

Chemical Hydrogen Storage

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Speakers: S. Suda, Y. Saito, A. Cooper, Y. Wu, K. Barral, T. Autrey, P. Prosini

12 Posters

Chemical Hydrogen Storage

- Liquid or solid fuel infrastructure may be possible
- A number of concepts have been demonstrated with high material hydrogen storage capacity
- Exothermic and endothermic catalyzed hydrogen generation reactions
- Regeneration is key
 - Off-board regeneration is likely
 - Energy efficiency
 - Recyclability of materials
 - Some processes may use hydrogen, others may not

Three Main Concepts Presented at Conference

- Sodium borohydride hydrolysis: $\text{NaBH}_4 + \text{H}_2\text{O}$
- Other boron compounds: H_3NBH_3
- Dehydrogenation of organics
 - Carbocyclic compounds (e.g. decalin = naphthalene)
 - Heteroatom-substituted systems (e.g. N-ethylcarbazole)
- Also, one poster on coordination complexes of NH_3

Sodium Borohydride Hydrolysis and Regeneration

- Exothermic hydrogen generation: catalysts and systems
 - H₂ generation systems
 - Wu (Millennium Cell), Prof. Suda, Posters
 - Stability of Solutions
 - Barral (Air Liquide)
 - On-board system (Natrium)
 - Abdel-Baset (Daimler-Chrysler)

- Regeneration: B-O to B-H
 - Energy Efficiency
 - Economic analyses and cost estimates
 - Barral (Air Liquide), Prosini (ENEA)
 - Improved processes/cheaper reducing equivalents
 - Suda, Wu

Regeneration Efficiency: Pathways

Boron-Nitrogen Compounds

- Avoid formation of stable B-O bond
- High material hydrogen storage capacity (significant potential)
- Several hydrogen generation concepts advanced
- Mechanisms, catalysts, substitution
 - Autrey (PNNL), RTI, Los Alamos, Industrial Research Lab (NZ)
- Regeneration Pathways
 - Thermodynamics appear to be reasonable
 - May not be able to use H₂

(BNH_x) Regeneration

Dehydrogenation of Organic Systems

- Endothermic hydrogen generation
 - Saito (Tokyo Univ of Science), Cooper (Air Products)
- Thermodynamics depends on structure
- Heteroatom substitution can favorably alter thermodynamics
 - Air Products, Los Alamos
- Catalyst development for dehydrogenation
 - Non-precious metal catalysts
 - Increased rates

Catalyst Development

Potential Areas for Collaboration-1

- Catalysis
 - Non-precious metals
 - Rates, heat management (endo/exothermic reactions)
- Coupling to Fuel Cell
 - Impurities and impurity tolerance (composition and quantities)
 - Heat and materials balance
- Infrastructure
 - Energy and/or hydrogen source
 - Analysis
 - Off-board regeneration infrastructure

Potential Areas for Collaboration-2

- Mechanisms and Kinetics
 - Molecular systems, spectroscopy
 - Theory and computation for thermodynamics, reaction intermediates
- On-board reactor
 - Reactor engineering, control interaction of material with catalyst
 - Overall system engineering, materials compatibility
- Off-board regeneration
 - Energy efficiency
 - Reaction pathways
 - Rehydrogenation
 - Other reduction chemistries
 - Cheaper reducing equivalents