Hydrogen Carriers for Bulk Storage and Transport of Hydrogen

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Outline

• Hydrogen carriers
  – concepts & definitions
  – objectives & goals

• ANL - base lining carriers
  – one-way
  – round trip
  – without H₂

• HyMARC
  – objectives
  – examples
  – identify gaps in knowledge
  – develop scientific tools
  – foundational research to enable rational design
  – summary

• Questions and Answers
Hydrogen Carriers - concepts

• As part of the H2@Scale concept, bulk storage and transport of hydrogen is of critical importance. Storage needs may range from daily to seasonal in duration, and transport distances may exceed hundreds of kilometers.

• The hydrogen carriers research effort is seeking new concepts and materials that have potential to provide advantages over conventional compressed and liquefied hydrogen for bulk storage and transport.
Hydrogen Carriers - definitions

• Hydrogen carriers are hydrogen-rich liquid or solid phase materials from which hydrogen can be liberated on-demand.
• Ideal hydrogen carriers have high hydrogen densities at low pressure and near ambient temperature.
• The formation of the carrier and release of hydrogen from the carrier should be as energy efficient as possible to minimize the energy penalty associated with the use of the hydrogen carrier to store and transport hydrogen.
Hydrogen Carriers: Objectives and Goals

Objectives:
To investigate pathways that will lead to the optimization of hydrogen carriers and to realize the most efficient, safe and economical approaches to:

(i) transport H₂ from a production facility to the city gate
(ii) facilitate geographically agnostic H₂ storage.

Goals:
(i) Development of novel hydrogen carriers (new concepts in liquids and solids).
(ii) Development of alternate approaches to prepare and release hydrogen from hydrogen carriers.
HyMARC Objectives in Hydrogen Carriers

- Defining the important properties of hydrogen storage materials beyond onboard vehicular.
- Determining the advantages and limitations for materials and approaches to hydrogen carriers for transport and long term storage.
- Investigating novel approaches to release or ‘adsorb’ hydrogen onto carriers.
- Characterizing novel approaches to preparing hydrogen carriers that do not require a discreet step of making gaseous hydrogen.
- Comparing approaches that can be used to prevent phase changes.
- Optimizing the balance of catalyst properties: Stability (TON), rates (TOF), $’s, selectivity, heterolytic vs homolytic hydrogen activation.
- Validating concepts for rational design.

Leveraging capability and expertise in HyMARC consortium for accelerating progress in hydrogen carriers
Formic acid provides ‘chemical compression’

Hydrogen release from formic acid is entropy controlled. $\Delta G$ is negative and $\Delta H$ is positive. Can generate 1000 bar pressure.

- $\text{H}_2\text{CO}_2 \Leftrightarrow \text{H}_2 + \text{CO}_2$

- What are approaches for separation of $\text{CO}_2$ and $\text{H}_2$?
- Controlling selectivity ($\text{CO}_2$ vs CO)?
- What are best approaches to make Formic Acid?
Summary of HyMARC role – analysis of alternate concepts

- Making \( H_2 \) carriers without \( H_2 \) (electrochemical)
- \( H_2O \) as a reactant to form \( H_2 \) (ROH and HCO\(_2\)-)
- Chemical compression (entropy controlled release of \( H_2 \))
- Controlling selectivity (\( CO_2 \) vs \( CO \))
- Integrated separation technologies (\( H_2 \) from \( CO_2 \), \( CO \))
- Preserving liquid phase throughout \( H_2 \) release and uptake
- Integrating electro and thermal catalysis processes
- Heterolytic sorption of \( H_2 \)