Session Summary

Session ID: 2022 STCH-1 (Anthony McDaniel Session Lead)
Title: HydroGEN 2.0 Metrics
Scribe: Ivan Ermanoski & Mural Board: Kent Warren

Summary of discussion

A summary of Hy2.0 plans for critically assessing STCH pathway viability was presented

Discussion centered around finalizing elements to the spider chart, which is a summary of material performance

Consensus among attendees that the spider chart content needs to be agreed on by the community, including the possibility of using the analytical hierarchy process to aid decisions

Consensus and/or dissenting opinions

- Outline of performance chart as presented is a good starting point, but more details and refinement are necessary (still a moving target)
- Material cost and physical and market availability matters in one opinion
- Availability and cost may or may not matter in another opinion, depending on the overall fraction of the plant/process cost that goes into the material
- Durability also matters, but this community continues to view durability as secondary to material discovery
- A measure of kinetics, cycle efficiency, and high conversion yield needs to be incorporated into the spider chart, details TBD
- Cycle efficiency can follow directly from an equation of state, but going a step further would be to modify the equation of state to maximize efficiency and inform materials work

Key Take-Aways

- Projecting material performance onto an easily digestible visual like a spider chart is an important outcome for Hy2.0
- Details captured by the spider chart table need to be agreed upon by the community

Action Items

- Formulate material metrics for comparing performance (version 1)
- Choose exemplar materials for comparative study against CeO2
- Assess selected material formulations
- Evaluate potential to meet DOE technology performance targets

Session Summary

Session ID: 2022 STCH-S2 Andrea Ambrosini (Session Lead)
Title: Promising STCH Materials
Scribe: Andrew Smith & Mural Board: Kent Warren

Summary of discussion

- Sophisticated computational and machine learning has enabled us to narrow pool of candidates from thousands to hundreds
- How do we narrow from there? What parameters do we screen on?
- What other materials or families may we be missing?

Consensus and/or dissenting opinions

- Group was mostly in consensus
- Down-select will be based on reports, DFT, calculations, literature, and chemical intuition
  - Will require development of new modeling capability
  - Can we predict melting point, nonstoichiometry/solid solution behavior, including solubility limits
- Combinatorial synthesis and characterization is a good goal, but what is the "sniff test" (characterization) to screen on?
- We should consider/revisit solid solution cations vs composites (e.g., Fe:YSZ), new form factors of existing materials, phase change materials

Key Take-Away

A mix of existing data and new capabilities will be required to down-select and screen predicted STCH materials

Action Items

- HydroGEN 2.0 will characterize several exemplar materials in further detail
  - May include BCM, CCTM, high entropy oxides, hercynite
- Using existing capabilities, stakeholders should collaborate to narrow the existing list of potential materials

Session Summary

Session ID: 2022 STCH-4 (Ivan Ermanoski Session Lead)
Title: Durability
Scribe: Dylan McCord & Mural Board: Kent Warren

Summary of discussion

- Last year recap and picked up next items
- Significant advances in materials necessitate, in-situ testing
- What do reactors look like, how much material, what outputs to measure?
- How many cycles and/or how much time at temperature?

Consensus and/or dissenting opinions

- Need *in-situ* durability testing
- Need realistic environment (temperature, cycle time, heat flux and temperature ramp rate…)
- Hours at temperature (~500-1000?) more important than # of cycles, but min. #of cycles necessary (5000?)
- Operation >1000h may be at the pilot scale
- Amount of material on the low end of 0.1-1 kg, primarily driven by large reactor size needed for a lot of material
- H_2 or CO production both ok
- *In-situ* test platform should be replicable
- Open Q: should *in-situ* be a real reactor or tube furnace-like

Key Take-Aways

- *In-situ* testing should WS and measure H_2
- Can we scale up materials for in-situ? 0.1-1 kg
- Material form factors are reactor-dependent
- Metrics: mass loss, sintering, performance loss
- No “standard reactor” exists, but it needs to be indicative of performance at scale
- Splitting CO_2 is easier and would be acceptable
- Need for industry input

Action Items

Solicit community input, including industry, on what Level 3 materials durability testing would look like and to what target TRL, so that STCH can advance toward commercialization

Session Summary

Session ID: STCH-5 (Eric N. Coker, Session Lead)
Title: STCH Thermodynamics
Scribe: Dylan McCord & Mural Board: Kent Warren

Summary of discussion

- Details of existing TGA protocol were reviewed
- Weak points of protocol were discussed, including:
  - Definition of "zero point"
  - How to speed up experiment without sacrificing accuracy
- Can the compound energy formalism (CEF) help speed up overall thermodynamic predictions, and what is the minimum amount of experimental data needed for accurate CEF?

Consensus and/or dissenting opinions

- Focus needs to be on methods to speed up thermodynamic property determination, e.g., through modeling/simulation
- "Simple" screening approach (i.e., Temperature Programmed Thermal Redox (TPTR) method recently published by CO School of Mines) may be useful first step

Key Take-Aways

- Reaching reduction equilibrium at low pO_2 and Temperature (T) is time consuming
- Extrapolation of mass-loss curve to steady state under particular T & pO_2 is non-trivial but ongoing developments
- CEF may allow faster determination of thermodynamic properties, but needs real data (on standard materials) to exercise the process
- Accurate determination of fully oxidized "zero point" is not trivial due to differences in intrinsic vacancies for different formulations

Action Items

- Still need definition of standard materials
- STCH community needs to reach consensus on a method to determine "zero point", i.e., intrinsic non-stoichiometry of STCH materials
- Need better specification of minimum data requirements (T-range, pO_2-range, number of points) for reliable prediction of thermodynamic properties

Session Summary

Session ID: 2022 S-6 (Jim Miller Session Lead)
Title: STCH Wrap-up/Bringing it to Closure and Next Steps
Scribe: Dylan McCord & Mural Board: Kent Warren

Summary of discussion

- HydroGEN 2.0 metrics – content of spider chart for material comparison; new 3.0 metrics?
- Materials – exemplars of different classes? Selection criteria beyond thermo screen?
- Durability – long term criteria: what is good enough and how to measure?
- Thermodynamics – emerging/unmet needs?

Consensus and/or dissenting opinions

- Shift towards proving out at a system level establishing performance vs alternatives
- Tentative identification of exemplar classes and examples
- No standard durability apparatus identified or in-place – centralized or distributed?
- Methods for Zero-pt. and equilibrium pt. determination is needed for thermo – key for models and speeding up process

Key Take-Aways

- Previous action items are complete or near complete
- New systematic tools needed to move beyond thermo screening, e.g., melting point prediction
- Need to have accurate thermo to develop accurate materials and systems models
- Interplay/interaction between experiment and modeling is crucial for validation and refinement of each

Action Items

- Establish consensus for metrics to create spider-chart
- Refine exemplar palette
- Engage industry – end-use and those with similar materials environments
- Refine value proposition against specific alternatives
- Cross-lab validation