

PROGRESS AND CHALLENGES OF A HYDROGEN ECONOMY

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Since the publication of the 2003 report on Basic Energy Needs for the Hydrogen Economy, many important advances in hydrogen research have occurred, a cadre of enthusiastic re-searchers has entered the field with great interest shown by students, and private industry has made significant commitment and investment to this technology worldwide. Concurrently, other energy technologies have made major strides forward. This overview discusses these topics and looks to the future.

1. Introduction

Energy availability for the masses is without doubt a dominant challenge of the 21st century. Driven by increasing world populations, an even faster increase in the per capita energy demand, a decreasing availability of traditional sources of energy through fossil fuels and the increasing concern about the need to curb the increase of CO₂ into the atmosphere, the need for a transformation to a sustainable energy supply from renewable sources has emerged as a dominant challenge of this century. President Bush in his 2003 State of the Union Message identified this as a major challenge of his administration, as have other national leaders worldwide. As a result of the Bush 2003 State of the Union Message, a hydrogen initiative was launched by the US Government Funding Agencies.

As a first step, a workshop was held in the spring of 2003, followed by a committee study which resulted in a report [1] which emphasized, on one hand, the appeal of hydrogen as an energy carrier whose release of energy produces only water as a by product without other pollutants or greenhouse gases, and takes advantage of the high efficiency enabled by hydrogen fuel cells. On the other hand, the report emphasized the challenges for the implementation of the hydrogen economy in terms of the enormous technical challenges to be overcome for its implementation, emphasizing that fundamental breakthroughs would be needed in understanding the physical processes involved in the production, storage and use of hydrogen. Understanding the atomic and

molecular processes that occur at the interfaces of materials with hydrogen was identified as crucial to producing the new materials that would be needed for these fundamental breakthroughs to occur. The report goes on to say that the discovery of the new materials, new chemical processes and new synthesis techniques that would be needed could only be achieved by initiating a major basic research program with these objectives. Such a research program was subsequently launched by the Basic Energy Sciences Office of the Department of Energy (DOE) following the recommendations of the report, working in close collaboration with the Energy Efficiency and Renewable Energy Office of the DOE, thereby uniting the basic and applied science thrusts through a highly interdisciplinary effort involving chemistry, physics, biology and engineering, all working together to solve the multitude of challenges and opportunities identified in the report. From these efforts, major research advances have occurred over a short period of time, amplified by the corresponding efforts occurring worldwide. The enthusiastic response of the research community and the great interest of students in joining this effort has been noteworthy, leading to a series of other studies and initiatives in other areas of energy research and development. Concurrently, industry has launched major initiatives so that the playing field is rapidly changing as breakthroughs are occurring in other areas. In the present brief report, emphasis is given to an attempt to identify an evolving role for the hydrogen economy within the larger energy challenge.

2. Strategic Issues

The framework for the hydrogen initiative, based on the 2003 Basic Energy Sciences Report “Basic Research Needs for the Hydrogen Economy” [1], was motivated by the charge to the study committee which focused on a hydrogen economy as an isolated entity and the use of hydrogen for transportation applications, exploiting the superior efficiency of the hydrogen and fuel cell combination relative to gasoline and the internal combustion engine. Based on the DOE hydrogen requirements for the years 2010 and 2015 (Table 1), the technology gaps for hydrogen as an energy carrier were identified (Fig. 1) and research directions for bridging these technology gaps were suggested in the report. In the meantime, the auto industry worldwide has taken a hydrogen based vehicle seriously and has moved rapidly in getting hydrogen fuel cell automobiles on the highways to gain experience with this new technology, using presently available methods for hydrogen production and storage, focusing mainly on hydrogen fuel cell development and the infrastructure needed for carrying out a hydrogen vehicle test program. While methods of hydrogen

production from natural gas are presently adequate for automotive needs, the use of a fossil fuel natural gas precursor defeats the long term goal of using a sustainable, renewable energy source to provide the large increase in hydrogen production (20-fold by the estimate in Figure 1) that would be required for transportation use. The development of a renewable route for large scale hydrogen production by methods, such as splitting water in a closed cycle water-hydrogen process or by a biologically inspired process remains a long term challenge where there are presently large opportunities for the research community.

The on-board storage of hydrogen to match US consumer appetites for a 500 km (~300mi) range for their family vehicle has been identified as the greatest challenge to the implementation of a hydrogen economy because even the filling of the present fuel tanks of an automobile with liquid (or solid) hydrogen would fall short of meeting the DOE 2015 targets. The auto industry has taken a different approach toward addressing the consumer appetites and is using increased operating efficiency, hybrid vehicle technology to lower the storage requirements. Using this approach, Toyota has recently demonstrated by a run from Osaka to Tokyo a 550 km (350mi) range for its hydrogen fuel cell vehicles based on presently available compressed hydrogen gas cylinder technology. Although researchers from the auto-industry would like to see the academic community and government supported research laboratories come up with a chemisorbed or physisorbed hydride solution for hydrogen storage, the auto industry does not now see the hydrogen storage problem as a technical show-stopper, though widespread public acceptance of the hydrogen gas cylinder technology has not been seriously tested. On the other hand, the auto industry is looking to the research community for major breakthroughs in renewable hydrogen production, reversible solid state hydrogen storage and higher efficiency hydrogen fuel cells to help make widespread adoption of the hydrogen fuel cell vehicle option a reality by mid-century. The arguments on the central role that new materials will play in these break-throughs, as presented in the 2003 hydrogen report [1] remain valid through the present time. What has changed in the interim is the vital role that industry is now playing and the need for the research community to be in close contact with industrial R&D, and to play a role in the incubation of start-up companies to develop the new technology that will be provided by future suppliers to the auto companies. Thus, one strategic issue for the planning of hydrogen research is the coordination, not only between basic and applied research by the multidisciplinary players, but also to look for opportunities where academic and

national laboratory research could have a large impact on future industrial product development.

A second strategic issue concerns scale. Projections of global energy needs imply a doubling in overall energy demand and a tripling of the electricity demands by the year 2050.

Table 1: Requirements for a hydrogen fuel cell automobile

Targeted Factor	2005	2010	2015
Specific energy (MJ/kg)	5.4	7.2	10.8
Hydrogen (wt%)	4.5	6.0	9.0
Energy density (MJ/L)	4.3	5.4	9.72
System cost (\$/kg/system)	9	6	3
Operating temperature (°C)	-20/50	-20/50	-20/50
Cycle life-time (absorption/desorption cycles)	500	1,000	1,500
Flow rate (g/s)	3	4	5
Delivery pressure (bar)	2.5	2.5	2.5
Transient response (s)	0.5	0.5	0.5
Refueling rate (kp/H ₂ /min)	0.5	1.5	2.0

Source: Milliken (2003).

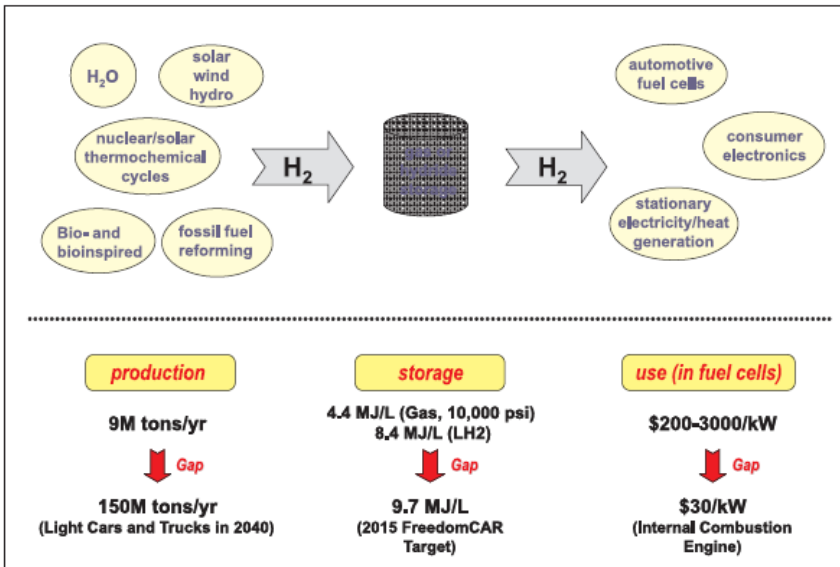


Figure 1: The technology gaps in hydrogen production, storage, and end use in a hydrogen Economy [2].

The only renewable energy source with sufficient capacity to meet these growing energy demands is solar energy. An increase from the present 14TW to 28-30TW by 2050 is expected to come from solar energy used for generating electricity (photovoltaic), providing fuels (biofuels, water splitting, close cycle synfuels), and supplying space and water heating (solar thermal). In this big picture, with solar electric, solar fuel and solar thermal as the energy sources, electricity and hydrogen are cited as complementary energy carriers. When thinking of hydrogen as a chemical carrier of energy, its role in energy storage from the electric grid emerges as an interesting opportunity, as does the generation of close-cycle renewable synfuels using a hydrogen from H₂O and carbon from CO₂ to produce a hydrocarbon fuel using sunlight [3]. The latter research direction, denoted by “transformation and recycling of CO₂ into a new material” was identified in the Declaration issued by the First World Materials Summit held in Lisbon in 2007 [4].

The need for break-throughs with high impact follows from the huge scale of the energy challenge involving a multi-trillion dollar business worldwide. Therefore major emphasis must be given to those research directions which will have the potential for large orders of magnitude impacts. This brings to mind Moore’s law which has provided road-maps for the electronics, optoelectronic and magnetic information storage industries for several decades. To have comparable impact on the energy industry, a Moore’s law road-map for the Energy Industry is needed. Here new materials will play a vital role, especially nanomaterials, because of the greater ability to modify and control their properties by varying the material’s size and composition, their greater surface area to promote catalysis which is based on an exponential $\exp(-E/kT)$ dependence, and the independent control of materials parameters which are interdependent in 3D systems.

could be interesting opportunities for hydrogen as an energy storage agent to be used in conjunction with this technology.

Another interesting direction where large-scale impacts on energy are occurring is in thermoelectric conversion where increases in the thermoelectric figure of merit and scale-up to samples with higher thermal capacities have been demonstrated. As a result, industrial development in this field is booming with about one million cooling/heating thermoelectric seats sold in 2007 for automotive use. When used in hybrid cars where fuel efficiency is readily monitored, it has been found that the local cooling of passengers by the thermoelectrically equipped seats causes a major decrease in the need for air conditioning for passenger comfort, resulting in a payback of less than 1 year for the thermoelectric car seats, with subsequent cost savings in future fuel consumption [6]. It would be interesting to explore what the effect of thermoelectric car seats would be on the efficiency of hydrogen fuel-cell autos.

The device utilization of the discovery of highly efficient carrier multiplication in semiconductor nanocrystals [7] allowing as many as 6 electron-hole pairs to be produced by a single optical photon incident on a PbSe nanocrystal is now being explored and may eventually result in enhanced photovoltaic device efficiency. If this scientific advance results in improved photovoltaic device efficiency, this may open new opportunities for hydrogen as an energy storage agent.

Finally, high throughput combinatorial screening allows a route for both experiment and theory to scan many variants of multi-component materials by composition, to optimize a material for a given property while at the same time allowing rapid measurement of several other properties of the material in the compositional range where the desired property is optimized. Such capabilities are necessary since a number of properties of a material affect its ultimate device performance, and these properties therefore need to be jointly optimized. For example, a material, which has excellent thermoelectric performance but is toxic, would not make it in the marketplace.

3. Strategies for the Hydrogen Economy

With the principles outlined in §2 in mind, we can identify a number of breakthroughs that have the potential for high impact on the hydrogen economy. As mentioned above, the use of improved catalysts have the potential for high impact because of their $\exp(-E/kT)$ dependence. Thus, a promising strategy is the search of new catalysts that lower the energy barriers for chemical reactions, can be made in the optimal small sizes (usually in the 2–5nm range), and can

contain cheaper and more plentiful elements. An example where such a specially tailored catalyst has been developed for the hydrogen economy is the Pt_3M catalyst. Density functional theory was first used to establish the concept of using a Pt surface layer of the catalytic particle to rapidly dissociate a hydrogen molecule. The introduction of a first subsurface layer with a PtM composition then provides a mechanism for attaching atomic hydrogen more easily [8]. Such an approach can provide strong binding and also rapid release on hydrogen. Variants of this concept could have an impact on hydrogen production, storage, and use in fuel cells. An implementation of this general concept has recently been made to increasing the catalytic activity of Pt by a factor of 10 in the oxygen reduction reaction by using a surface Pt layer and a subsurface PtNi layer to break the O–O bonds to form O–H bonds. Weak surface bonds prevent the splitting of O–O bonds, while strong surface bonds attract guest species to adhere to the surface, thereby blocking access of other reactants to the catalyst. In the case of the oxygen reduction reaction, the 10-fold increase in catalytic activity for the oxygen reduction reaction which occurs at the anode of hydrogen fuel cells was achieved by using both the (111) crystal orientation of the catalytic particle and its compositional variation [9].

A number of other impressive advances have been made in the laboratory at the research level, and a small number are cited here as examples. One noteworthy example is the identification of a route to increase the tolerance of hydrogen production by a genetically modified Fe–Fe hydrogenase bacterial structure that yields a 100-fold increase in H_2 activity relative to the natural algol enzyme. Simplified and robust analogs of bacterial hydrogenase have the potential to lead to the development of a commercial-scale hydrogen production route that may be scalable to large scale production, self-sustaining and cost effective [10].

An interesting approach to lowering the release temperature of hydrogen through increased destabilization is the use of a second compound in a chemical reaction, and for example $\text{LiNH}_2 + \text{LiH} \rightarrow \text{Li}_2\text{NH} + \text{H}_2$ releases hydrogen at $\sim 150^\circ\text{C}$ which is significantly lower than LiNH_2 (at 200°C) or LiH (at 500°C). This study is of significant scientific interest. However the storage capacity for the joint reaction is only 6.5%, which could be too low for commercial development [12, 13] On the other hand, the destabilization pair of $\text{LBH}_4 + \text{MgH}_2$ with a storage capacity of 11.5% could be more interesting for further commercial development [14].

Some new ideas have recently been introduced into increasing the temperature of operation of PEM membranes and increasing the power density

of the fuel cell operation. Some membranes have been developed that conduct protons at temperatures up to 200°C in the absence of water [15]. A new class of chemically cross linked membranes fabricated at low temperature from liquid precursors significantly enhance proton conductivity by allowing additional acid loading, enhance thermal and mechanical stability by increased cross-linking, while at the same time increasing electrical and chemical exchange with the electrode by enhancing the effective surface area [16].

The advances in hydrogen research are mostly at an early stage with further progress in understanding and in material performance expected in the near term. Applications to industrial products are expected to follow.

4. Concluding Remarks

Because of its special and unique attributes, hydrogen is likely to be one of a mix of future sustainable energy technologies. New materials and nanoscience are necessary to its development as they are to many of the other pertinent energy technologies. The strong interplay between basic and applied sciences, interdisciplinary approaches and the coupling between theory and experiment are all vital. Working closely with industry will be important for identifying research directions with high potential impact. Attention to major advances in other key technologies is equally important for the identification of new priority directions for hydrogen R&D. Because of the highly complementary focus of energy research in different countries, based on their different climatic and cultural constraints, international cooperation and networking should be encouraged and supported. Linking to and coordinating between international groups (such as the World Materials Summit) promoting materials research for energy applications regionally and internationally would be important, so that policy makers worldwide get a clear message about progress in hydrogen research and its potential contribution to the larger picture of providing a sustainable energy supply world-wide.

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