CeO_2 standard
- Reaching reduction equilibrium at low pO_2 and T is time consuming

Action Items

- Edit and refine current draft of the protocol
- Round robin of CeO_2 to ensure different labs are consistent using the protocol
- Determination of perovskite standard
- Identify additional characterization techniques, particularly for low pO_2, e.g., stagnation flow reactor

Session Attendee List

Session ID: STCH-3
Title: STCH THERMODYNAMICS (PROTOCOL)

Name	Affiliation
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Charles Musgrave	University of Colorado Boulder
Dylan McCord	University of Florida
Elizabeth Gager	University of Florida
Ellen B. Stechel	Arizona State University
Eric Coker	Sandia National Laboratories
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Ivan Ermanoski	Arizona State University
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Session Attendee List

Session ID: STCH-3
Title: STCH THERMODYNAMICS (PROTOCOL)

Name	Affiliation
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Michael Sanders	Colorado School of Mines
Shang Zhai	Stanford University
Steven Wilson	Arizona State University
Zhiwen Ma	National Renewable Energy Laboratory

Session Summary

Session ID: 2021 STCH-4 (Ivan Ermanoski Session Lead)
Title: Durability

Summary of discussion

- Recapped last year's discussion and picked up with remaining items
- Largely achieved consensus on early and advanced durability testing, with *in-situ* testing yet to be addressed in detail

Consensus and/or dissenting opinions

- Following level 1 and 2, the additional *ex-situ* tests that make sense are:
  - Material compatibility. This might even creep into levels 1&2, in case there are any concerns regarding putting materials into instruments
  - More cycles: Maybe ~1-2k, otherwise similar to level 2
- Diminishing returns in more ex-situ tests
- Need to design/build and then exercise materials in reactors
- Testing protocols should be as approachable and accessible as possible

Key Take-Aways

- At some point *ex-situ* durability tests start to diminish returns.
- With few materials likely to pass Levels 1 and 2 of durability testing, the next best step is likely to exercise materials in reactors – potentially after a couple more *ex-situ* compatibility and cycling tests
- What do test reactors and equipment look like? They need to be as accessible as possible. This is an area where more understanding is needed

Action Items

- Publish Level 1 and Level 2 Durability Protocols after review by several in the community

Session Attendee List

Session ID: STCH-4
Title: STCH DURABILITY (PROTOCOL)

Name	Affiliation
Al Weimer	University of Colorado Boulder
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Dylan McCord	University of Florida
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Michael Sanders	Colorado School of Mines

Session Attendee List

Session ID: STCH-4
Title: STCH DURABILITY (PROTOCOL)

Name	Affiliation
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Tadashi Ogitsu	Lawrence Livermore National Laboratory
Zach Bare	University of Colorado Boulder
Zhiwen Ma	National Renewable Energy Laboratory

Session Summary

Session ID: 2021 STCH-5 (Chris Muhich Session Lead)

Title: Density Functional Theory

Summary of discussion

- A protocol is unlikely to achieve the aims of the project as agreed in 2019
- A paper or report of “Best Practices” including pitfalls, and structural/magnetic ordering effects, and functional & lab-to-lab results comparisons will be completed

Consensus and/or dissenting opinions

- All agreed that a protocol is not feasible but best practices would be valuable
- A minimum list of areas that a best practices paper should include were discussed

Key Take-Aways

- A group was formed to start addressing the best-practices paper
- That group will determine what will be included and how to structure the paper

Action Items

- Establish list of those interested and willing to co-author the best practices paper
- Begin meeting about best practices manuscript and round-robin calculations

Session Attendee List

Session ID: STCH-5
Title: STCH DENSITY FUNCTIONAL THEORY

Name	Affiliation
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Jonathan Scheffe	University of Florida
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Robert Wexler	Princeton University
Sai Gautam Gopalakrishnan	Indian Institute of Science
Shang Zhai	Stanford University
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Session Attendee List

Session ID: STCH-5
Title: STCH DENSITY FUNCTIONAL THEORY

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Stefan Brendelberger	German Aerospace Center (DLR)
Stephan Lany	National Renewable Energy Laboratory
Steven Wilson	Arizona State University
Tadashi Ogitsu	Lawrence Livermore National Laboratory
Zach Bare	University of Colorado Boulder
Zachary Clifford	Rutgers University

Session Summary

Session ID: 2021 STCH-7 (Anthony McDaniel Session Lead)
Title: Metrics -Units and Operating Boundaries (Protocol)

Summary of discussion

- Discussed three major points
  1) review and approval of prior metrics
  2) the need for a Rigone-type plot to compare redox materials
  3) best practices for calculating process efficiency
- Discussion on equitable comparison of material performance; more materials are being discovered and reported in literature, hence the need
- Discussion about best practices for predicting solar-to-hydrogen conversion efficiency (aka process efficiency)

Consensus and/or dissenting opinions

- H_2 productivity should be normalized as "mole H_2 /mole atoms" (including active and inactive phases)
- 1-sun H_2 production rate (kg H_2/s m^2) is useful; area on the mirrors; not the only important metric
- No agreement on standardizing cycle conditions for comparison purposes; thermo is not enough because it lacks "cycle time" information – likely optimized for material with some boundary conditions.
- Process efficiency needs a detailed model; computational tools, methods, and assumptions all matter; possible to standardize some assumptions

Key Take-Aways

- Given the resources it takes to critically assess material performance via measurement and modeling, a tiered approach should be taken
- Materials must first pass fast and simple screening tests before investing more resources to determine viability
- Standardizing protocols and performance metrics is possible to some extent, but it is premature to prescribe global parameters and operating boundaries. In other words, metrics and operating boundaries remains a material-specific issue

Action Items

- Finish metrics definition draft and distribute to members of the community for publication in Frontiers in Energy Research – Benchmarking and Protocols Research Topic
- These will be recommendations including rational, not requirements

Session Attendee List

Session ID: STCH-7
Title: STCH METRICS: UNITS AND OPERATING CONDITIONS

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Kangjae Lee	German Aerospace Center (DLR)
Kent Warren	University of Colorado Boulder
Kim Cierpik-Gold	DOE Contractor (BGS)
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Rohini Bala Chandran	University of Michigan
Shang Zhai	Stanford University
Stefan Brendelberger	German Aerospace Center (DLR)
Steven Wilson	Arizona State University

Session Attendee List

Session ID: STCH-7
Title: STCH METRICS: UNITS AND OPERATING CONDITIONS

Name	Affiliation
Tadashi Ogitsu	Lawrence Livermore National Laboratory
Zach Bare	University of Colorado Boulder
Zachary Clifford	Rutgers University
Zhiwen Ma	National Renewable Energy Laboratory

Session Summary

Session ID: 2021 STCH-8 (Zhiwen Ma Session Lead)
Title: STCH Systems Modeling and Techno-economics)

Summary of discussion

- Systems Modeling and STCH materials are inter-connected. Defining STCH materials help define system configuration and components, which are analysis bases of techno-economics analysis (TEA)
- STCH materials are the foundation of STCH system and maintain ongoing researches in the field that currently cross HFTO, SETO, and international programs. Hybrid thermochemical/ electrochemical processes may be explored for its benefits and potentials.
- Developing STCH approaches/ consensus on system design will be key to system modeling and TEA.

Consensus and/or dissenting opinions

Community connection helps develop, regularly update, and coordinate working progresses to be effective. Material data to be standardized are recommended to embody into community-accepted database via internet access and analysis program. Systems modeling may consider process software in addition to technoeconomics (such as H2A tool). It would also be useful if system modeling and Technoeconomics software could generate component design and performance to enable cross-technology applications.

Key Take-Aways

STCH material development may lead the system modeling and methodology currently needed by the STCH community.

Establishing connections between STCH material development and system integration can facilitate a promising STCH path.

The need of communication across material development and system integration is necessary to inform industry of the technology status and evaluation tools.

Action Items

- Interface with activities initiated under SolarPACES Task II and the international community for roadmap, code (including software modeling package), and standard development
- Should consider industry involvement to promote a commercialization path. With solar fuel startups Heliogen, Synhelion), industry should be audiences of the STCH outcomes
- Volunteers from the session will reach out to others in the community to gauge interest in forming a system modeling and Technoeconomics U.S. working group

Session Attendee List

Session ID: STCH-7
Title: STCH SYSTEMS AND TECHNOECONOMICS

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Session Attendee List

Session ID: STCH-8
Title: STCH SYSTEMS AND TECHNOECONOMICS

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Zhiwen Ma	**National Renewable Energy Laboratory**

Session Summary

Session ID: 2021 STCH-9 (Jim Miller Session Lead)
Title: STCH Wrap-up

Summary of discussion

- Materials focused sessions mostly focused on fine tuning protocols
- TEA and Roadmap – what is the appropriate level of detail? There is linkages and interdependence here
- Metrics – retired several discussions, will continue with HydroGen 2.0

Consensus and/or dissenting opinions

- Normalization/universal standards, error bars, reproducibility & replication, sensitivity analysis
- Don't eliminate something prematurely
- Materials, reactors, or both?
- Work from end point back to define constraints/what is reasonable and identify main sensitivities?

Key Take-Aways

- Community has developed a lot of consensus
- A key challenge for further consensus lies in the chicken and egg issue of the materials vs. reactors
- We have to lead by example in our own work and reporting
- We can achieve additional progress through HydroGEN 2.0 and leverage, e.g., with SolarPACES, industry, foreign partnerships …

Action Items

- Finalize/publish protocols or best practices for kinetics, durability, DFT, thermo
- Data sharing methods, .e.g., in DFT
- Round robin calculations (DFT) and tests (thermodynamics TGA)
- Define targets and metrics (Roadmap, TEA)

Session Attendee List

Session ID: STCH-9
Title: STCH WRAP UP

Name	Affiliation
Andrea Ambrosini	Sandia National Laboratories
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Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Brief Overview of the Solar Thermochemical Pathway Breakouts for Closing Plenary

March 8, 2021

Ellen B. Stechel, presenting

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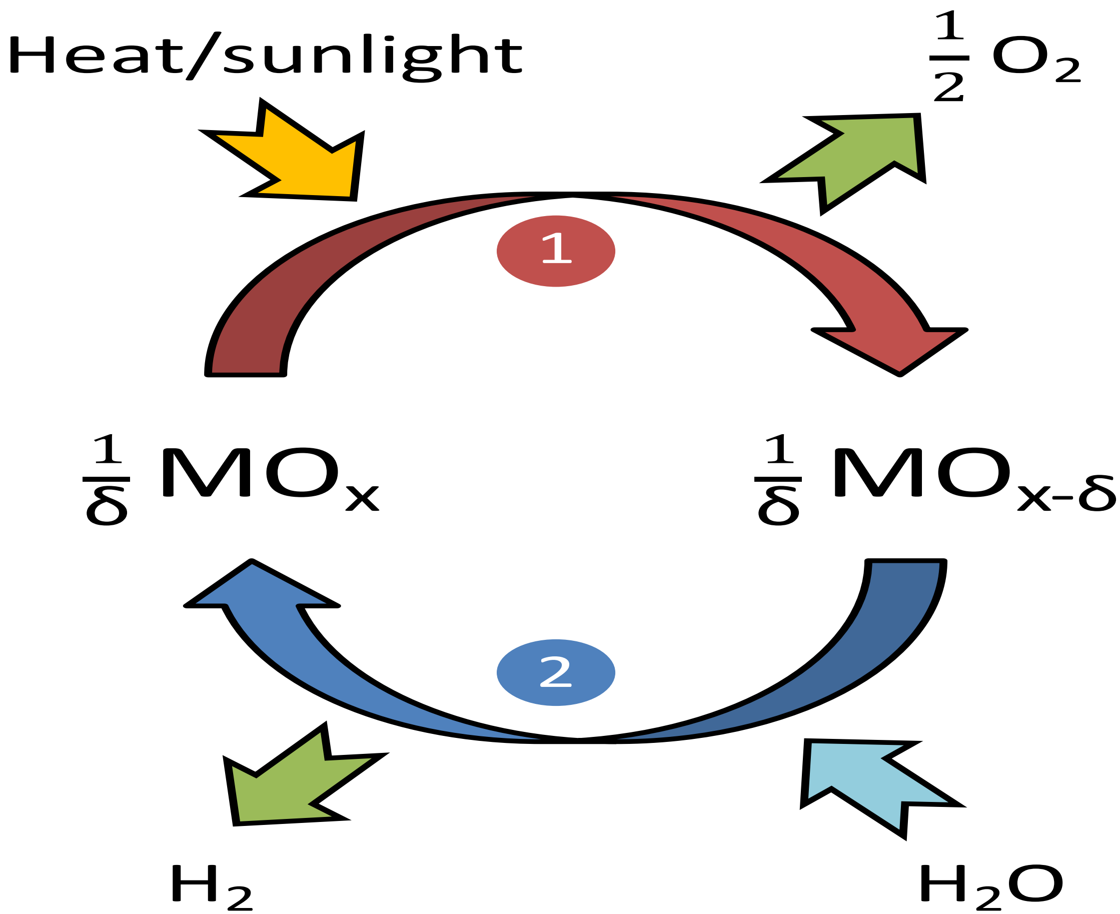
Two-step Redox-Active Metal Oxide Water Splitting Cycle



STCH: Solar Thermo-Chemical Hydrogen

STCH Conducted Eight Breakout Sessions

- Four on materials properties: (1) Thermodynamics, (2) Kinetics, (3) Durability, and (4) Computation (Density Functional Theory)
- Three higher level: (1) Elements of a Roadmap, (2) Systems Modeling/Technoeconomics, and (3) Metrics/Operating Conditions
- The eighth was a wrap up session

			Session Leads
STCH-1	Tues	STCH Kinetics (33)	Jonathan Scheffe
STCH-2	Tues	STCH Technology Roadmap (33)	Tony McDaniel
STCH-3	Tues	STCH Thermodynamics (20)	Andrea Ambrosini
STCH-4	Tues	STCH Durability (22)	Ivan Ermanoski
STCH-5	Wed	STCH Density Functional Theory (26)	Chris Muhich
STCH-7	Wed	STCH Metrics and Operating Conditions (22)	Tony McDaniel
STCH-8	Wed	STCH Systems Modeling and Techno-economics (22)	Zhiwen Ma
STCH-9	Thurs	STCH Wrap-up Session (22)	Jim Miller

Special Thank you to the Note Takers

- Andrea Ambrosini (STCH-4)
- Robert Bell (STCH-8)
- Ivan Ermanoski (STCH-8)
- James Park (STCH-3, STCH-9)
- Jonathan Scheffe (STCH-2)
- Kent Warren (STCH-1)
- Steve Wilson (STCH-3, STCH-5, STCH-7)

Common Themes

- Significant consensus in the community down to many details
  - Much more than at the first workshop and the second workshop
  - Especially regarding establishing metrics, thermodynamics, kinetics, and durability protocols, and sharing best practices in density functional calculations
- Need to predicate our testing protocols in terms of screening levels 1, 2, and 3
  - If they fail at Level 1, they get tossed, ditto at Level 2
  - STCH has used a Materials Genome like approach to identify candidates by predicting from computation (Level 0 – helpful but not the only route to candidates)
  - Unfortunately, there are limitations to such predictions as they often fail at or before Level 1 (cannot be synthesized, melt at too low a temperature, do not cycle)
  - But still it is a highly valuable approach as it limits the number of experiments given the overall candidate pool is too large for a purely empirical approach
- The field faces “unique” challenges as there is no reactor test platform in the U.S. that can exercise materials in realistic operating conditions (Level 3)

Roadmap and Systems Modeling

- Unclear to the community on value, need, or resources available to refine a roadmap
  - Who would be the audience
  - Are multiple roadmaps needed depending on the audience
  - What would be the goals
- If this community does not develop a R&D roadmap, then somebody else will do it for us and we may not agree with that outcome
- Discussion on working backwards from target metrics and bounding metrics for components
- Lots of discussion on “chicken and egg” problem on materials vs. reactors
- Need all the key system components before can develop a credible technoeconomic assessment – so inter-relationship

Thermodynamics

- Want to first show that the material will split water
- For thermodynamics the "workhorse" characterization is thermogravimetric at a number of relevant temperatures and partial pressures of oxygen
  - These are time-consuming and require a simpler Level 1 measurement of capacity, measured as moles H_2 per mole atom of the working material (different than lit)
- Discussion focused on the Protocol for determining thermodynamic relationship between the off-stoichiometry δ, temperature (T), and partial pressure of O_2 (pO_2)
  - Lot of discussion on how to achieve very low pO2 levels and potential issues
- Agreed to show reproducibility between labs with a round robin using CeO2 as the reference (three labs)
- Agreed need to identify a reproducible perovskite reference that splits water (does not have to be state of the art)
  - Haven't found a ternary perovskite that passes Level 1 screening including splitting water - may have to agree to use a quaternary

Kinetics

- The kinetics discussion focused on the Protocol for using a laboratory flow reactor to assess water oxidation kinetics for materials' candidates
  - Agreed that powders 10-100 µm to start; however, larger pellets are also necessary as we know that ferrites will work when kept small but not at more practical sizes
  - Need to determine regime for which kinetics is independent of particle size
- Kinetics only follows if material passes Level 1 durability and stability screening
- Can thermally or chemically reduce (latter may be easier in some labs)
- Need at least three different temperature measurements but not prescribing which temperatures
- The kinetics model should be determined empirically rather than mechanistically

Durability

- General agreement reached with Level 1 and Level 2 durability criteria protocol
  - At least Level 1 necessary before doing extensive thermodynamics or kinetics measurements
- Unclear but likely a reactor test stand or new specialized instruments will be necessary for Level 3 (to test in realistic operating conditions)
- Discussed the importance of testing for material's compatibility in addition to durability
  - Might even creep into Levels 1 and 2, in case there are concerns regarding putting materials into laboratory instruments

Density Functional Theory

- The discussion centered on preparing a publication of best practices for calculating materials general properties and oxygen vacancy formation energy
  - Will include some non-experts and experimentalist
- Also discussed the range of challenges and considerations such as
  - Magnetics, spin ordering, effective mass, spin-orbit coupling, alloying, phase changes, local structure around defects.
- Candidate searching should be done broadly over large chemical space
- Planned for doing a round robin calculation on a material with the different approaches, will be included in the publication.
- CeO_2 can be difficult due to contribution of f electrons, but must be included as it is the "state-of-the-art" and best studied

Thank you for your attention and to all the session leads, note takers, and participants, in these highly productive discussions