

## IV.A.5q Catalyzed Nano-Framework Stabilized High Density Reversible Hydrogen Storage Systems

Daniel A. Mosher (Primary Contact),  
Sarah Arsenault, Thomas H. Vanderspurt,  
Susanne M. Opalka and Xia Tang  
United Technologies Research Center  
411 Silver Lane  
E. Hartford, CT 06108  
Phone: (860) 610-7011; Fax: (860) 660-1284  
E-mail: mosherda@utrc.utc.com

DOE Technology Development Manager:  
Ned Stetson  
Phone: (202) 586-9995; Fax: (202) 586-9811  
E-mail: Ned.Stetson@ee.doe.gov

DOE Project Officer: Paul Bakke  
Phone: (303) 275-4916; Fax: (303) 275-4753  
E-mail: Paul.Bakke@go.doe.gov

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- Sandia National Laboratories  
Livermore, CA and Albuquerque, NM
- Albemarle Corporation, Baton Rouge, LA

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### Introduction

Current complex hydrides have yet to meet the 2010 DOE systems targets, presenting a continuing challenge for the discovery of high capacity, reversible hydrides. For example, metal borohydrides  $[M(BH_4)_n]$  have the potential to meet the targets, but some materials are unstable (such as those containing Ti, Al, or Sc cations) and decompose within minutes or days. Other metal borohydrides (such as those containing Li, Na, K or Ca cations) decompose at temperatures that are higher than what is desired for proton exchange membrane (PEM) fuel cell integration and cannot be recharged with gaseous hydrogen at moderate pressures. Thus, there is a need to develop novel techniques that enable high capacity that is maintained over numerous absorption/desorption cycles. The current project will address this by incorporating solvated and other forms of complex metal hydrides, with a focus on borohydrides, into

nano-scale frameworks of low density, high surface area skeleton material to stabilize, catalyze, and control desorption product formation associated with such complex metal hydrides and modify thermodynamics of the processes.

### Approach

The United Technologies Research Center (UTRC), Sandia National Laboratories (SNL), and Albemarle Corporation will team to develop catalyzed framework structures (CFS) designed for specific advanced hydrogen storage materials (HSM). The team will initially examine the HSMs developed by UTRC/Albemarle under a previous DOE contract, "Complex Hydride Compounds with Enhanced Hydrogen Storage Capacity," and by SNL under previous Metal Hydride Center of Excellence efforts, these HSMs being borohydrides.

UTRC will use an iterative atomistic/thermodynamic modeling and experimental approach to develop nano-framework structured (NFS) materials. Some new high capacity HSMs are only stable in solvents or with ligands such as amines. Stabilization of these hydrides will be performed instead by the interaction with the NFS cell walls. In addition, nanometer scale catalytic sites within the NFS cells will activate  $H_2$ , and through hydrogen spillover, facilitate reversibility (rehydrogenation). Containing the HSM constituents after hydrogen discharge within the NFS cells will reduce decrepitation (irreversible phase segregation, separation, or degradation) such as the formation of refractory metal borides. UTRC, utilizing expertise in self assembly of engineered nano-structures, will synthesize NFS materials with  $\geq 90\%$  porosity. SNL and Albemarle will provide HSMs or their precursors while UTRC and SNL will incorporate these HSMs into the NFS materials.

The CFS approach has the potential to increase material relative volumetric packing from  $\sim 60\%$ , achievable with advanced powder densification techniques developed by UTRC under a previous DOE contract, to values in the neighborhood of  $80\%$ . UTRC will also carry out subscale cyclic tests and heat/mass transfer experiments to demonstrate the CFS approach, provide data for preliminary system designs and support performance projections.