H2NEW Hydrogen from Next-generation Electrolyzers of Water

U.S. DEPARTMENT OF ENERGY

HydroGEN and H2NEW Data Hub

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3/14/2023

H2NEW In-Person Meeting, Napa, CA

https://datahub.h2awsm.org/

NREL Transforming ENERGY | INL Idaho National Laboratory | Argonne NATIONAL LABORATORY | BERKELEY LAB Bringing Science Solutions to the World | Lawrence Livermore National Laboratory | Los Alamos NATIONAL LABORATORY EST. 1943 | NETL NATIONAL ENERGY TECHNOLOGY LABORATORY | OAK RIDGE National Laboratory | Pacific Northwest NATIONAL LABORATORY

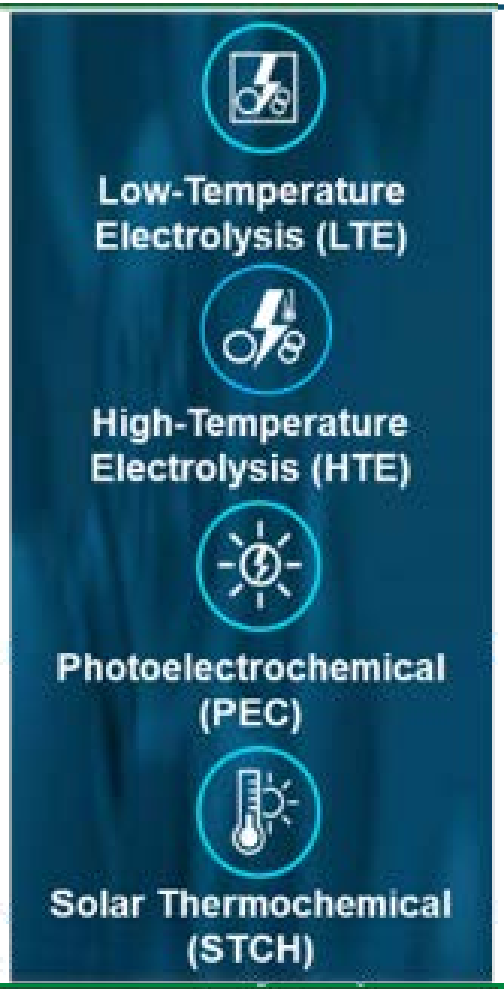
HydroGEN Consortium

Website: https://www.h2awsm.org/

Goal: Accelerating R&D of innovative advance water splitting (AWS) materials and technologies for clean, sustainable and low-cost hydrogen production.

Challenges
- Cost
- Efficiency
- Durability

Water



National Lab Consortium Team

NREL National Renewable Energy Laboratory
Berkeley Lab
Idaho National Laboratory
Sandia National Laboratories
Lawrence Livermore National Laboratory

H_2 Production target ≤ $1 kg

Hydrogen

HydroGEN is advancing Hydrogen Shot goals by fostering cross-cutting innovation using theory-guided applied materials R&D to accelerate the time-to-market and advance all emerging water-splitting pathways to enable clean, low cost, and sustainable low-cost hydrogen production

HydroGEN and H2NEW Data Hub

Data Hub Objectives:

1. **Data Repository**
   - Storage and sharing of research data/Public vs. Private data
2. **DOI/Publication of Data**
   - Internal vs. external data
3. **Provide Security Mechanisms**
   - User login
   - Project level access management
4. **Visualization and Analysis Capabilities**

*Collaborative **EMN** data hub that also houses **H2NEW** Data

Active Data Hubs

HydroGEN Advanced Water Splitting Materials

HyMARC Hydrogen Materials Advanced Research Consortium

DuraMAT Durable Module Materials Consortium

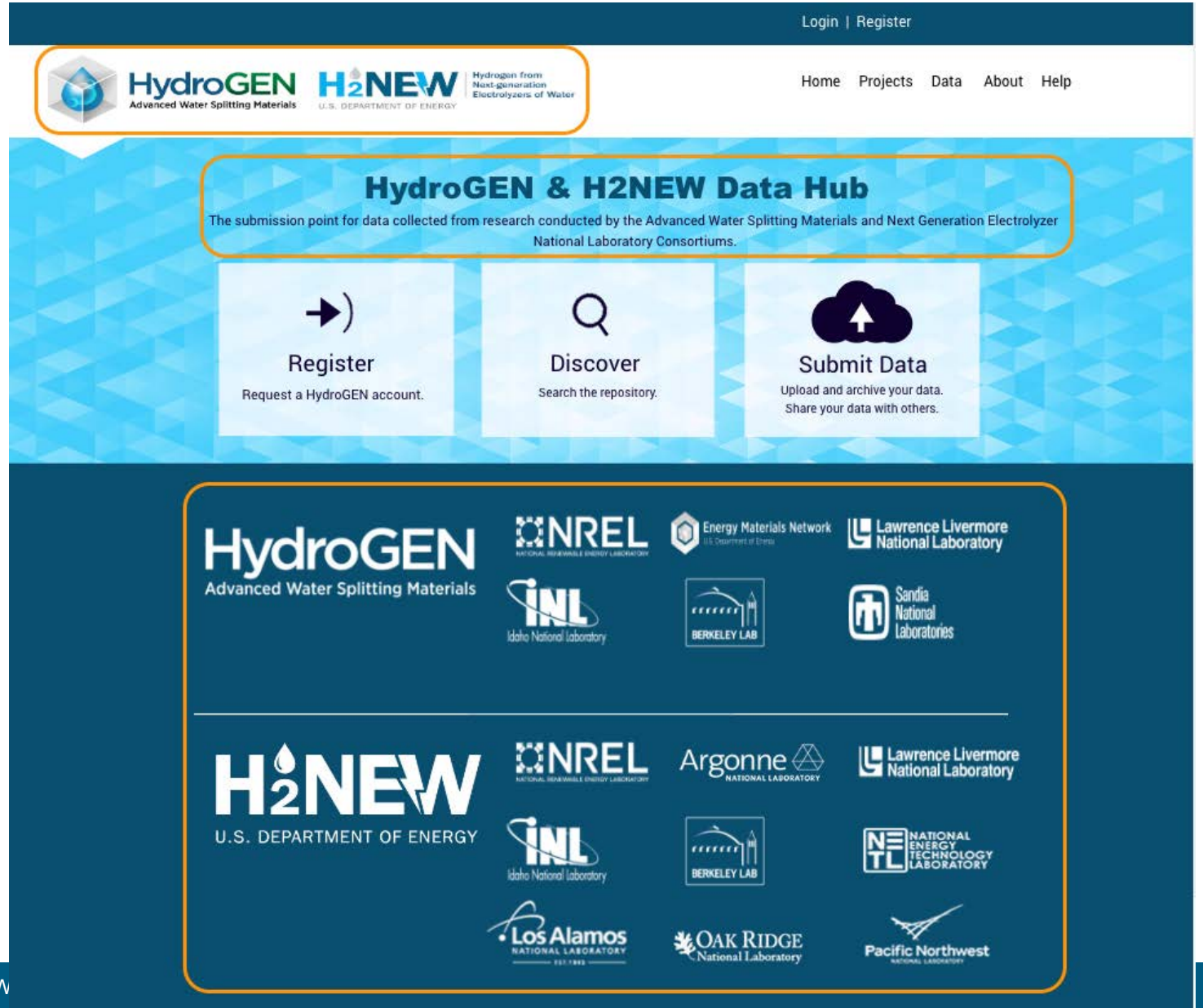
Perovskites PV Data Hub

Battery Data Hub ENERGY.GOV

ElectroCat Electrocatalysis Consortium

ChemCatBio Chemical Catalysis for Bioenergy

Upcoming Development Changes: Collaboration, Representation Matters



Upcoming changes to accommodate and represent H2NEW on the data hub:

Front End:

- Addition of H2NEW primary logo
- Primary tagline description change to include H2NEW
- Addition of H2NEW Contributor Logos

Data

- H2NEW Project Creation

Projects

All Projects

Project Tree

- H2NEW AE
- H2NEW Benchmarking
  - PEME Benchmarking
  - SOEC Benchmarking
- H2NEW SOEC
  - Durability (SOEC)
  - Performance (SOEC)
  - Characterization (SOEC)
  - Scale Up (SOEC)
  - Modeling (SOEC)
- H2NEW PEME FOA Projects
- H2NEW SOEC FOA Projects
- H2NEW PEME
  - Durability (PEME)
  - Performance (PEME)
  - Characterization (PEME)
  - Scale Up (PEME)
  - Modeling (PEME)
- ANL PGM Free
- ASU Perovskites
- Hydrogen Benchmarking
  - LTE
  - HTE
  - STCH

Search projects...

Order by: Name Ascending

1 2 3 4 »

H2NEW AE

Hydrogen from Next-generation Electrolyzers of Water (H2NEW) Low-Temperature...

H2NEW Benchmarking

Benchmarking: Hydrogen from Next-generation Electrolyzers of Water (H2NEW)...

Sub-projects:

PEME Benchmarking

SOEC Benchmarking

H2NEW SOEC

Hydrogen from Next-generation Electrolyzers of Water (H2NEW) Consortium High...

Making Digital Data Accessible

- Secure project space for team members
- Experimental and Modeling Data
- Metadata tools and improvements to support advanced search

Many Types of Experimental Data

Material characterization

- XRD, SFR, XPS, XRF, SEM, TEM, Raman

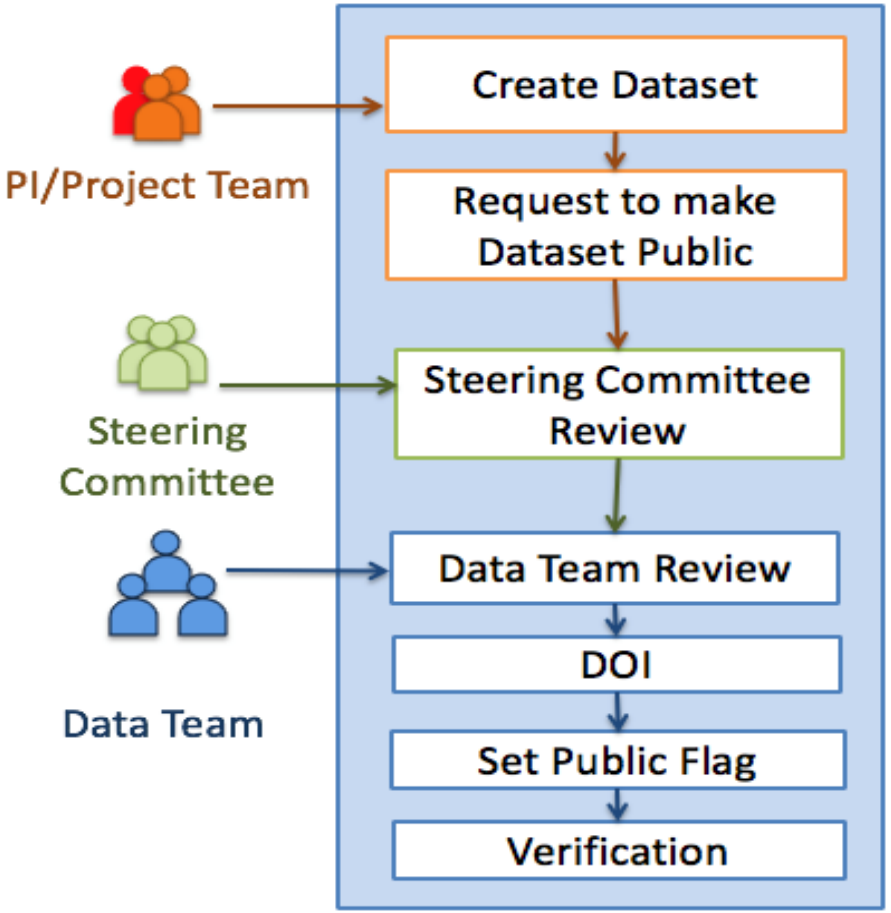
Device performance

- Electrolysis, PEC J-V, IPCE, Tafel plots

Materials durability data

- TGA, membrane conductivity

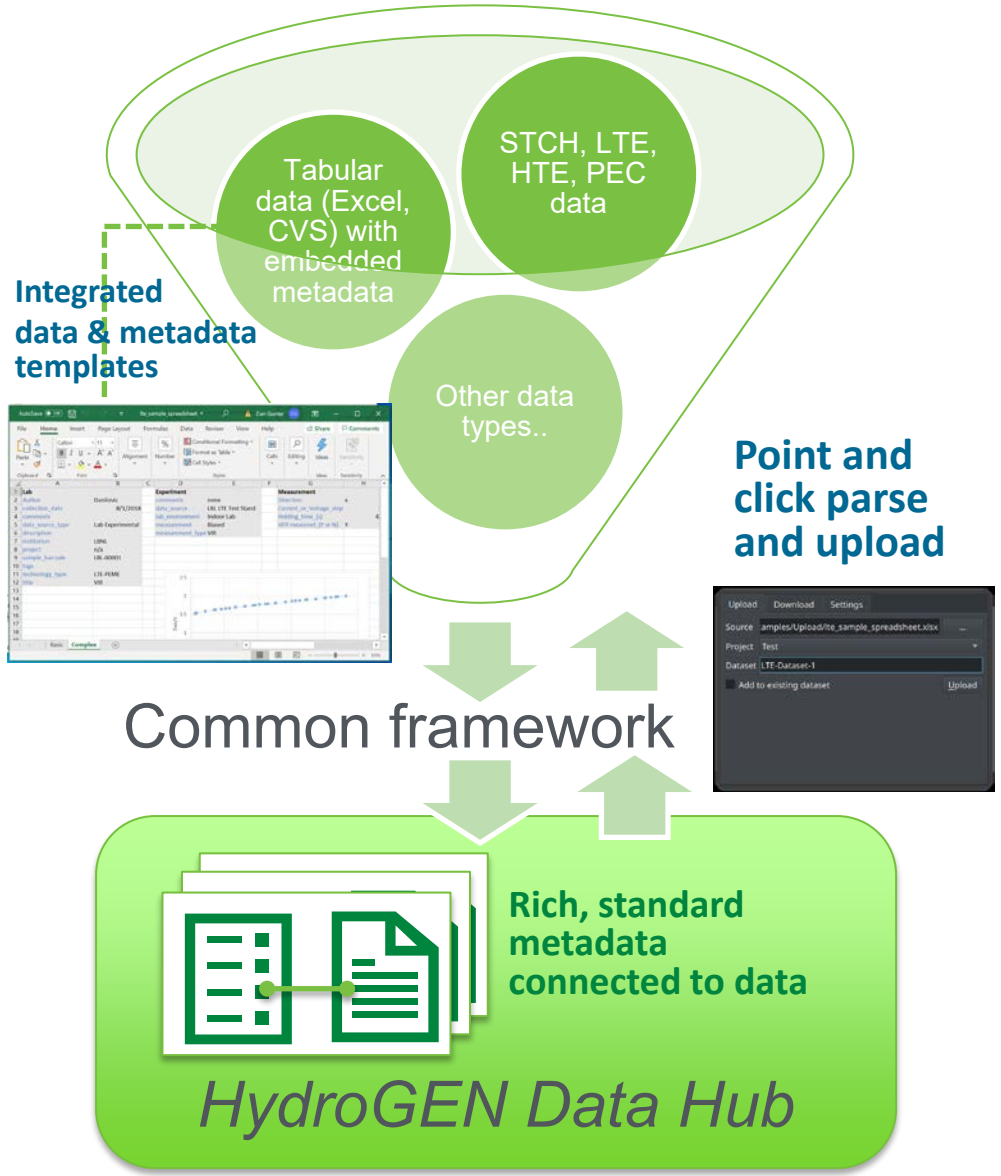
Data Publication Process



Metadata automation and standardization

Metadata is crucial to data utility and re-use

- Need to capture all information about Lab, Experiment, Sample, and Measurement
- Automated this data capture
  - Extract metadata into a standard form, automate upload/download to/from the Data Hub
- Enabling more uploads & more powerful search across datasets
- Wrote a Python parsing architecture that lets new data types “plug-in”, with collaboration on shared code in Github



LTE Metadata

	A	B
1	Key	Values
2	**Lab**	
3	Researcher's Name	Allen Kang
4	Researcher's Email	allen.kang@nrel.gov
5	Researcher's Institution	National Renewable Energy Laboratory
6	MEA Creator's Name	Allen Kang
7	MEA Creator's Institution	National Renewable Energy Laboratory
8	HydroGEN Project Name	LTE Supernode
9	HydroGEN Dataset Name	
10	Data Collection Date	
11	Data Source Type	Lab Experimental
12	Technology Type	LTE
13	Measurement Type	
14	Sample Name	
15	Description	
16	Comments	

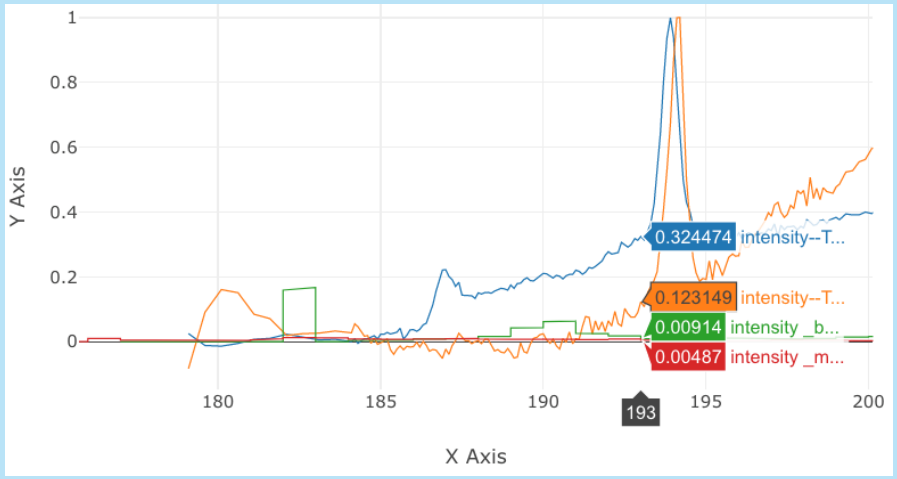
18	**Cell Assembly**	
19	Active Area (cm2)	25
20	Hardware Set ID	
21	Hardware Station ID	
22	Hardware Origin/Vendor	
23	Compression Type	
24	Bolt Torque	
25	Number of Bolts	
26	Flow Field Flow Alignment Type	
27	Lab Temp (oC)	25
28	Lab Pressure (Bar)	
29	Cathode Flow Field Flow Type	triple serpentine
30	Anode Flow Field Flow Type	triple serpentine

32	**Materials**
33	Anode Catalyst Material
34	Anode Catalyst Particle Size (nm)
35	Anode Catlayst Support
36	Anode Catalyst Synthesis
37	Anode Catalyst Vendor
38	Anode Gasket Material
39	Anode Gasket Material Thickness (mm)
40	Anode Ionomer Vendor
41	Anode Ionomer Type
42	Anode Ionomer IEC
43	Cathode Catalyst Material
44	Cathode Catalyst Particle Size (nm)
45	Cathode Catalyst Support
46	Cathode Catalyst Vendor
47	Cathode Gasket Material
48	Cathode Gasket Material Thickness (mm)
49	Cathode Ionomer Vendor
50	Cathode Ionomer Type
51	Cathode Ionomer IEC
52	Membrane Ionomer
53	Membrane Thickness
54	Membrane Ion Exchange Capacity (IEC)
55	Membrane Prep Conditions
56	Membrane Type
57	MEA Prep Custom Notes
58	Membrane Vendor/Origin

60	**MEA**
61	Anode Catalyst Loading (mg/cm2)
62	Anode Catalyst Thickness (um)
63	Anode Catalyst Deposition Method
64	Anode GDL Thickness (um)
65	Anode Porosity
66	Anode Ionomer:Catalyst Ratio
67	Anode Catalyst:Support Ratio
68	Anode DI:Solvent ratio
69	Anode Solvent Type
70	Cathode Catalyst Loading (mg/cm2)
71	Cathode Catalyst Thickness (um)
72	Cathode Catalyst Deposition Method
73	Cathode GDL Thickness (um)
74	Cathode Porosity
75	Cathode Ionomer:Catalyst Ratio
76	Cathode Catalyst:Carbon Ratio
77	Cathode DI:Solvent ratio
78	Cathode Solvent Type
79	Membrane Pre-treatment
80	MEA Type (Anode/Cathode)
81	Electrode Type

83	**Cell**
84	Anode FF Material
85	Anode FF Pattern
86	Anode FF Coating
87	Anode FF Coating Method
88	Anode PTL (model or ID #)
89	Anode PTL Vendor
90	Anode PTL Thickness (um)
91	Anode PTL Porosity
92	Anode PTL Coating
93	Anode PTL Coating Thickness (nm)
94	Cathode FF Material
95	Cathode FF Pattern
96	Cathode FF Coating
97	Cathode FF Coating Method
98	Cathode PTL (model or ID #)
99	Cathode PTL Vendor
100	Cathode PTL Thickness (um)
101	Cathode PTL Porosity
102	Cathode PTL Coating
103	Cathode PTL Coating Thickness (nm)

Data Tools



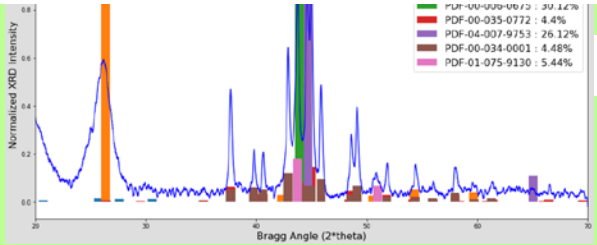
The interactive **Advanced Multi-Spectra Data View** allows many spectra files (any csv or tabular file format) to be visualized at one time, from one or many files.

https://bit.ly/2Vss96E

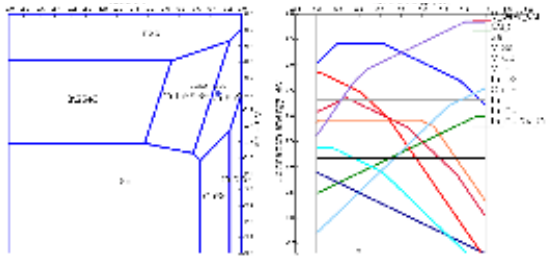
Data Tools for

- EMN collaboration
  - Data exchange and exploration
  - Data analysis and visualization (A&V)
- External users
  - Access to comprehensive database
    - Experimental and computational
  - Materials properties
    - Spectroscopy, phase stability, etc.
  - Device performance

Structural information: XRD interface in collaboration with ElectroCat



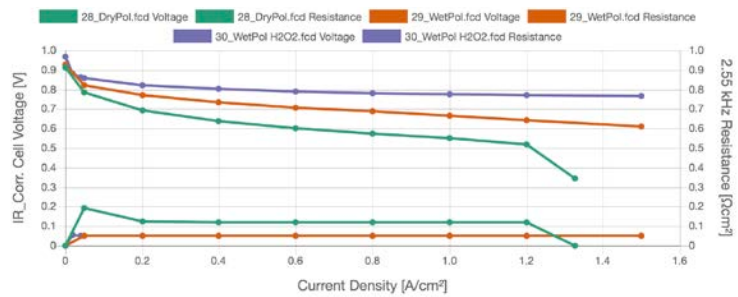
Phase stability & Defect properties



Device performance

(A&V example)

Electrolysis Performance curve



Links to Data Hub User Resources

- **Data Hub Help & Tutorial**
  - https://datahub.h2awsm.org/dataset/h2awsm-data-hub-tutorial
  - https://datahub.h2awsm.org/dataset/help-and-tutorial
- **Bulk Upload Feature & EMN Multiple File Uploader**
  - https://datahub.h2awsm.org/dataset/bulk-upload
  - https://datahub.h2awsm.org/dataset/emn-multiple-file-uploader
- **Demo: Electrolysis & Fuel Cell Pol Curve Data Tool**
  - https://datahub.h2awsm.org/dataset/electrolysis-pol-curve
  - https://datahub.h2awsm.org/dataset/fcd-format-view-data-tool
- **Demo: XRD Unmix Data Tool**
  - https://datahub.h2awsm.org/dataset/demo-xrd-unmix-data-tool
- **Demo: MgB2 and B203 Simulation Data versus experimental MgB2 Multi-Spectra Data View**
  - https://datahub.h2awsm.org/dataset/multi-spectra-data-tool

Initiatives: Near & Long Term

1. Maintain Security Compliance

2. Build New Software Deployment Infrastructure

3. Improve Data Searchability

Save the Date for 5th AWSM Benchmarking Workshop

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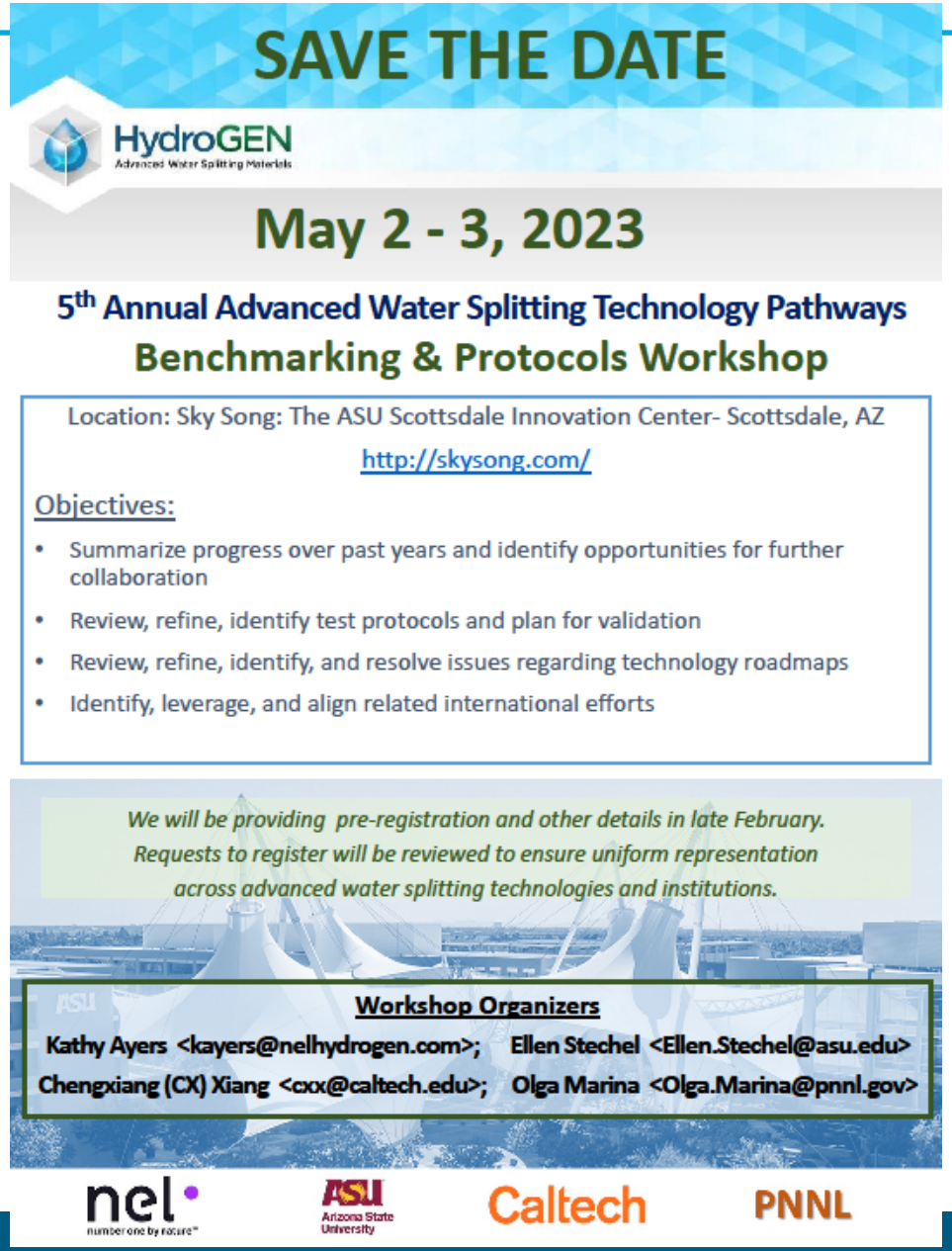
Goal: Develop best practices in materials characterization and benchmarking: Critical to accelerate materials discovery and development

Best Practices in Materials Characterization

Kathy Ayers, Nel Hydrogen (LTE)
Ellen B. Stechel, ASU (STCH)
Olga Marina, PNNL (HTE)
CX Xiang, Caltech (PEC)
Consultant: Karl Gross, George Roberts

- Strong community engagement and participation, nationally and internationally
- 19 test protocols submitted to Frontiers in Energy special issue for publication



Previous Benchmarking Workshop Presentations and Break-out Summaries on the Data Hub

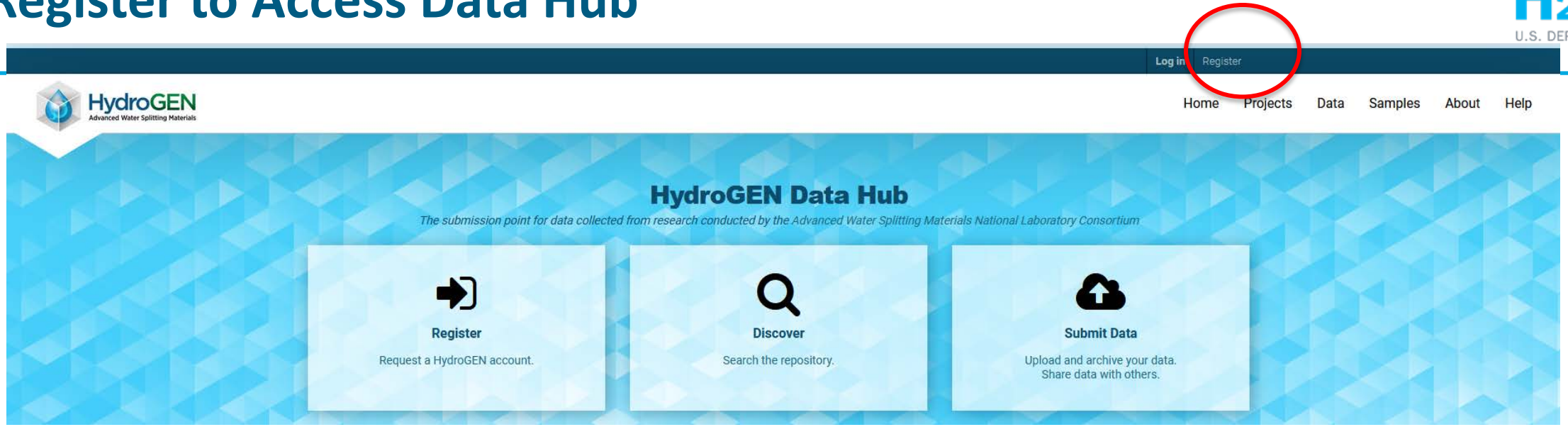
https://datahub.h2awsm.org/project/benchmarking

Frontiers in Energy Research Publications:

Of the 19 papers published, 7 are for LTE. They are free to download on the Frontiers in Energy Research site. https://www.frontiersin.org/research-topics/16823/advanced-water-splitting-technologies-development-best-practices-and-protocols#articles.

1. Rotating disk electrode standardization and best practices in acidic oxygen evolution for LTE
2. Gas permeability test protocol for ion-exchange membranes
3. Standard operating protocol for ion-exchange capacity of AEMs
4. Assessing the oxidative stability of AEMs in oxygen saturated aqueous alkaline solutions
5. Protocol for screening water oxidation or reduction electrocatalysts activity in a three-electrode cell for AEME
6. Measurement of resistance, porosity, and water contact angle of porous transport layers for LTE technologies:
7. Standard operating procedure for post-operation component disassembly and observation of benchtop electrolyzer testing

Register to Access Data Hub



Please register as a user on the Data Hub

- click **Registration** at the top right
- visit: https://datahub.h2awsm.org
- complete registration form, Create Account (we suggest you use the same login name and password as that for the SharePoint site)
- email Emily Harrel (emily.harrel@nrel.gov) with your username so that she can give you access to the appropriate project data space.
  - Let her know which projects you are working on

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Thank you! Q&A?

https://datahub.h2awsm.org/

Huyen.dinh@nrel.gov

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