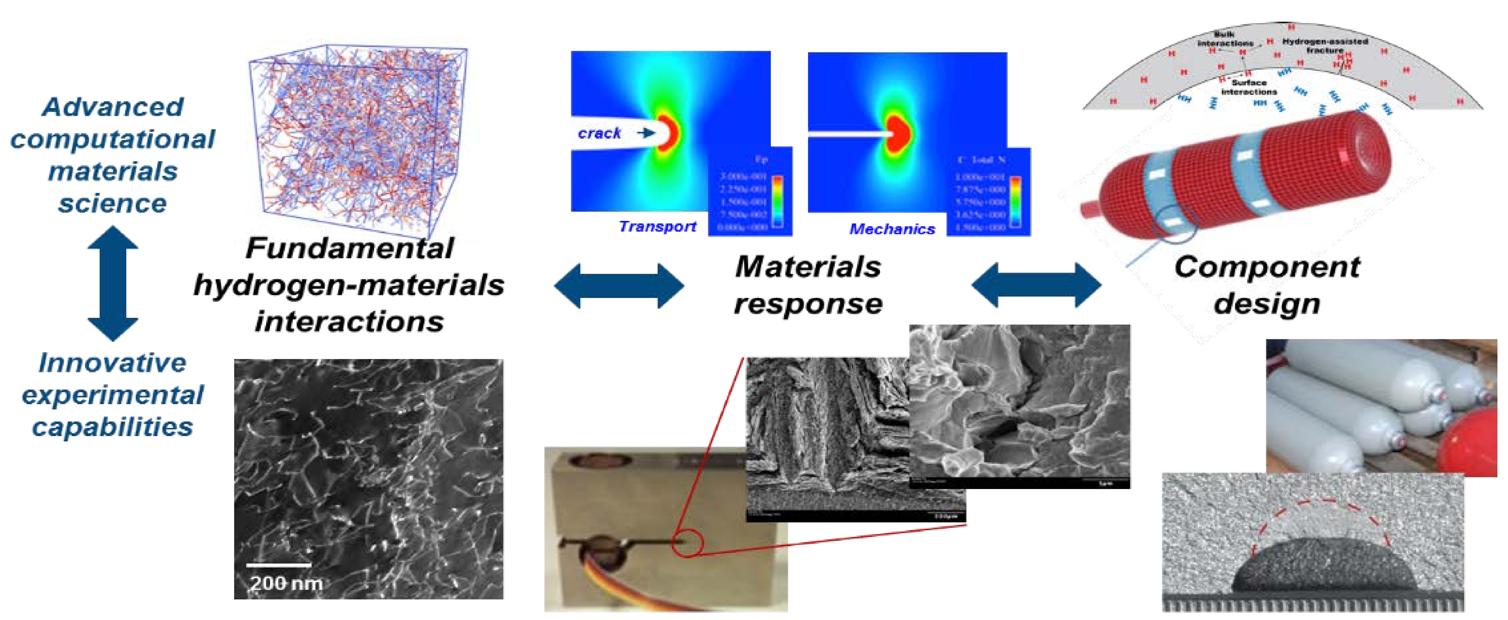
H-Mat: Enhancing Hydrogen Compatibility of Metallic and Polymeric Materials through Early-Stage R&D

Emerging multi-lab network to understand hydrogen-materials interactions across length scales

Foundational Materials Science is Key to Next-Generation Technology

- Understanding of hydrogen-metal interactions across length scales to inform **multiphysics models** of hydrogen-mediated damage and failure. Gaps in known physics include:
  - Hydrogen-dislocation interactions
  - Hydrogen-deformation interactions with interfaces and grain boundaries
  - Compositional effects on hydrogen-mediated deformation and fracture
  - Influence of microstructure and residual stress on materials behavior in hydrogen



Thermodynamics of H-interactions at nm-scale

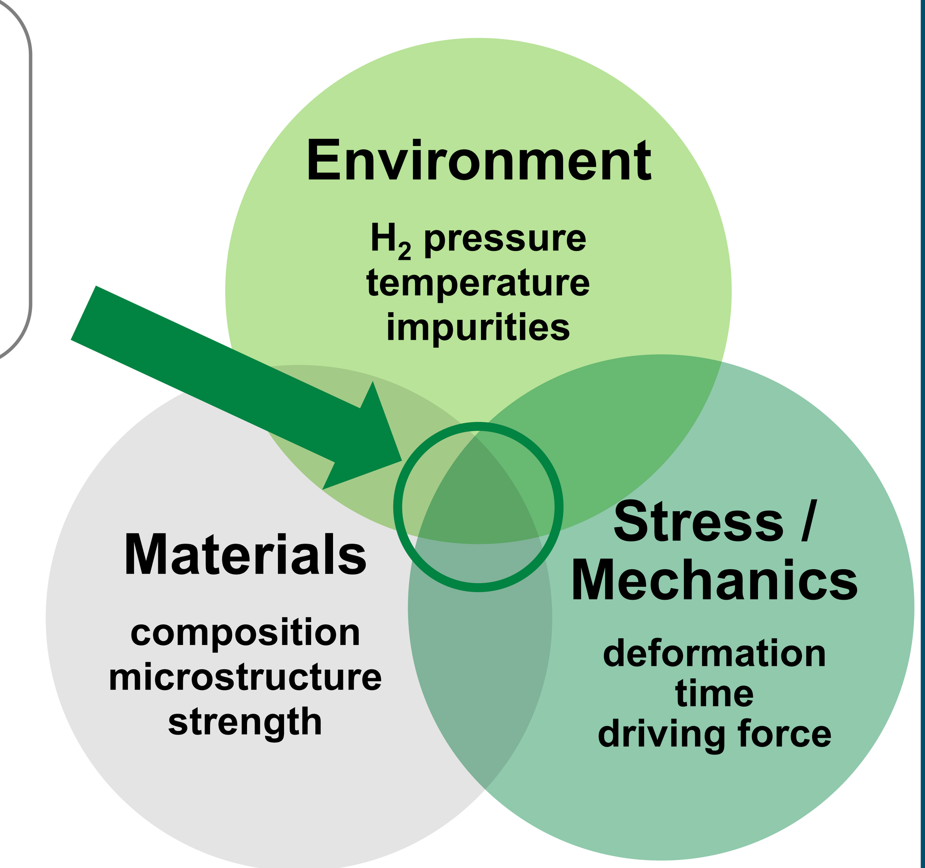
Micromechanisms of materials behavior at µm-scale

Structural performance at the engineering scale

- Predictive damage models **based on microstructural characteristics** (e.g., fillers, crystallinity) to describe degradation of structure of polymers subjected to high-pressure gases
- Scientific framework to understand **tribological behavior of materials** in high pressure gases
- Mature capabilities to assess performance of materials in **extreme environments** (e.g., thermal extremes)
- **Methods and metrics to assess performance** of various materials classes in hydrogen service (e.g., high-strength steels)
- **Strategies to mitigate hydrogen effects** and predictive lifetime assessment tools for mitigation strategies

Hydrogen Effects Depend on Multi-physics Phenomena that Vary Across Length Scales

*Hydrogen compatibility depends on **Materials** characteristics under the influence of **Stress** in hydrogen **Environment***



<u>**High-priority challenges include:**</u>

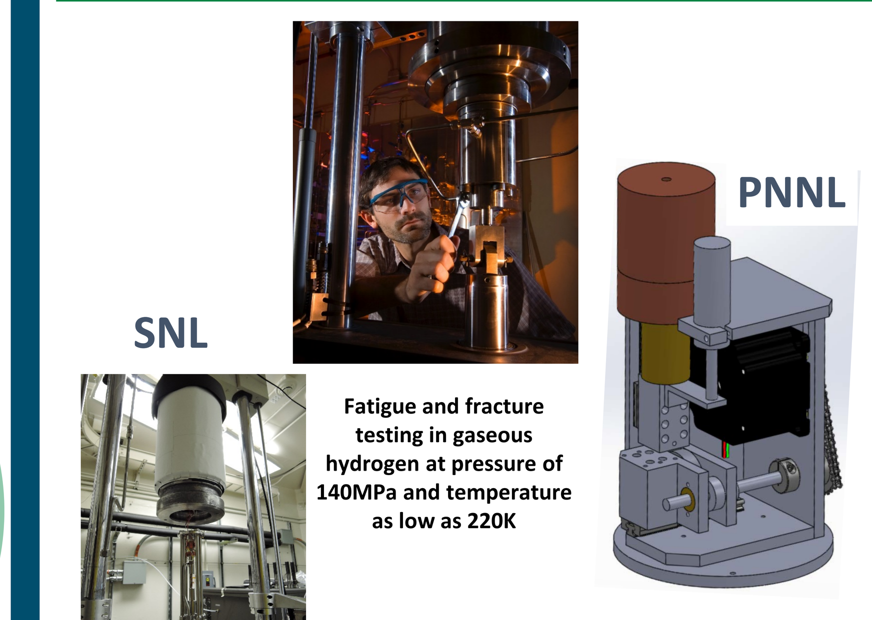
- **Advanced imaging** of hydrogen at the intersection of materials-environment-mechanics variables
- **Analytical tools** in high-pressure hydrogen at temperature extremes
- Characterization of the **temporal interactions** of hydrogen at the surface and in the bulk

Examples of Current Stakeholder Collaborations

- <u>Industry</u>
  - Collaboration with **25 industry stakeholders** to identify polymeric materials of interest to hydrogen infrastructure, followed by failure modes and effects analysis and experimental characterization, led by Pacific Northwest National Laboratory and Sandia National Laboratories
  - **MOU between Sandia, FIBA Technologies, Tenaris, and Japanese Steel Works** to identify and characterize pressure vessel steels for high-volume storage of hydrogen
- <u>Government agencies</u>
  - **Interagency research** including universities, national laboratories and industry to integrate R&D activity across the technology spectrum
    - 2016 MOU between DOE's Fuel Cell Technologies Office and the National Institute of Standards and Technology to facilitate collaboration in materials compatibility research
    - DOE and DOT jointly funded R&D on pressure vessels and pipelines
- <u>Academia</u>
  - University partnerships to advance fundamental experimental and computational studies of hydrogen-microstructure interactions toward **Integrated Computational Materials Engineering (ICME)**

World-Class Capabilities at the National Laboratories

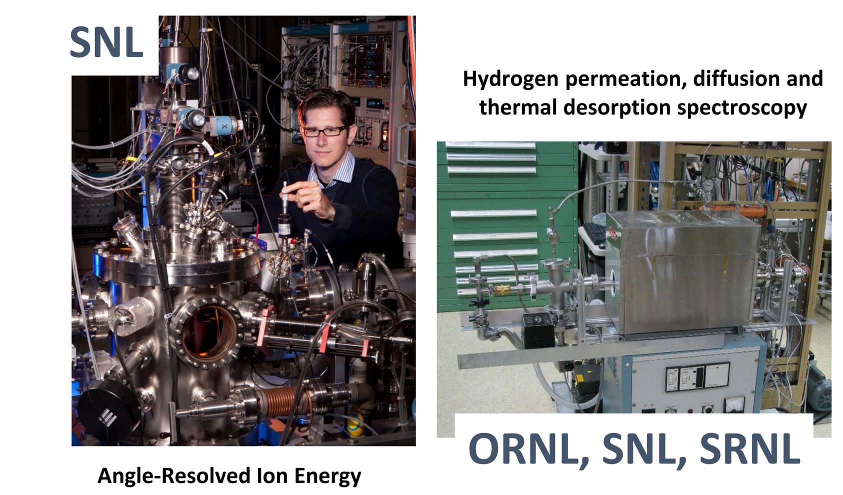
Mechanical Testing in High-Pressure Hydrogen



Fatigue and fracture testing in gaseous hydrogen at pressure of 140MPa and temperature as low as 220K

In situ tribology in hydrogen and other gases at pressure up to 35 MPa

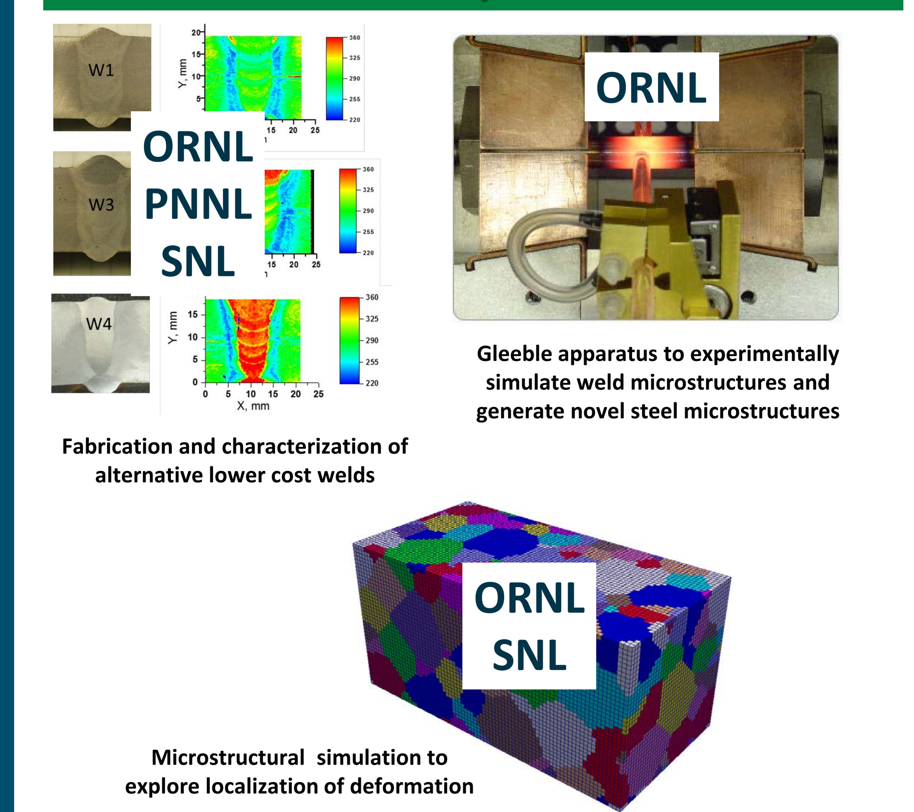
Hydrogen Surface Interactions, Hydrogen Transport and Trapping



Angle-Resolved Ion Energy Spectrometer (ARIES) for study of hydrogen-surface interactions

Hydrogen permeation, diffusion and thermal desorption spectroscopy

Microstructural Simulation and Development

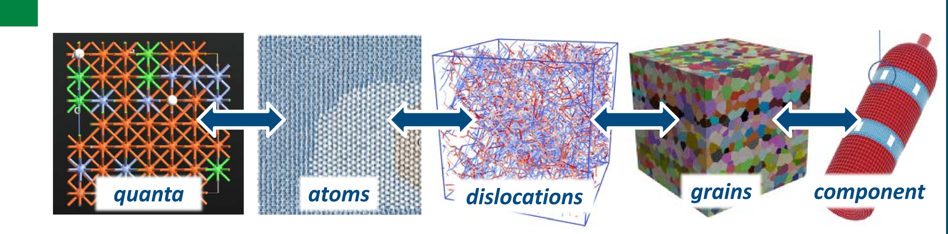


Fabrication and characterization of alternative lower cost welds

Gleeble apparatus to experimentally simulate weld microstructures and generate novel steel microstructures

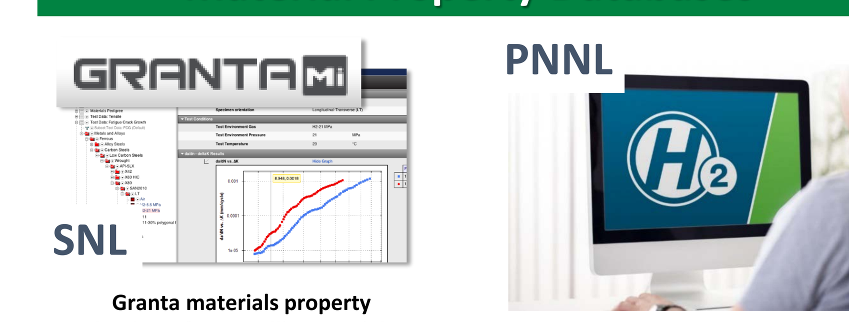
Microstructural simulation to explore localization of deformation

Advanced Computational Materials Science for Hydrogen-Materials Interactions



Computational materials science exploiting study at different length scales from quantum phenomena to atomistic to defects and grains to component

Material Property Databases



Granta materials property database for metallic materials

H2Tools.org, which will host a new polymer properties database

Ideas for Future Collaborations

- Deploy national laboratory resources to support industry-led research projects in materials compatibility.
- Conduct regular stakeholder engagement with industry and academia to obtain feedback on ongoing R&D and identify priorities for future research
- Align future research priorities with those of other federal agencies to create critical mass of investments in cross-cutting challenges
- Form university partnerships to grow U.S. expertise in materials compatibility, and align fundamental activities with applied research and H2@Scale