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The use of hydrogen and fuel cells to power light-duty vehicles offers an effective pathway as part of a portfolio of technologies to reduce greenhouse gas emissions and petroleum usage.¹ In addition to the challenges associated with improving the power density and durability of polymer electrolyte membrane fuel cells while reducing their costs, there are challenges in developing hydrogen storage technologies that offer high specific energy and energy density at acceptable costs for use onboard vehicles.² Working with the U.S. automotive manufacturers through the FreedomCAR and Fuel Partnership (now U.S. DRIVE), the U.S. Department of Energy (DOE) established in 2003 a comprehensive set of performance metrics for onboard hydrogen storage systems based on comparison with gasoline fueled vehicles. The metrics included 2015 system-level targets for specific energy and energy density of 3.0 kWh/kg (9 wt.%) and 2.7 kWh/L (81 g H₂/L) respectively.³ In 2009, after re-evaluating the performance metrics with comparisons to available fuel cell, hybrid, and electric vehicle performance data, the DOE issued a revised set of performance targets that included “Ultimate Full Fleet” system-level targets for specific energy and energy density of 2.5 kWh/kg (7.5 wt.%) and 2.3 kWh/L (70 g H₂/L) respectively.⁴ Considering the energy density target alone as an example, compressed hydrogen at ambient temperature has a density of about 40 g H₂/L; liquid hydrogen at its normal boiling point of 20 K has a density of 71 g H₂/L. Since the energy density targets are for the complete system, neither normal compressed hydrogen nor liquid hydrogen is theoretically able to meet the system-level targets. Therefore it was recognized that advanced hydrogen storage technologies would need to be developed if all the performance metrics were to be achieved.

When hydrogen interacts with other materials or elements, either as the dihydrogen molecule or as monoatomic hydrogen, hydrogen densities greater than that of compressed hydrogen gas or liquid hydrogen, can be obtained. For instance, dihydrogen can be adsorbed onto high-surface area, porous materials, where even at low pressures of a few bar, the hydrogen density of the adsorbed layer can approach the density of liquid hydrogen. When atomic hydrogen bonds to other elements, either through metallic-type bonding as in interstitial metal hydrides, covalent bonding as in complex hydrides, compounds such as ammonia borane and even water, or ionic bonding as in binary alkali metal hydrides such as sodium hydride, hydrogen densities up to twice that of liquid hydrogen can be obtained.⁵ It was therefore recognized that materials-based hydrogen storage might provide a pathway to high energy density storage of hydrogen at low pressure and near ambient temperature with the potential to meet the DOE performance targets. The materials-based storage technologies can be roughly categorized into three groups: sorbents, reversible metal hydrides, and offboard regenerable chemical hydrogen storage. Prior to the 2003 timeframe, most materials-based hydrogen storage technology development had focused on reversible interstitial metal hydrides, hydrolysis of chemical hydrogen storage materials, specifically sodium borohydride (NaBH₄), and investigation of carbon nanotubes and nanofibers as hydrogen adsorbents.

In an effort to accelerate the development of materials-based hydrogen storage technologies, in 2004 the DOE announced the formation of three “Materials Centers of Excellence” to develop reversible metal hydrides, chemical hydrogen storage materials, and high-surface area hydrogen sorbents.⁶ Each of the three centers consisted of multiple partner institutions which worked in a

concerted, synergistic way to carry out hydrogen storage materials discovery, characterization, and development for the three categories of hydrogen storage materials. Each center included computational analysis, materials synthesis, and materials characterization capabilities. The centers continued their efforts for approximately five years and were concluded in 2010. The following three sections include the executive summary of the final report for each center.