Hydrogen Storage for Automotive Vehicles

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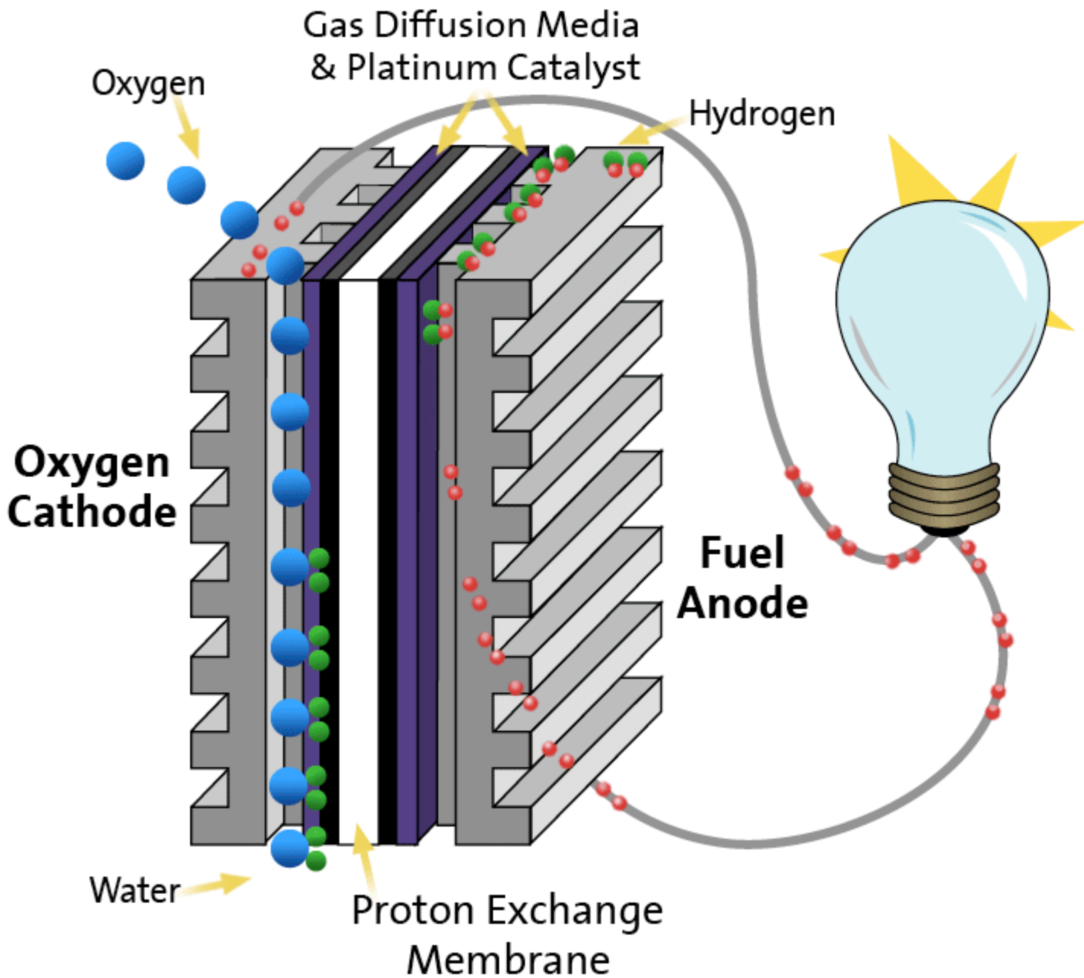
OUTLINE

- Why hydrogen fuel cell electric vehicles?
- Hurdles to hydrogen mobility
- Options for storing hydrogen
  - physical storage
  - chemical storage
    - ❖solid state materials
- Summary
- By special request – E-Flex & *Volt* !

Fuel Cell 101

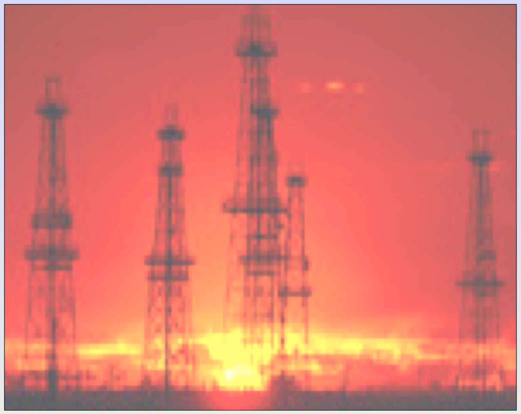


Why Hydrogen Fuel Cell Cars?

GM

Hydrogen Addresses the Societal Drivers

Petroleum Dependence



Balance of Payments

Hydrogen

Local Air Quality

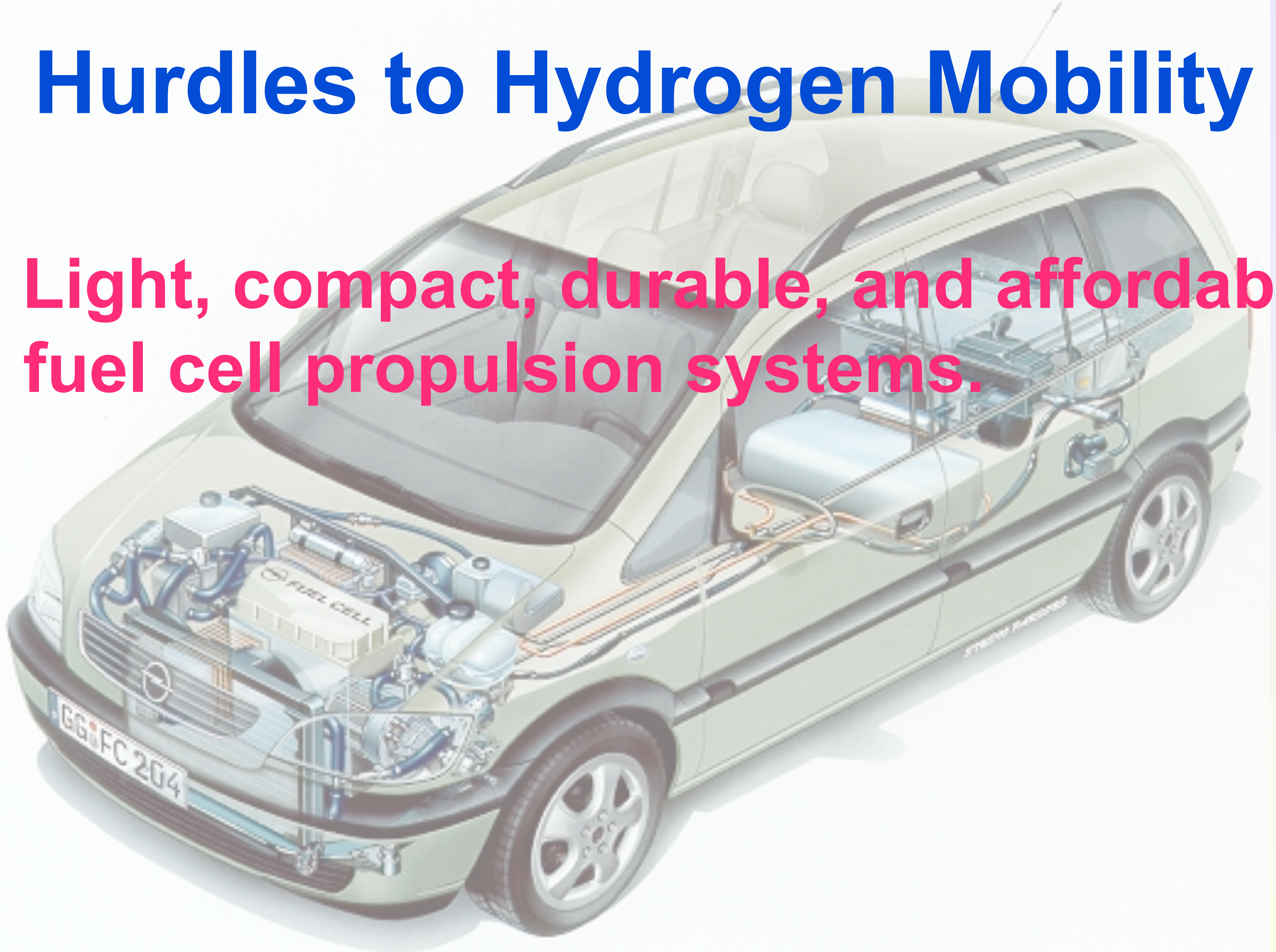
Global Climate Change

R&D CENTER

Hurdles to Hydrogen Mobility

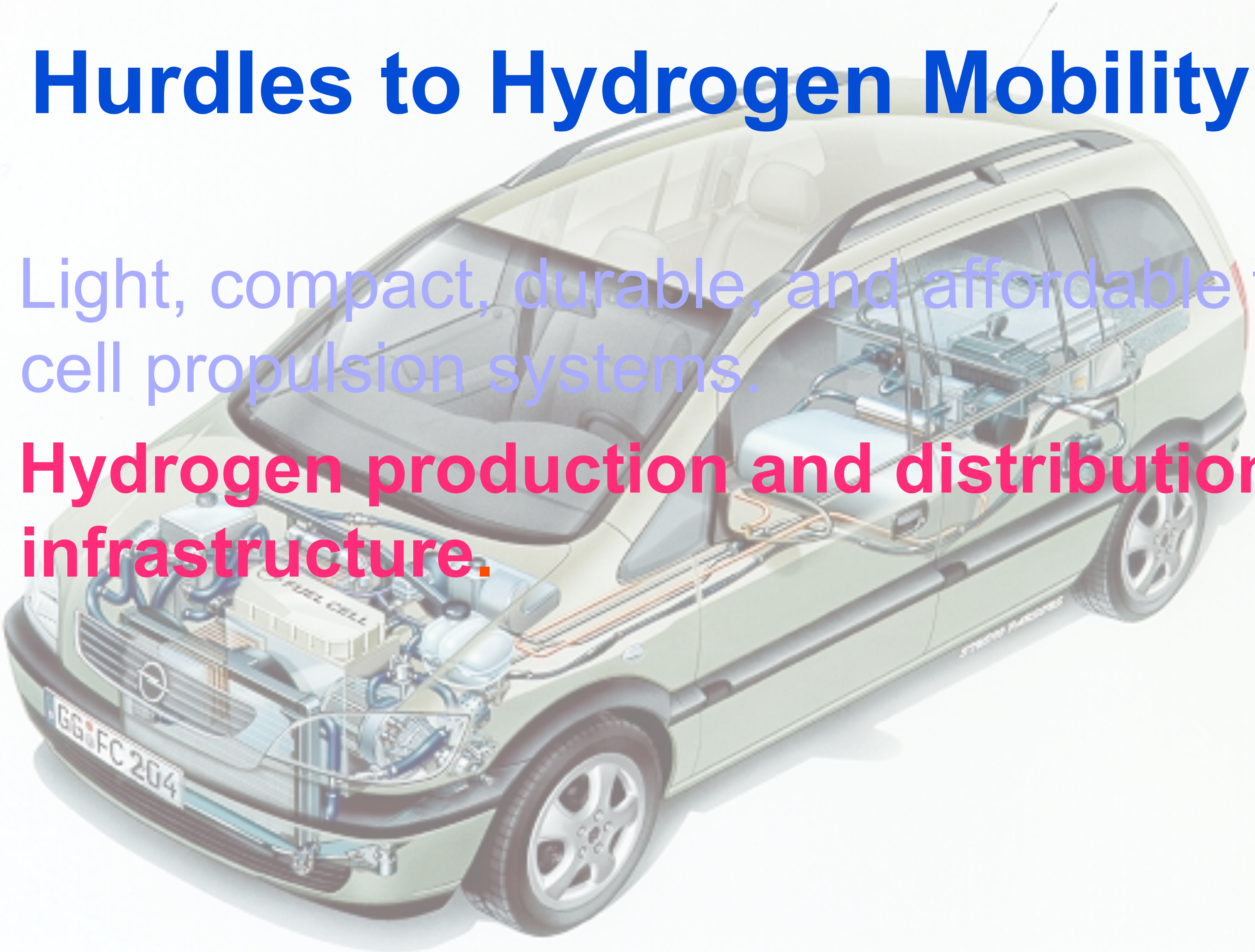
Hurdles to Hydrogen Mobility

1. Light, compact, durable, and affordable fuel cell propulsion systems.



Hurdles to Hydrogen Mobility

1. Light, compact, durable, and affordable fuel cell propulsion systems.
2. **Hydrogen production and distribution infrastructure.**



H_2 Production

- Now : reforming of natural gas
- Future: splitting of H_2O via non-carbon energy sources
  - electrolysis with electricity from solar, wind, hydro, nuclear
  - direct H_2 production using sunlight and semiconductors
  - nuclear/solar thermochemical cycles
  - biological and bio-inspired

DOE Research Areas in Hydrogen Production

Fossil fuel reforming

Molecular level understanding of catalytic mechanisms, nanoscale catalyst design, high temperature gas separation

Solar photoelectrochemistry/photocatalysis

Light harvesting, charge transport, chemical assemblies, bandgap engineering, interfacial chemistry, catalysis and photocatalysis, organic semiconductors, theory and modeling, and stability

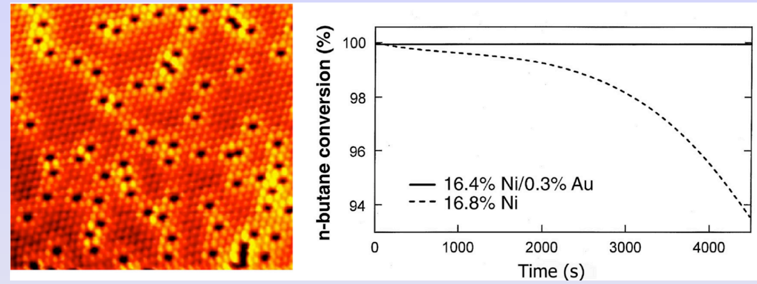
Bio- and bio-inspired H_2 production

Microbes & component redox enzymes, nanostructured 2D & 3D hydrogen/oxygen catalysis, sensing, and energy transduction, engineer robust biological and biomimetic H_2 production systems

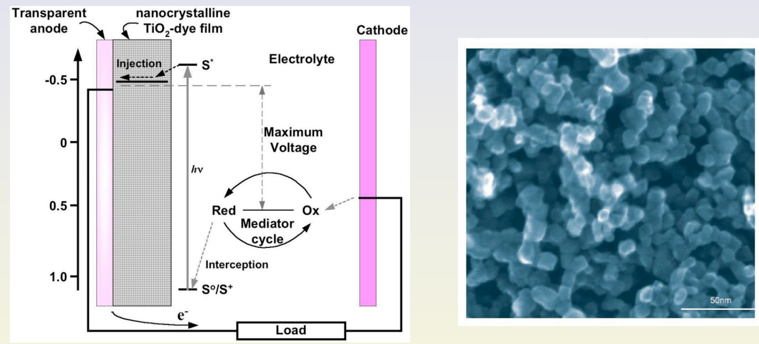
Nuclear and solar thermal hydrogen

Thermodynamic data and modeling for thermochemical cycle (TC), high temperature materials: membranes, TC heat exchanger materials, gas separation, improved catalysts

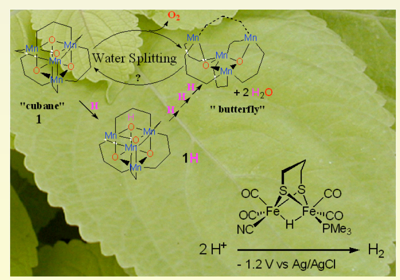
(Courtesy G. Crabtree, ANL)



Ni surface-alloyed with Au to reduce carbon poisoning



Dye-Sensitized Solar Cells

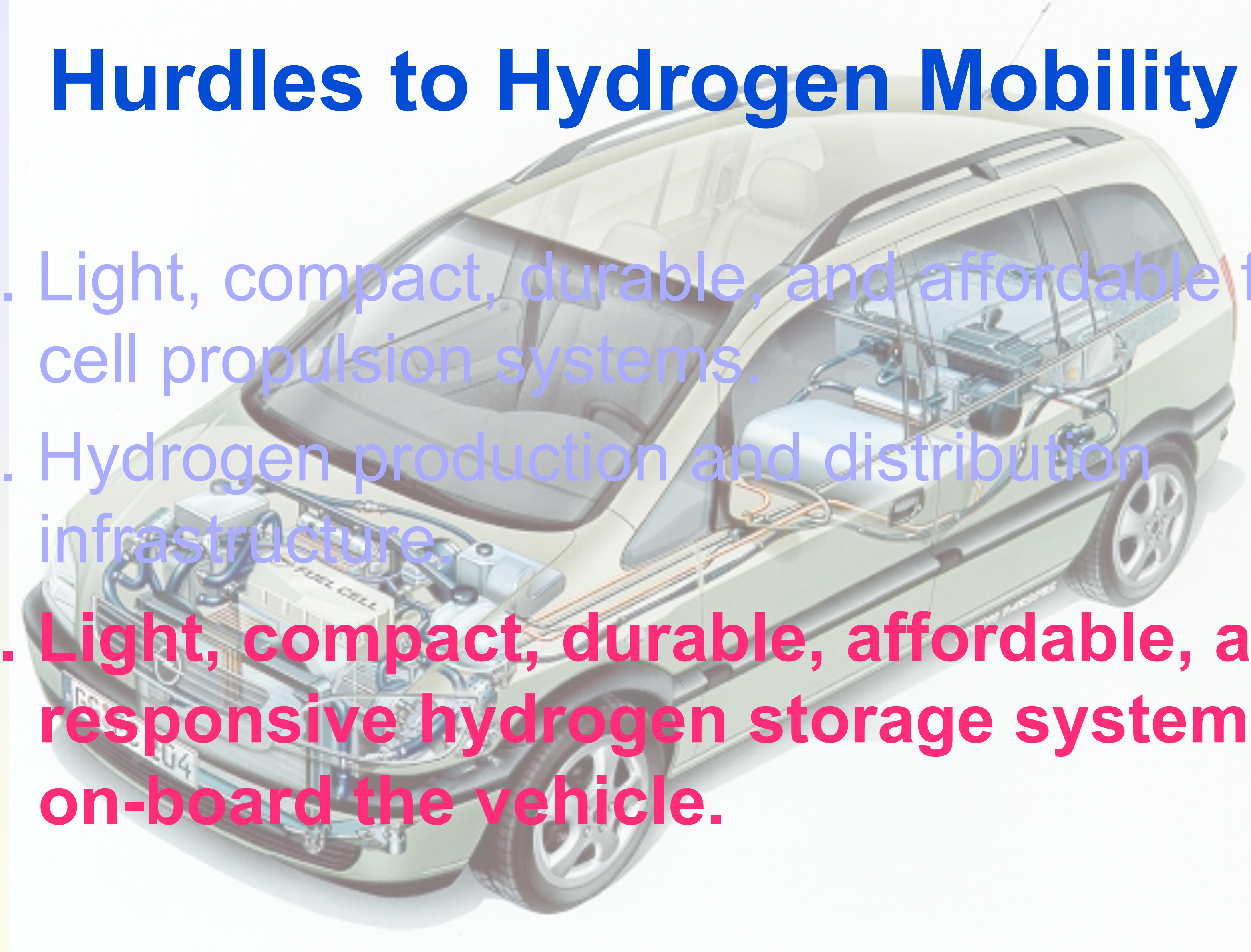


Synthetic Catalysts for Water Oxidation and Hydrogen Activation

H_2 Infrastructure

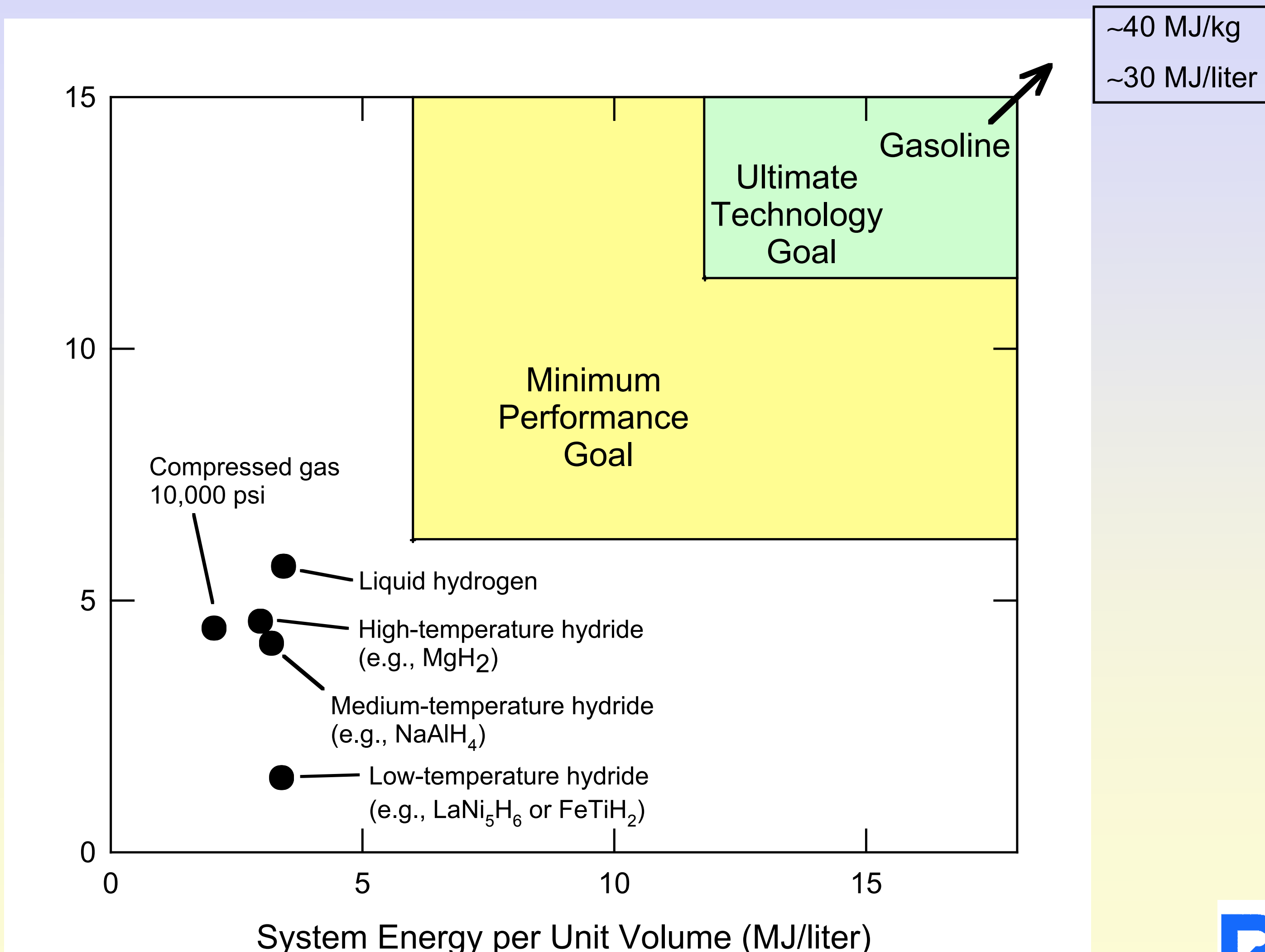
- Dependent on methods for H_2 production and storage
  - centralized: pipelines, delivery trucks
  - distributed: electrolyzers, photocatalyzers, or reformers at gas stations, homes

Hurdles to Hydrogen Mobility



1. Light, compact, durable, and affordable fuel cell propulsion systems.
2. Hydrogen production and distribution infrastructure.
3. **Light, compact, durable, affordable, and responsive hydrogen storage system on-board the vehicle.**

Gravimetric Energy Density vs. Volumetric Energy Density of Fuel Cell Hydrogen Storage Systems

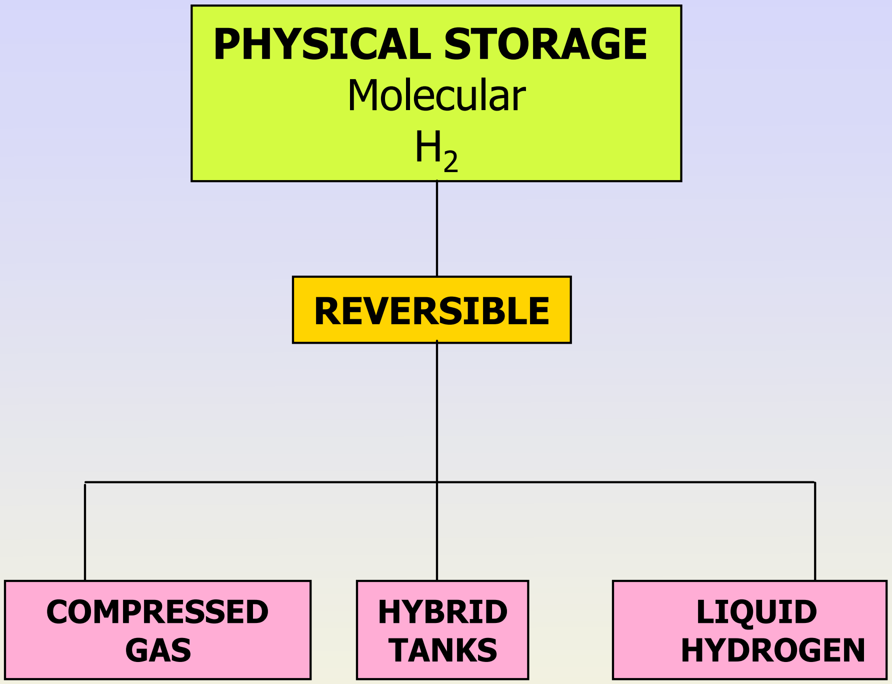


HYDROGEN STORAGE PARAMETER GOALS

METRIC	GOAL
• System energy per unit weight for conventional vehicles with 300-mile range	> 6 MJ/kg
• System energy per unit volume for conventional vehicles with 300-mile range	> 6 MJ/ℓ
• Usable energy consumed in releasing H_2	<5 %
• H_2 Release Temperature	~80 ºC
• Refueling Time	<5 minutes
• H_2 Ambient Release Temp Range	-40/+45 ºC
• Durability (to maintain 80% capacity)	150,000 miles

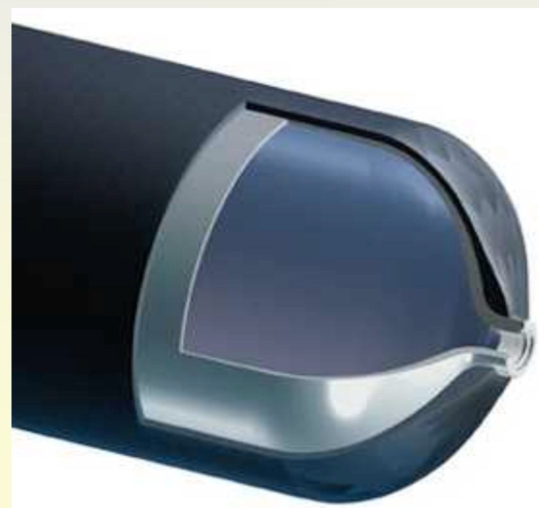
Options for Storing Hydrogen Today

HYDROGEN STORAGE OPTIONS_



Compressed Storage

- Prototype vehicle tanks developed
- Efficient high-volume manufacturing processes needed
- Less expensive materials desired
  - carbon fiber
  - binder
- Evaluation of engineering factors related to safety required
  - understanding of failure processes



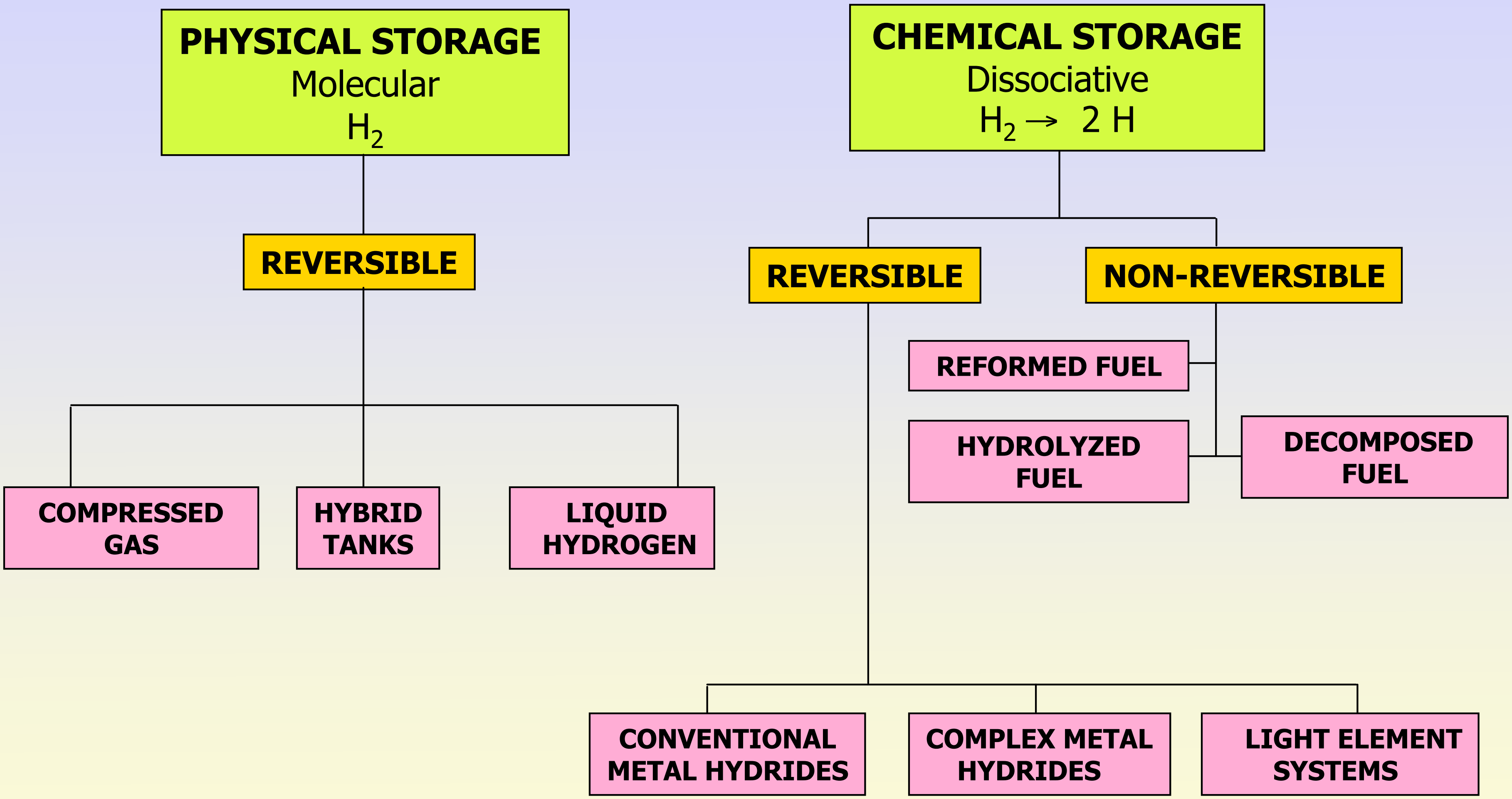
Liquid Storage

- Prototype vehicle tanks developed
- Reduced mass and especially volume needed
- Reduced cost and development of high-volume production processes needed
- Extend dormancy (time to start of “boil off” loss) without increasing cost, mass, volume
- Improve energy efficiency of liquefaction

Hybrid Physical Storage

- Compressed H_2 @ cryogenic temperatures
  - – H_2 density increases at lower temperatures
  - – further density increase possible through use of adsorbents ***– opportunity for new materials***
- The best of both worlds, or the worst ??
- Concepts under development

HYDROGEN STORAGE OPTIONS



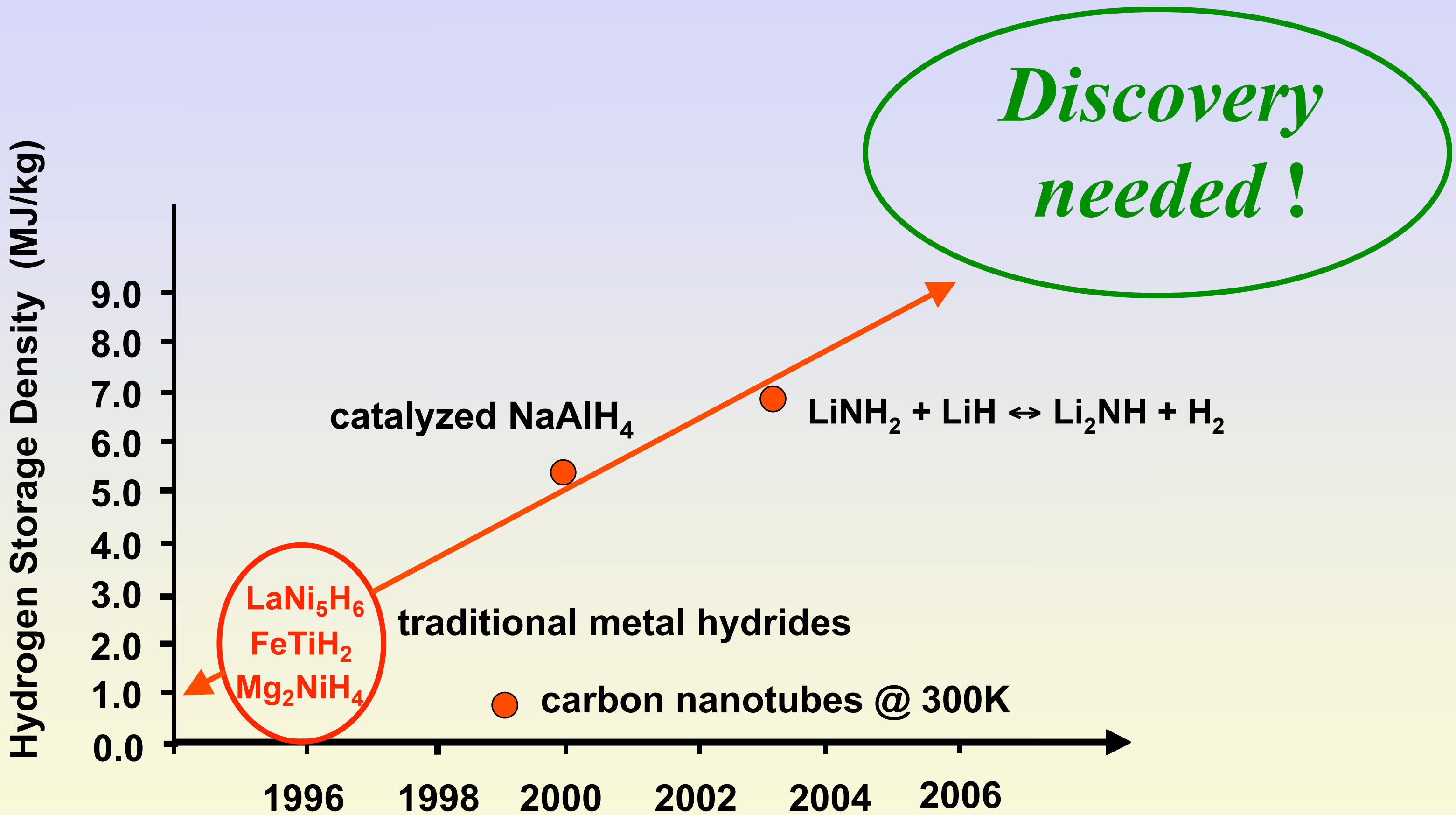
Non-reversible On-board Storage

- On-board reforming of fuels has been rejected as a source of hydrogen because of packaging and cost
  - energy station reforming to provide compressed hydrogen is still a viable option
- Hydrolysis hydrides suffer from high heat rejection on-board and large energy requirements for recycle
- On-board decomposition of specialty fuels is a real option
  - need desirable recycle process
  - engineering for minimum cost and ease of use

Reversible On-board Storage

- Reversible, solid state, on-board storage is the ultimate goal for automotive applications
- Accurate, fast computational techniques needed to scan new formulations and new classes of hydrides
- Thermodynamics of hydride systems can be "tuned" to improve system performance
  - storage capacity
  - temperature of hydrogen release
  - kinetics/speed of hydrogen refueling
- Catalysts and additives may also improve storage characteristics

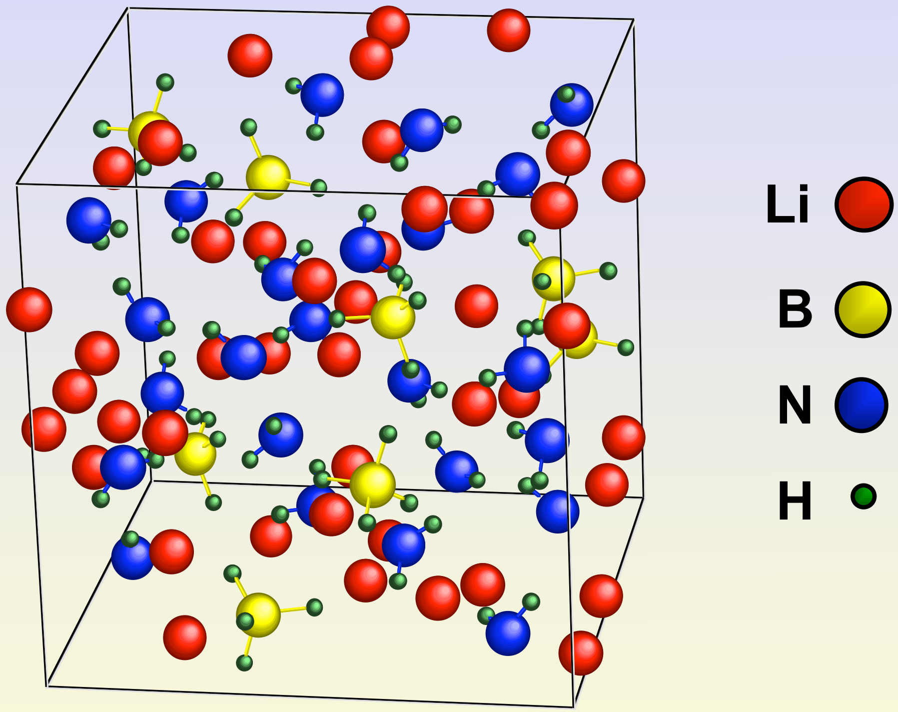
Reversible On-Board Storage Capacity



Recent Developments in Hydrogen Storage Materials

New Hydrides

$Li_4BN_3H_{10} = (LiBH_4)(LiNH_2)_3$



- releases ~11 mass% H_2
- attempts to reverse with catalysts, additives so far unsuccessful

Destabilized Hydrides

- Equilibrium pressure P and operating temperature T set by enthalpy ΔH of hydride formation:

  $\ln P(\text{bar}) = \Delta H/RT - \Delta S/R$ (van't Hoff relation)

- Light metal hydrides tend to have large ΔH
  ⇒ moderate by reacting with something else:

  $LiNH_2 + LiH \leftrightarrow Li_2NH + H_2$ (6.5 mass% H; T(1 bar) ~ 275°C)

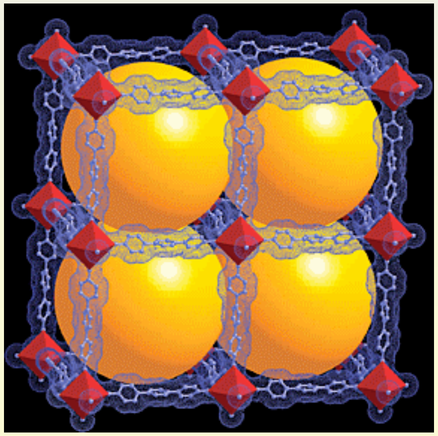
  $2LiBH_4 + MgH_2 \leftrightarrow 2LiH + MgB_2 + 4H_2$
  (11.5 mass% H; T(1 bar) ~ 225°C)

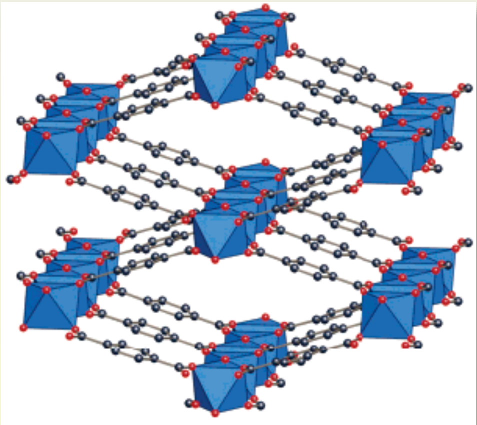
  $6LiBH_4 + CaH_2 \leftrightarrow 6LiH + CaB_6 + 10H_2$
  (11.7 mass% H; T(1 bar) ~ 420°C)

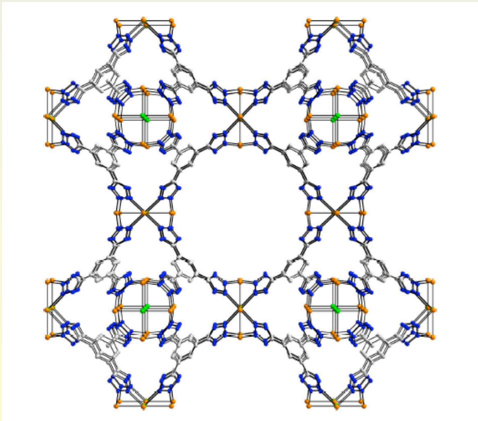
  – ***so far T(1 bar) too high, hydrogenation reaction too sluggish***

Cryogenic Materials for Hybrid Tanks

- H_2 molecules can bind to surfaces at low temperatures
- Materials with large surface area might enable tank with enough improved capacity to offset penalty for cooling
- Considerable research underway on such materials
  - activated carbon: ≤ 2500 m^2/g (1 oz ↔ 17 acres!); 5 mass% @ 77K
  - metal organic frameworks (MOFs): ≤ 5000 m^2/g; 5-7 mass% @ 77K

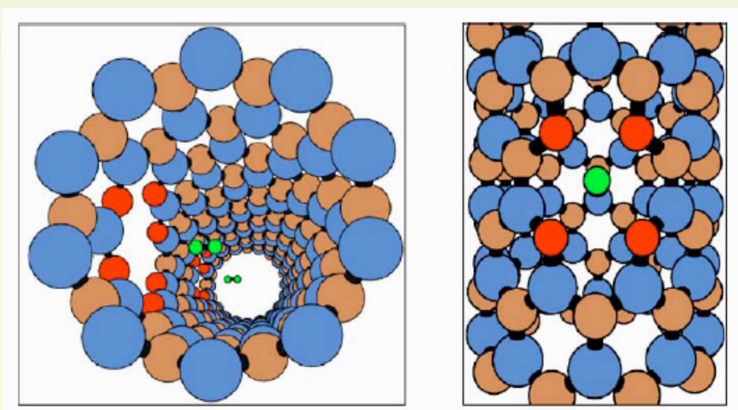




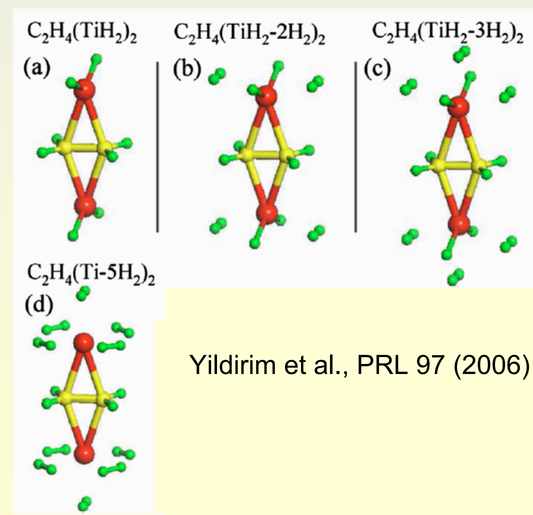


Modeling New Materials with Density Functional Theory

- DFT has become a valuable tool in research on H_2 storage materials
- Great promise for imaginative use of DFT to guide discovery and development of new hydrides
- Recent (hypothetical!) materials:
  - organometallic buckyballs [C_{60} + transition metals (TMs) such as Sc]
  - TM/ethylene complexes
  - polymers (e. g., polyacetylene) decorated with TMs
  - activated boron nitride nanotubes



Jhi, PRB 74 (2006) 155424



Yildirim et al., PRL 97 (2006) 226102

SUMMARY

- Liquid and compressed hydrogen storage
  - Technically feasible; in use on prototype vehicles
  - Focus is on meeting packaging, mass, and cost targets
  - Both methods fall below energy density goals
  - Unique vehicle architecture and design could enable efficient packaging and extended range
- Solid state storage
  - Fundamental discovery and intense development necessary
  - “Idea-rich” research environment

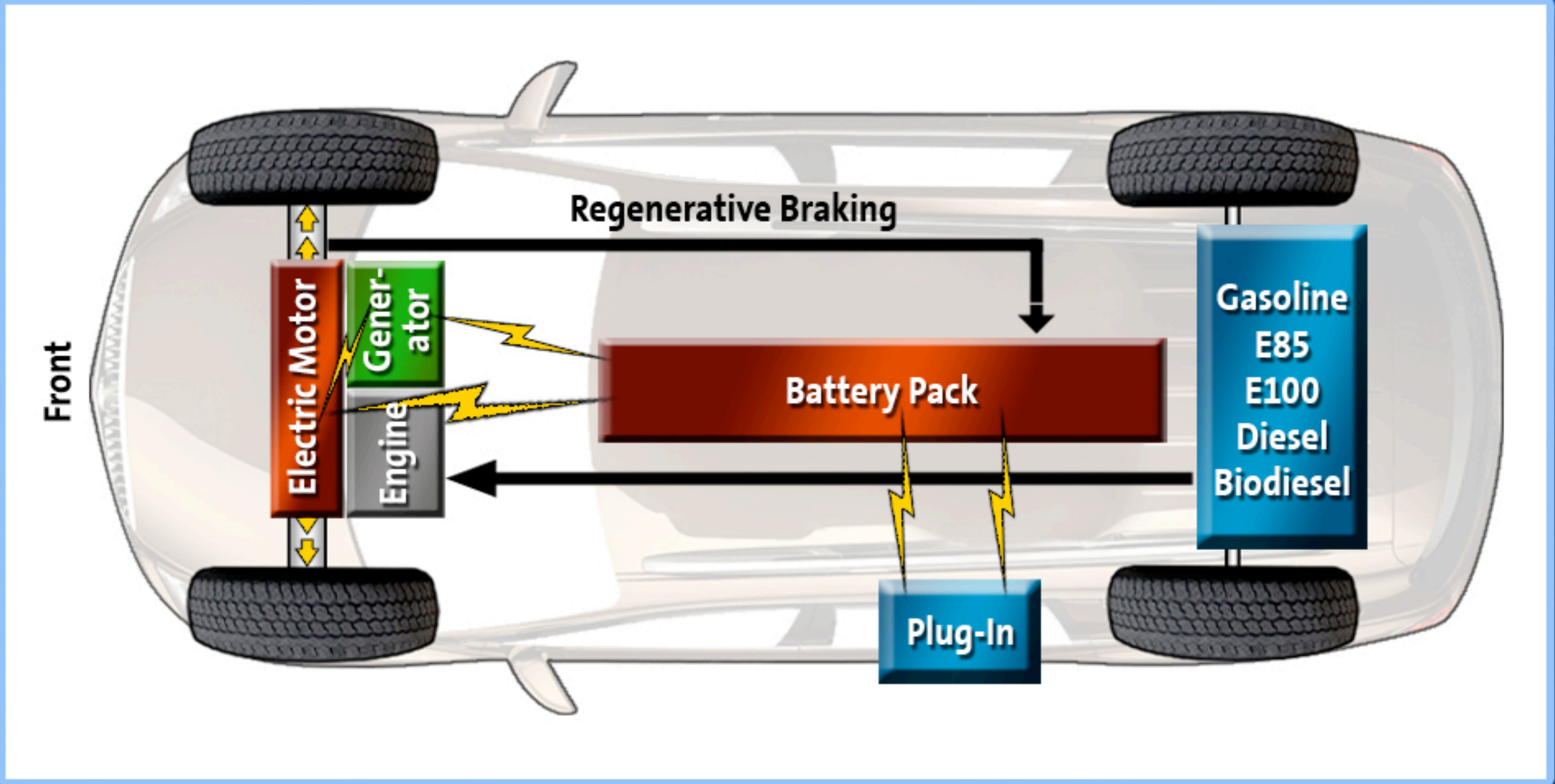
E-Flex & Chevy Volt

GM E-Flex

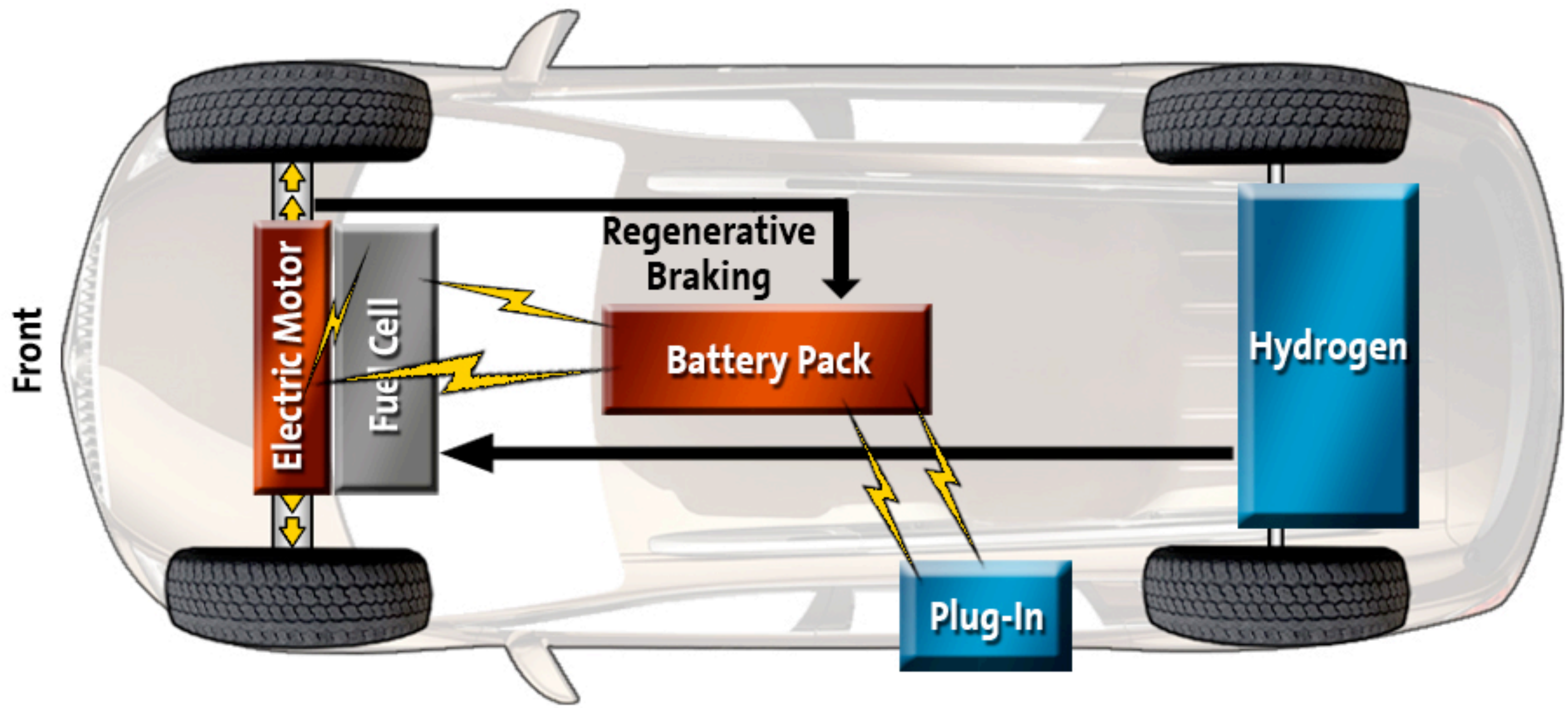
– Flexible electric drive system enabling variety of electrically driven vehicles
  - Common electrical drive components
  - Create and store electricity on board


GM
VOLT
E FLEX

E-Flex System: Engine-Generator



E-Flex System: Fuel Cell



GM

Extended-Range EV

FUEL CELL