Hydrogen for Energy and Information Sciences (HEISs)
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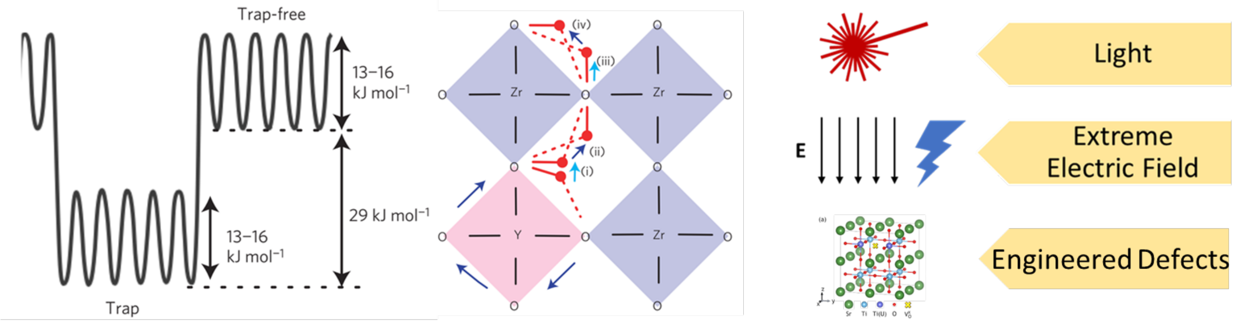
Lead Institution: Northwestern University
Class: 2022 – 2026

Mission Statement: *To advance the fundamental understanding and discovery of multihued hydrogen transport in inorganic solids of earth-abundant elements, and of its transfer along and across interfaces within such materials, where 'hydrogen' includes all charge states of the element: H^+ (proton), H^0 (atom), and H^- (hydride ion).*

The transport characteristics of hydrogen are distinct from those of other elements owing to its small mass, which is comparable to the electronic effective mass of some heavy-Fermion solids, and its ambipolar nature. Dominant transport via tunneling at ambient temperatures is possible for protons, with appreciable kinetic isotope effects. Its redox flexibility, occurring as either a cation or an anion and potentially transforming between states within a given host material, is accompanied by a dramatic change in ionic/atomic radius, from effectively 0 in H^+, to 0.6 Å in H^0, and 1.1 Å in H^-. Furthermore, the hydride ion is far more polarizable than other anions of comparable ionic radius, O^{2-} and F^-, suggesting a route to tailoring bond covalency and enabling high mobility.

Recognizing the unique characteristics of hydrogenic species transport, HEISs proposes to exploit external static and dynamic electric/strain fields to **design** the energy landscapes for mobile and reactive H-containing species in bulk crystals as well as at interfaces. Of particular interest and value are exceptionally **high electric fields** and **photon** illumination, where the latter additionally induces **phonon** modulation. These external drivers couple to the energy landscape of hydrogenic species and can serve as a means of engineering higher dimensional defects, can alter the dominant charge state of H and distribution within trap sites, and can also drive transport and reaction dynamics at strongly nonlinear field-strength regimes.

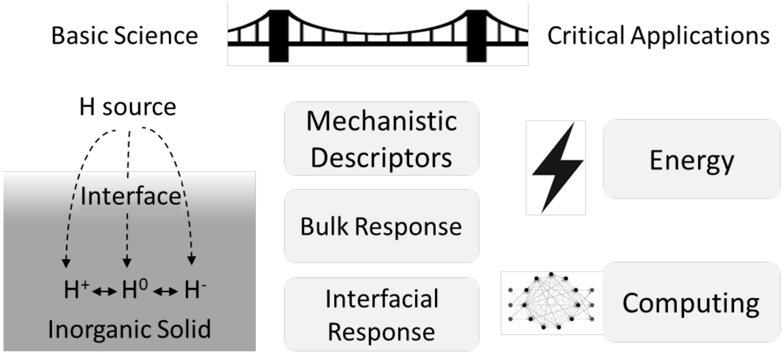


Beyond its special place in physical chemistry, hydrogen is of tremendous societal importance in energy technologies and of growing importance in energy-efficient computing. In both arenas, the relevant devices are limited by hydrogen kinetics, whether it be electrochemical reaction at an interface or diffusion through the bulk, and whether the material be an electrolyte, a semiconductor, or a metal. HEISs will establish the governing mechanisms and physical descriptors of the transport and interfacial incorporation mechanisms needed to achieve precision-guided discovery and design across these classes of materials. In particular, HEISs will address the following critical open questions:

- What are the rate-limiting steps in hydrogen transport and incorporation mechanisms, and the electronic, structural, and dynamic descriptors thereof?

- Can we vary the hydrogen oxidation state within a given material? Is the oxidation state fixed at the point of incorporation, or can it be dynamically tuned?
- What is the nature of traps that inevitably display affinity for hydrogen species? Traps typically retard bulk transport, but can extended defects serve as high mobility highways? And can surface trap sites be designed to achieve desirable surface incorporation pathways?
- Can we exploit stimuli beyond heat, such as light and extreme electric field, to accelerate hydrogen dynamics?
- What underlying transport principles apply across multiple classes of oxide materials (wide band-gap electrolytes, small band-gap semiconductors, metallic conductors), and which transport features are unique to a particular class?

With a deliberate focus on use-inspired, ambient-to-intermediate temperatures, the scientific advances and insights gained will provide a foundation for controlling electrochemical transformations critical for carbon-neutral energy (including nitrogen and carbon dioxide reduction) and for modulating electron transport in materials for brain-inspired computing.



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