

## Hydrogen Storage

### Summary of Annual Merit Review Hydrogen Storage Subprogram

#### Summary of Reviewer Comments on the Hydrogen Storage Subprogram:

Reviewers consider hydrogen storage to be a critical enabling technology for the success of the President's Hydrogen Fuel Initiative. Overall, the R&D portfolio was judged to be well-managed, appropriately diverse and focused on addressing technical barriers and meeting performance targets. Progress was considered good, despite the newness of the effort, the level of funding and the difficulty in the task. The general opinion was that the Centers of Excellence will enhance integration of efforts, collaboration, cooperation, and overall effectiveness of the subprogram. In addition, the interface and collaboration with DOE's Office of Science was noted as desirable and appropriate. The proposed annual solicitation process was considered critical and a good aspect of program management.

The reviewers also highlighted a number of challenges and recommendations, summarized as follows:

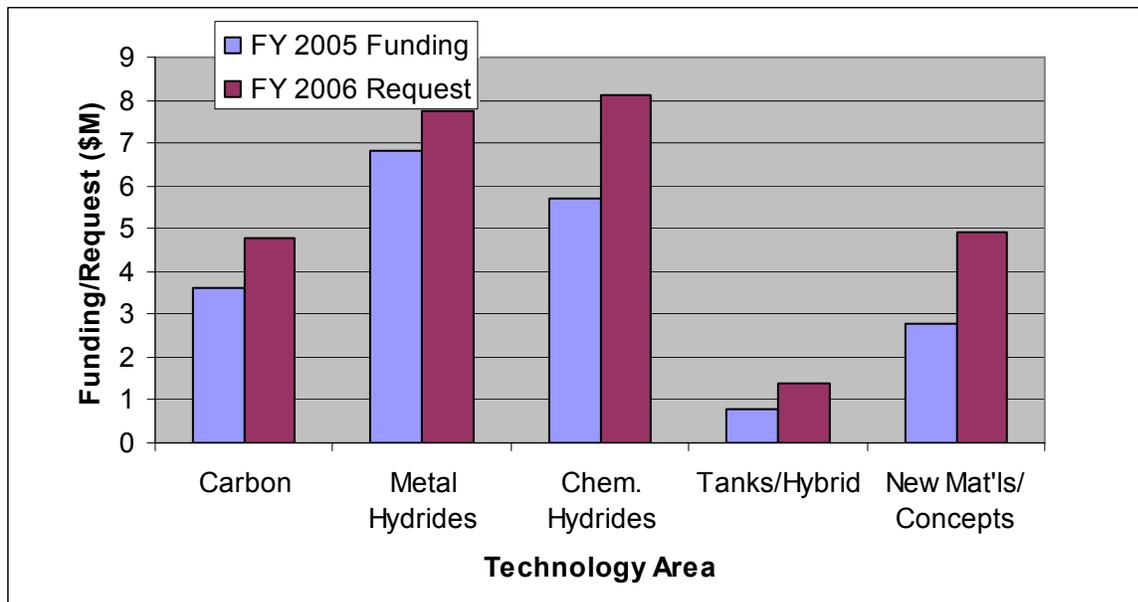
- Considering that hydrogen storage is a key hurdle and given that the effort is newer than others, such as fuel cell activities, DOE's management approach from a funding perspective was considered suboptimal.
- In addition, as projects move into more advanced stages, there was concern that more resources would be required to adequately monitor and manage projects.
- The Centers of Excellence were considered to be a challenge to manage to ensure the full value of broad collaboration and synergy of the efforts.
- The redirection of funds to congressionally-directed projects and its impact on the program continues to be a concern.

It was also noted that the hydrogen storage subprogram has substantially more university participants compared to prior years. The differences between Office of Science and EERE funding approaches was mentioned, highlighting that while basic science projects may last several years, effective management of applied programs may require termination of projects. Research that is clearly not helping to reach the technical goals should not be funded for many years. In some cases, reviewers stated that approaches that do not have potential to meet 2015 targets should be deemphasized.

In general, comments discussed how the incorporation and accomplishment of go/no-go decisions are critical and a "real test for management." Some reviewers believed that the storage subprogram still has at least a few projects that do not deserve funding, based on the fact that they either duplicate higher caliber work in other projects or are not very likely to produce meaningful results in a timely manner. A recurring recommendation was to continue to address system level issues to help direct materials R&D.

#### Hydrogen Storage Funding by Technology:

The funding portfolio for hydrogen storage addresses primarily long-term materials R&D to meet 2010 and 2015 targets for on-board applications. The requested FY2006 funding profile, subject to congressional appropriations, and the Centers of Excellence address the National Academies' report recommendations to "shift...away from some development areas towards more exploratory work" and that "the probability of success is greatly increased by partnering with a broader range of academic and industrial organizations..." Continued funding, at a low level, for compressed hydrogen/cryogenic tanks emphasizes cost reduction and novel conformable designs. In addition, it is recognized that materials-based solutions will require low-cost, conformable tanks and would benefit from current R&D in this area. A major milestone in FY2006 will be the go/no-go decision on R&D for single-walled carbon nanotubes with a metric of reproducibly achieving 6 wt.% (material basis) hydrogen storage capacity.



### **Majority of Reviewer Comments and Recommendations:**

In general, the reviewer scores for the storage projects were average to low, with scores of 3.3, 2.7 and 1.5 for the highest, average and lowest scores respectively. All projects reviewed were into at least their second year of effort. The three Centers of Excellence were presented but not reviewed, because of their late start due to funding. The scores are indicative of discriminating reviewers, perceived scope of work, and perceived insufficient technical progress in view of the challenging task (and in some cases, relative to funds received). In most cases, scores were lower than implied by written comments. Key recommendations are summarized below. DOE will act on reviewer recommendations as appropriate for the scope and coherency of the overall hydrogen storage research effort.

- **Carbon:** Implement go/no-go decision points. While some reviewers showed concern for the level of investment in this higher-risk area of materials research, most reviewers were very supportive of the broadened scope of work, beyond single walled nanotubes, and the added risk mitigation provided by complementing more traditional research areas, such as metal hydrides. Continue to shift emphasis to address the broader area of carbon-based materials and other high surface area adsorbents. Emphasize go/no-go decision points in the project research plans.
- **Metal Hydrides:** Continue to refocus efforts on new materials with potential to meet the long term storage targets. Sodium alanate work should be phased out. There is perceived overlap, particularly in the independent projects. DOE is urged to facilitate collaboration across the program to leverage efforts with the metal hydride center of excellence and apply lessons learned from mature projects. Thermal management, another system-level issue, should receive greater emphasis. Emphasize go/no-go decision points in the project research plans.
- **Chemical Hydrogen Storage:** Continue to address life-cycle efficiency, particularly for off-board regeneration of spent fuel, early in the program. Emphasize go/no-go decision points in the project research plans.
- **New Materials & Concepts:** The bulk of these Grand Challenge projects were not formally reviewed because they had just started. However, informal feedback indicated that there exists overlap with existing independent projects and center work. DOE needs to help facilitate more focus and coordination. Greater emphasis on new approaches to meet long-term targets is positive in the DOE plan.
- **Tanks:** Continue to focus on cost reduction and conformability. More fully justify the benefits of cryo-compressed approaches to increase capacity.

- **Testing and Analysis:** Testing and analysis are viewed as important cross-cutting enabling activities. In particular, it is important to develop tools that allow for rapid system-level storage capacity estimation tools using material-based properties. For essentially all areas, defining a list of system components and their respective weight, volume, and cost, is recommended. Additional recommendations include analyses of possible alternative options and rapid translation of results from a materials perspective into system performance and vice versa. More emphasis should be given to testing and analysis, which is a cross-cutting enabling issue.

One overall recommendation was for DOE to advise presenters for next year's review to state the status of the performance of the material (e.g. wt.% hydrogen, kWh/L, and refill times) compared to previous year levels to help gauge progress. This recommendation may be generally applied across all subprograms to more clearly distinguish progress from year to year.

**Project # ST-01: Hydrogen Storage**

*Satyapal, Sunita; U.S. Department of Energy*

**Brief Summary of Sub-Program**

The purpose of the Storage Overview is to describe goals/objectives, budget, barriers/targets, approach to R&D, technical accomplishments, interactions and collaborations, solicitations and awards, and future directions. As such, it sets the stage and puts into context the R&D and analysis projects which will be presented in this sub-program area during the Annual Merit Review and Peer Evaluation Meeting.

**Degree to which the Sub-Program area was adequately covered and/or summarized**

- Yes, the program was covered very well.
- Excellent presentation of state-of-the-art and technical goals, and the DOE R&D program in this area.
- The Team Lead has completely described the sub-program structure, objectives, and the funded projects. The presentation clearly states the basis for the structure of the sub-program and the preparation work. The main project areas and major achievements have been well presented with a summary of objectives and participants, with indications (websites) for more details.
- Did a good job of summarizing and explaining a broad range of projects in the technology area.
- Sub-program very well covered and status presented clearly. Presentation well structured, concise, and comprehensive.
- Program was explained well, including new Centers of Excellence.
- The sub-program areas were covered well, providing good guidance to principal investigators in managing and conducting their research activities.
- Excellent guidance to PIs has been provided in the presentation. Specific requirements for storage materials have been clearly stated to PIs in order to meet DOE targets on storage system basis.
- Targets, progress, and roadmap were all well covered by the Team Lead. Basic needs were also covered by the Science presenter. Nature of the challenge was well demonstrated.
- A very clearly presented/comprehensive description of the Hydrogen Storage sub-program.
- In general, very well summarized. Good, quick overview of accomplishments so far. Targets covered well relative to present state-of-the-art limitations (especially solid media). The many sub-program players and relationships (CoEs, independent, etc.) made clear with some good graphics. Sub-program is large and complex. Hard to show all the nuances adequately.
- Targets covered well. Partnerships and coordination with other group well laid out. Well done!
- BES research is based on basic fundamental material behavior. Was confusing who was managing the sub-program.
- Good summary of sub-program, goals, and accomplishments.
- Covered the sub-program well. Comprehensive, yet succinct.

**Were important problem/issue areas and challenges identified/discussed, including plans for addressing these items in the future?**

- Yes, the slide on the range was one of the highlights of the meeting.
- The presentation shows in a convincing manner the major needs for key technical parameters (priority on specific requirements). The major scientific and technical problem/issues are adequately summarized and identified. The short- and longer-term plans and expectations for the future activities and major decisions are well organized and structured.
- Yes. The importance of hydrogen storage to achieving the goals of the DOE Hydrogen Program was emphasized and thoroughly explained. Plans for hydrogen storage Centers of Excellence were also well described.
- Main problem areas were clearly identified along with the challenges and future directions. Specific examples were employed to clarify some of the challenges and the respective performance targets. Very nice overview of status, key accomplishments, and future plans.
- Areas and challenges for the future were addressed with various projects to overcome barriers. At this point, however, there is no clear-cut solution to overcome the barriers.

- Yes. All sub-program accomplishments as well as gaps and challenges have been clearly stated in order to guide R&D activities as well as Tech Team activities.
- Yes, the targets and what is needed to reach them were well covered. The presenter also noted that the targets were often misused as material targets and emphasized that they were system targets.
- Yes. In particular, the Centers of Excellence will start to make things gel in terms of unequivocally meeting at least the 2010 “system” goals.
- Problems and issues well summarized, in general. The on-board refueling time problem for solid media (heat rejection) was not addressed. Safety was not addressed. Timetables give the R&D community what is expected for success. Go/no-go decisions are important.
- Addressed "system" well. Showed where funding will concentrate. Well done. Must continue to stress systems issue and how PI's must consider all characteristics in their material discovery.
- Displayed and highlighted system issues of materials well. Energies of three classes were explained well. LHV [lower heating value] is confusing. What is the defining line between hydrogen storage EERE research and BES research? Many look the same.
- Good concise explanation of the thinking behind the targets. Discussion of 2005 versus 2007 [targets] seemed a bit confusing. Said that 2005 targets were very close to being achieved with compressed and liquid storage. However, on “status” slide, the numbers do not seem to back up this statement: 0.5 and 0.8 kWh/L for 350 and 700 bar, compared with the 2005 target of 1.2 kWh/L. Also, it does not appear that compressed is anywhere near the 2005 cost target either.
- For the most part, yes. It is important to re-visit the magnitude of the “challenge” and why it is called "Grand." It is also important to stress a result-oriented program and PI accountability.

**Does the Sub-Program area appear to be focused, managed well, and effective in addressing the Hydrogen Program R&D needs?**

- The sub-program presents well organized and structured activities to meet Hydrogen Program R&D needs. The management appears adequate to face the day-by-day needs and to properly follow sub-program progress.
- Yes. Hydrogen storage is a critical area. DOE appears to be doing as well as can be expected to fund and manage this program area given fiscal and staffing constraints. However, concerned that as the projects move into more advanced stages, more resources at DOE will be needed to monitor and manage the projects.
- Sub-program area very well managed and coordinated. The concept of Centers of Excellence will enhance integration of efforts, collaboration, cooperation, and overall effectiveness. This area is well aligned with the Hydrogen Initiative and the EERE Multi-Year R&DD Plan.
- The Hydrogen Storage sub-program is one of the best managed efforts within the Hydrogen Program. Communication is very strong and transparent. The team is open to new ideas and processes to improve.
- Clearly covering the broad spectrum of research that is needed. Management has organized the large volume of work into centers to help administrate and coordinate. Significant improvement has occurred over the last years, which the DOE program has participated in. Connection shown to BES is desirable and appropriate. Go/no-go decisions will be the real test of the management. Continued stream of new solicitations is critical and a good aspect of program management.
- Yes. Good program management is being provided in order to guide and focus R&D activities in hydrogen storage areas.
- From the point of view of the Team Lead’s presentation, one would say yes to this question. However, after hearing most of the oral storage presentations and viewing several of the posters, I find that there are at least a few projects that are not deserving of funding, based on the fact that they either duplicate higher caliber work in other projects or are not very likely to produce meaningful results in a timely manner.
- Yes, no problems in this area.
- Appreciated the definition of BES versus EERE system distinction. Showed Tech Team outputs. The Storage and the Fuel Cell Team Leads have the best managed tech teams of all USCAR activities.
- How is funding split between Tech Teams -- if at all? Will take a few years to eliminate overlap.
- Good focus on technical targets and diverse portfolio aimed at achieving materials discovery, systems engineering, etc., to enable these targets.
- There has been significant progress and it is getting better all the time. The field and the tasks are very difficult. Considering the resources and time, yes, it is managed well.

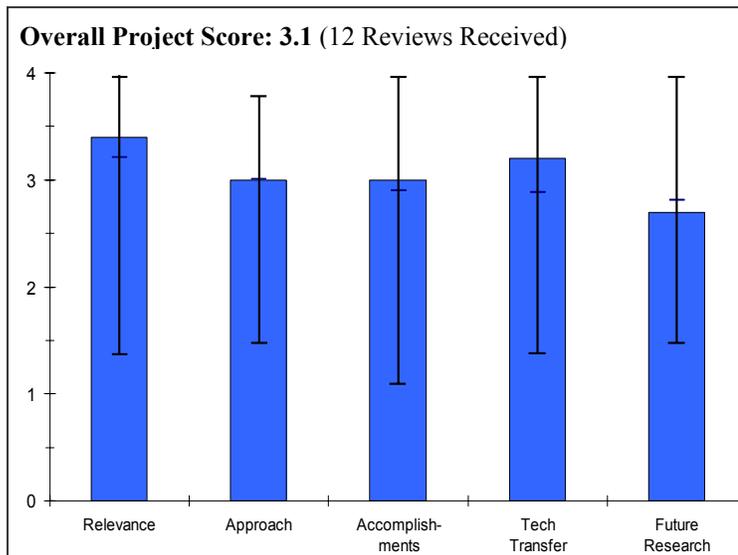
**Other comments:**

- Excellent job.
- The close interaction and synchronization with BES in funding is a welcome step.
- Team Lead appears as a strong, well-focused leader with a good vision. Team Lead is flexible enough to recognize potential and the need to redistribute funds when necessary, as stated in the presentation. Recommendations:
  - Earlier in the program, conduct analyses on possible alternative options and ‘translate’ as fast as possible, the results from materials perspective into systems performance.
  - Recommend a move from materials to system targets.
  - More emphasis should be given to testing and analysis, which is a cross-cutting enabling issue.
  - Closely follow the coordination of partners and projects under the Centers of Excellence – it could be a management challenge due to the size of the consortium and the range of research areas.
  - Investigate the impact, if any, on the program due to the incurred delays in Grand Challenge awards and possibilities of speeding-up progress.
- The DOE team assigned to this sub-program has a high level of expertise and is effective in managing their PIs.
- A difficult challenge, which needs all the funding it can get. If this is really the key hurdle, and given that the program is younger than the fuel cell effort, then one would think it would get more funding than fuel cells. This is clearly not true, and from the level of funding perspective, the management approach may be sub-optimized. While the needs of universities to maintain graduate students is clear, the idea that university programs will not be turned off makes management of these programs effectively impossible. In [DOE] BES programs, this is not a conflict, but in EERE programs it is; work that clearly is not helping reach the goals should not be funded for many years. [DOE comment: Because of the basic nature of the research, BES projects typically get three-year funding and are almost always continued through that time period. EERE projects, being applied research or demonstrations, are reviewed annually and may be terminated due to lack of progress, other Program priorities, etc.]
- The sub-program is and should remain open to really “new” ideas, given reasonable a priori gravimetric, volumetric and thermodynamic justifications. A little too much “hand waving” sometimes obscures reality. There is too much emphasis remaining on the alanates. (This opinion results from more than just the ST1 presentation.) Given the well-established weight, volume and safety shortcomings of the alanates, maybe some go/no-go gates should be considered? The Team Lead understands that alanate projects cannot be stopped on a dime, but careful future focus must be made.
- In my opinion, the strategy of having 2005, 2010, and 2015 goals is misleading. Decide on what the tangible goals should be for an economically tenable hydrogen storage system for a vehicle and orchestrate a program that works towards those goals. If, for example, the current 2015 targets are the right goals, many of the systems currently under study could be eliminated from consideration immediately by simply making a straightforward determination of the upper limit of their best possible performance level.
- UTRC sounded like task was Mg-amide based.
- BES [DOE Basic Energy Sciences] is fairly new to many of us.
- The progress and results of the previous hydrogen storage work on carbon does not seem to warrant the same level of support as in other promising areas (e.g., complex, metal, chemical hydrides). This definitely seems like a much higher-risk, more exploratory area of research. Why did DOE decide to launch an entire multi-million dollar center based on the relatively high-risk topic of carbon and other nanostructured materials?
- Need to further stress "system" targets (there could be new people, etc.). Very good job/presentation. Stress PI accountability more. For example, when a question was asked about funding or termination of an academic program, it should have been said that PIs are taking a risk and before applying for funding they need to understand it fully.

**Project # ST-02: Development of Metal Hydrides at Sandia National Laboratories***Wang, James; Sandia National Laboratories-Livermore CA***Brief Summary of Project**

Metal hydride research at Sandia National Laboratories continues to develop new high-capacity hydride materials capable of achieving at least 6 wt.% hydrogen for vehicular applications (system basis). This project review is on Sandia's work in hydrogen storage for FY05.

Sandia employs a parallel approach through work in each of the following areas: (1) Investigate new complex hydrides and other reversible hydride-based materials to achieve higher capacities; (2) Develop new synthesis and doping processes to improve both absorption/desorption kinetics and ultimate capacity; (3) Experimentally characterize the materials' properties; (4) Determine hydriding mechanisms through experimental analysis and modeling; and (5) Determine important engineering materials properties of the materials to ensure that complex hydrides are on track for eventual commercialization.



Sandia has been selected to lead the DOE Metal Hydride Center of Excellence (MHCoe), which is composed of 8 universities, 3 industrial partners and 5 other national/federal laboratories. Current materials under study for the center include advanced complex hydrides, destabilized binary hydrides, novel intermetallic hydrides, and other reversible hydride-based materials. The Center activity will be formally reviewed in FY06. This review is for FY05 work by Sandia.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.4** for its relevance to DOE objectives.

- The relevancy could be and should be higher. However, the program appears to have reached a technical stagnation plateau over the period of 2004 -2005. The scope lacks sharp definition as compared to 2004.
- The PI showed a complete spectrum of metal hydride investigations suitable for properly addressing the Hydrogen Storage Program Objectives.
- Hydrogen storage is the highest priority research area supporting the vision of hydrogen economy. Centers of excellence are important initiatives supporting development of hydrogen storage technologies.
- Project works on high [capacity] systems that are likely to be critical for potential consideration in the President's Hydrogen Fuel Initiative.
- It is not clear if this work can be successful in meeting H<sub>2</sub> storage targets. There is not explicit progress to DOE goals. The down-select process will be key to not expending scarce resources on dead-ends.
- The project objectives (as those are stated) are consistent with DOE strategies and targets. Technical barriers are stated clearly.
- These materials and systems are steps toward the 2010 target, and are most appropriate. It is suitable and beneficial that there is engineering, material, theory and experimental work together leading to potential synergy.
- This project addresses one of the two key roadblocks to a hydrogen fueled vehicle economy - H<sub>2</sub> storage. MHCoe plans give encouragement that a better organized, more comprehensive and more focused hydrogen storage program will emerge in the coming years.
- No hydrides are discussed with the potential to meet storage targets.

- Most of the materials studied within the project have relevance to meeting the targets.
- There is a good focus on high density materials. This is relevant to the area of materials discovery, since this team is studying a diversity of systems.
- Metal hydride material research is a key enabling technology to improve hydrogen storage, if [operating] temperatures are reduced to FCV [Fuel cell vehicle] waste heat levels, the system could potentially be very simple.

### **Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- The group needs to define more criteria for material selection. Look at systems modeling earlier in order to provide more valuable criteria for selecting materials to research (such as material thermal conductivity which has a large effect on tank sizing). Ammonia loss cannot be resolved through "engineering" because it is still a base material loss that will substantially affect material cycling capacity.
- Technical barriers are acknowledged but the priority to address them is not properly arranged. For instance, the approach for material discovery versus the storage system requirement (e.g., container and balance of plant for storage) is not defined. What characteristic should an ideal alloy have to achieve 2010 system targets? Wt.%? Heat of formation? Packing density? Minimum thermal conductivity? Expansion rate? Kinetics? Thermodynamics? The PI has been asked these questions in several other occasions previously and was asked again at this review meeting but failed to answer the question. This is a critical step.
- The approach addresses major scientific and technical barriers that may help to identify new and more suitable metal hydrides for on-board applications. The creation of a MHCoe is very instrumental for a complete coverage of scientific and technical barriers. The MHCoe uses adequate and complementary expertise and techniques to have a complete survey of the present and future metal hydride alternatives. The lack of quantitative objectives for the materials related to the DOE system goals may affect the project's progress and deliverable. The system engineering part is not well presented and appears not functional to meet DOE goals. The final goal of a 1-kg [hydrogen] system appears poor and not ambitious with respect to the resources. [The 1-kg hydrogen prototype system is a DOE specified deliverable.]
- Although the center is just being launched, the approach seems reasonable. There is a concern on the large number of researchers listed which only add to 6 FTEs. Question significance of each contribution when some can only spend a small fraction of their time on the project. Ought to list only the significant contributors.
- Approach includes a variety of materials characterization approaches applied to systems of interest. The nature of the choices and alternatives in the systems chosen were not explained, however relevant systems were being examined.
- Approach well thought out for research underway. Integration into Metal Hydride CoE will help this project.
- It is not clear how various approaches are being selected for the project. There was no techno-economical justification for the approaches except references to some empirical literature data. Examples: incorporation of Si and Mo - the approach appears to be "try and see what happens." Needs systematic approach to new materials discovery.
- Mix of materials experiment and engineering is good. Many processes seem to be focused on seeing how desorption behaves and then see if absorption works. This is fine since thermodynamic data do not exist; but try to define the products and calculate (or failing that test) its possible reversibility as a highest priority. Work on role of Ti is a good addition.
- Lots of people in a 6 FTE effort; task-to-task responsibility structure is not obvious. A variety of characterization methods are used in appropriate ways. I am encouraged to see nanophase materials and combinatorial methods emphasized in MHCoe.
- Good variety of tools to attack problem. Project manager needs to assure that tools are used effectively and results shared and used across program.
- Formation of  $\text{NH}_3$  in amide desorption needs even more effort than presented. Cycling weight loss not insignificant in amide, but no effort to address the issue. There is not enough effort on  $\text{AlH}_3$ . There is not enough effort on borohydride. The  $\text{NaAlH}_4$  surface catalysis model does not seem to go anywhere or fit any data. What is the significance? Some of the materials analysis experiments not very convincing in terms of stated conclusions. There are too many people on project for funding level.

- Wide-ranging approach, studying a variety of promising materials. Good to see that approach is nimble enough to quickly switch to more promising materials (e.g., the current shift towards Mg-modified amides more than Na alanate). It is not clear what next steps will be in the Mg-modified amide systems. What are the ideas to improve the thermodynamics further?

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- Although the material capacity accomplishments are decent, they are potentially misleading. Do not assume that all metal hydride systems will incur a 0.5x reduction in capacity; every material will result in varying system efficiencies. It is becoming obvious that higher storage capacities will be required in order to account for metal hydrides poor packing capacity and poor thermal conductivity.
- The progress must be measured against the amount of resources a program has received. In that respect while there is marginal and stepwise progress in some technical areas, the overall output and the results are disappointing. There was no mention of progress on some of the engineering areas that was being done last year.
- The PI summarizes excellent scientific results. The project is progressing well with respect to its objectives. The limited comparison with DOE goals makes hard, future selection and choice decisions. The results on Mg-based materials are well below the state-of-the-art and far from a possible use.
- Numerous accomplishments were cited, but none in enough detail to determine which were actually done in the prior year. PI needs to find way to allocate time to provide more in depth discussions of key technical accomplishments rather than one slide on each of over 12 technical topic areas.
- The program is aware of DOE program goals and has structured its plans in order to meet those goals. It will shift from materials R&D to storage system design in a timely manner to maximize probability of meeting program goals.
- 50% through project from time standpoint and overcoming some barriers, but how far to FreedomCAR & Fuel Partnership goals or DOE goals?
- There was no indication as to how the DOE targets can potentially be met with the approaches selected for future work. However, basic knowledge obtained up-to-date appears to be very useful for future research.
- Progress seems to have slowed since last year, but still good for 6 FTEs. Dropped desorption by 40°C, though at loss of kinetics. Characterized the material with X-ray, thermal desorption and Infra-red. Used PCT to show low NH<sub>3</sub>, but it [ammonia] is inhibited in that system. Work started on several new systems.
- Lots of work on alanates; adding Mo to borohydrides; loss of ammonia; AlH<sub>3</sub>, modified with LiH. This group utilizes theory and modeling and explains the effect of Ti addition. The presenter glossed over many of the data slides.
- Good work on NaAlH<sub>4</sub>. Materials degradation study is relevant and well done.
- Lowering of amide release temperature good result. AlH<sub>3</sub> looks promising.
- Many novel results in a variety of materials classes. Said that main focus this year was really on Mg-modified amides. However, major result (reduction of temperature upon Mg addition) seems to be similar to last year's data?

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- None indicated. Unless they are working with the same partners indicated in the MHCoe, they did not indicate that they had any partners or industry collaboration (GM aside! but that is supposed to be separate). GE was an industrial partner for manufacturing- should they not include more relevant tank suppliers for either stationary or automotive?
- There is much collaboration within national labs and outside universities. Significant progress on establishing the center of excellence.
- The coordination appears working among MHCoe members and a few external institutions. The three presentations of the PI and GE and HRL do not show good coordination because the various project parts

appear not clearly integrated. The interactions with other institutions and project involved in the DOE Sub-program are not specified.

- Broad and comprehensive.
- A broad group of external collaborators are working with the PI and his colleagues.
- Incorporation into MHCoe is good. New communication tools will be very valuable for further collaboration within this project and the MHCoe.
- Nice interaction and much more to come in the new center. I do not think this is a problem, as SNL is big enough they are effectively 'partnering' internally - they gain the benefits of other minds and equipment that partnering yields.
- The reviewed portion seems like a collection of in-house projects that the MHCoe has now incorporated into an organized/focused program with numerous substantive outside collaborations; hopefully, next year's program will show how all the pieces of the MHCoe fit together.
- Little collaboration is obvious.
- The group is having key collaborations established through center activities.
- Good collaborations; but as the Center gets kicked off, the group will need to be diligent in keeping others in the field "in the loop" in a collaborative way.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- The approach appears to be more of the same semi-empiricism deployed since 1995.
- While continuing the same work, they need to establish MHCoe partnerships and ensure more industry input. Relying on nano-synthesis as a panacea may not work. Nano-particles tend to agglomerate quickly and thus cycle data may degrade quicker than desired.
- The approach for continuing the work is clearly based on experimental deliverables and results. A well defined multi-year plan is positive in driving the work with changes suggested by results. The engineering part is too limited to favor clear material selection.
- Biggest challenge is going to be managing the center and getting the maximum value out of all the diverse subprojects listed. Will be interested in seeing results from some of the proposed projects.
- Future research plans appear reasonable.
- Continue to build on progress to date, but add effort to on-board storage module work.
- The main focus for 2005 has been stated as Mg-amides modified with Li. At the same time the goal for 2006 has been stated to be new materials discovery. Does it mean that the  $2\text{LiNH}_2 + \text{MgH}$  approach is a "no-go?" It is still not clear if the proposed future work has a good probability of success of meeting the DOE targets (needed technical justification for that to be presented).
- Although the planning seems exciting, it could benefit from a few, more precise scenario plans, for example by sticking to higher capacity systems. In some regards this is moot because the Center takes over this work.
- The plans for the MHCoe are the ones that matter here.
- Not obvious that investigator has identified plans for a systems approach? Will work be folded into Center of Excellence?
- Not evaluated because this program will roll into center work.
- Center of Excellence is main future research, and proposal is excellent. Topics for future work at Sandia are good; however, proposed plan for achieving new materials is unclear.

#### **Strengths and weaknesses**

##### Strengths

- There are many years of metal hydride experience with almost all the identified materials. The MHCoe will strengthen their research and expand their vision of materials and systems.
- Excellent technical resources and instrumentation. Experience in material science and engineering. Good collaboration.
- The MHCoe has an excellent coverage of expertise and resources. The present focus of the project is on the most promising candidates.

- There is a good technical team with good facilities.
- Breadth of characterization equipment applied to materials under investigation.
- Strong collaboration; new collaborative tools and the MHCoe will make project even stronger.
- Excellent technical expertise, instrumentation, facilities significant amount of experimental work being conducted that creates useful knowledge of the systems.
- Broad approach with significant theoretical and experimental thrusts interacting with each other. The material classes have some chance to make all goals; specific study materials could theoretically make 2010 goals. Very strong team!
- This is an institution with a lengthy history of performing metal hydride research. A seemingly solid plan for going forward with the MHCoe
- The group leverages materials strengths of national lab. They are talented researchers. They utilize outstanding facilities.
- This project has an excellent team, good research focus, and good technical results. Continue to focus on improved storage densities at desorption temperatures/pressures of interest.

#### Weaknesses

- Lack of direction from industry. OEMs need to do better job to define real system requirements and what real storage capacities of material will be required. There is a lack of good planning to identify new materials.
- There is inadequate/unclear technical approach. De-emphasis of tank and system requirement. There is low productivity. There are no clear internal targets when screening new materials.
- The material R&D is not properly driven by the DOE goals, because of the lack of clear quantitative objective on materials which are related to system performances. The project approach is not appropriate to facilitate a timely selection of materials for the scale-up and final system delivery. The system engineering is too limited and not adequate for driving activities towards DOE goals. According to the Project Plan, the new material discovery is not flexibly incorporated in the future work, as it should be. The MHCoe appears to be "a closed forum" in which possible future collaborations with new institutions, proposing new materials or solutions can be hardly incorporated.
- Concerned about ability to manage breadth of research planned under the center.
- The presentation did not present logic of materials systems choices/chosen for evaluation. It gave appearance of a survey of all work under support. While the individual efforts appear quite strong, one would wish to give lead PI opportunity to explain logic of systems chosen for further investigation and coupling between efforts supported. When asked, it was apparent that coupling could be stronger between modeling and experiment. Was informed that it would be utilizing theory better in informing choices of systems for study in the MHCoe.
- The progress toward system level targets not addressed. With 24 people working on project, the group is only accumulating 6 FTEs of time does not provide much opportunity for personal ownership by any of those involved. Research is good, but more focus on where it is leading and why, would be valuable.
- Selection of approaches is still empirical. They lack the really innovative "out-of-box" ideas. Philosophy of selection of new materials is still based on looking for known systems from literature that has low probability of success for the new materials discovery.
- 3kWh/kg system at 2.7kWh/L will require a material about 1.5x that capacity; none on the slate. That is OK for now, but some plan to get there would be nice. Concluding NH<sub>3</sub> suppression from PCT data is dangerous because NH<sub>3</sub> pressure inhibits further formation; it is TGA that shows the loss. Note that while capacity fade of LiMgN system is low, one still loses 1/2 of total capacity in 500 cycles. The D<sub>2</sub> experiments do not clearly show the H<sub>2</sub> pulls Ti to the surface.
- The published results of decades of work on metal hydride systems tend to suggest that the material of choice for meeting 2015 H<sub>2</sub> Storage system goals will not be a metal hydride. The presentation was not planned out very well for the time available; the speaker had to speed through portions of the talk near the end that I would like to have heard more about.
- It is not obvious that investigators are working as a team trying to obtain goal rather than individual PIs working on their individual programs. See next comment in this regard. There is real concern over 6 FTEs spread across 24 people. You need smaller groups to insure project ownership by investigators. FreedomCAR targets not mentioned in presentation. They should be focus of program rather than an afterthought. Still too materials focused. Need to combine with analysis to assess materials.
- Too diffuse with too many people doing different things. Materials analyses studies do not seem to be completed sufficiently to address issues and come up with solutions, mechanisms, etc.

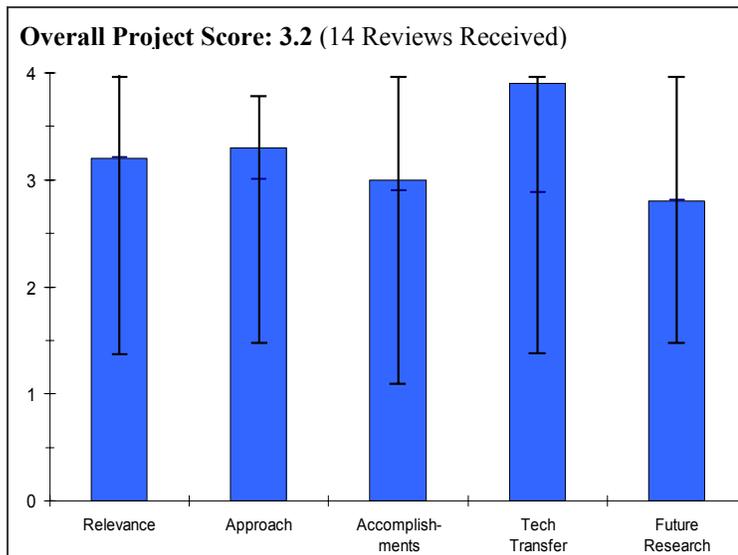
- Diversity of materials classes along with the large number of people working on this program gives the impression that coordination of effort could be improved.

### **Specific recommendations and additions or deletions to the work scope**

- Add effort to on-board storage module work.
- Look at systems modeling earlier in order to provide more valuable criteria for selecting materials to research (such as material thermal conductivity which has a large effect on tank sizing).
- Review ANL [Argonne National Lab] storage system analysis and TIAX LLC analysis to raise their material capacity goals and address thermal conductivity issues.
- The project needs to realign its work scope with the 2010 desired system outcome. Tank and system requirements need to be addressed equally and simultaneously when a material candidate is selected for further testing (for example much work has been done on sodium alanate in the past 10 years but an early overall system analysis would have been able to rule its adequacy). Material safety and its stability have to be a prime factor in screening new materials.
- The system analysis must start earlier in the plan and drive the selection of materials towards DOE goals. The MHCoE work should include also prenormative activities as a result of experimental tests on novel materials that poses safety concerns and may require specific code & standards development: e.g. sensors, testing procedures, and so on: the existence of an independent project on testing may be supported by in-house preparation work.
- Invite lead PI to make an additional presentation on program management and coordination aspects to DOE HQ staff prior to next formal peer review.
- Add system targets to presentation and status to those targets.
- Use more systematic selection of approaches. For example, it can be done by defining all properties of materials required to meet DOE targets (system basis) first. Using these properties as input parameters, conduct modeling of potential structures and compositions that can theoretically meet the system targets (if that is possible) and use combinatorial approach to try to synthesize those materials.
- Probably the addition of the Center will add more aspects that we could recommend. They seem to be trimming less productive routes voluntarily.
- In future reviews it would be good to have a prior year to current year status comparison to help gauge progress. In future MHCoE overview talks that are backed up by other poster or oral presentations, do not spend time putting up lots of data slides if there is no deeply meaningful point to be made from them - especially if other presentations will cover the same material. I suggest to the DOE staff that they allow at least 15 minutes for questioning/discussion of Center of Excellence presentations in future reviews.
- Need to present definite plans for systems analysis and approach.

**Project # ST-03: Catalytically Enhanced Hydrogen Storage Systems***Jensen, Craig; University of Hawaii***Brief Summary of Project**

The University of Hawaii is developing catalytically enhanced hydrogen storage materials capable of being used in vehicular applications. The objectives of the research are to determine the chemical nature and mechanism of the species that are responsible for the enhanced kinetics of Ti-doped NaAlH<sub>4</sub> and to apply the insights gained from fundamental studies of Ti-doped NaAlH<sub>4</sub> to the design and synthesis of hydrogen storage materials that will meet DOE hydrogen storage system targets. This project ends in FY05. New work by C. Jensen will continue within the DOE Metal Hydride Center of Excellence initiated in FY05.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- Work is aimed primarily at understanding how catalysts work on metal hydrides or alanates.
- The project is highly pertinent to the DOE's R&D goals.
- The subject matter has been investigated for many years. The current system and detailed cost data suggest that sodium alanate cannot meet the DOE objectives. There have been some limited technical side benefits which may be useful for some other materials.
- The project is fully in line with DOE goals and the President's Initiative. The project, already concluded, and started before the definition of present DOE goals, maintains high relevance for the scientific achievements and the establishment of benchmark results.
- Hydrogen storage is the highest priority research area that supports the vision of a hydrogen transportation economy. This project investigated new classes of storage materials.
- The project is in line with the program objectives. Understanding of the fundamentals of the Ti-doped alanates hydrogen cycling kinetics will assist the development of materials that can meet the DOE targets. Valuable experience has been gained and the PI has wide expertise that can benefit the work program (see Metal Hydrides Center of Excellence).
- Work is of high relevance to attainment of goals of the President's Hydrogen Fuel Initiative.
- Project was originally aimed at fundamental understanding of the effects of catalytic doping of sodium alanate phases and the effects on hydrogen adsorption-desorption kinetics. Project targets were set in 2000, i.e., before the DOE storage targets were finalized.
- While [sodium] alanate will not directly meet the goals, it is a fairly well understood surrogate with several mysteries still unexplained in the improvement of its kinetics. Understanding this material may well help us catalyze other hydrides with higher capacity, and alanate may be a component to alter other hydrogen carriers, another reason to understand it in detail.
- The group focused on dehydrating/rehydrating kinetics of Ti-doped Na-Al-H. This project has been a path-finder activity that has generated much excitement and germinated work of a related/connected nature at other institutions.
- Explained and improved performance for first potentially practical complex hydride for H<sub>2</sub> storage.

- The project is looking in great detail at the classic new generation hydride, doped sodium alanate. This was the first EERE project on the alanates and was then quite relevant to DOE objectives. Nowadays, in addition to potential safety problems, it is becoming well known that this system will not meet DOE targets, so project should soon “move on” to stay highly relevant to ultimate DOE objectives.
- The focus has been on understanding the reaction mechanisms in [titanium-doped] NaAlH<sub>4</sub>.
- Although, admittedly, NaAlH<sub>4</sub> is not the material that will achieve the DOE objectives, a good case was made for this type of fundamental studies of kinetic properties, and how that will likely impact future materials classes.

### **Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- The research group seems to be spending too much time on ball milling techniques which will be difficult to scale-up in a practical manufacturing process. Anelastic [relaxation spectroscopy] technique sounds interesting but too little time was devoted to explain method and real value.
- The project covered all the bases and effectively used partners to obtain the necessary expertise for the wide scope involved.
- This was pre-“Grand Challenge” project. The approach was not designed to meet DOE objectives. Consequently, the technical work diverged in areas with little end benefits to DOE. It was never clear if there was any systematic approach beyond traditional empiricism. In the last one and a half year, there was sign of stagnation.
- The approach focused strictly on key scientific and technical barriers. The project has opened the road to a comprehensive R&D including materials “guided” design. The study of the phenomena involved has required the integration of a variety of characterization techniques, of more general applications. The formulation of novel complex hydride has had an impact on further choices on alanates.
- Well respected research.
- The work was innovative with an exhaustive characterization task. An excellent case of fruitful collaboration, even at international level, for tackling scientific challenges. The work as such does not strictly address the technical barriers but the insights gained, will be applied in the design and synthesis of materials that may just be able to do that.
- The approach is reasonable to the objectives of the project. PI is to be complimented for searching out collaborations to supplement in-house capabilities.
- Although, not meeting the immediate hydrogen storage targets, the results provided insights to understanding of the behavior of various chemical hydride systems.
- Dr. Jensen has used a broad range of tools to investigate the actual atomic scale mechanism. He has engaged others when needed to do tasks he is not equipped to do. It would be nice to see this applied to production of higher capacity or faster kinetic material in future work.
- The approach is rather fundamental, as opposed to engineering. It is looking in detail at the doping mechanism in a multi-pronged scientific approach. Good, and hopefully this will be extendable to other complex hydrides. The extension of this effort to developing really new hydrides should be a byproduct of this alanate work. That seems to be slower in coming than I would have expected.
- For the most part, the characterization methodologies were intelligently selected and applied. Important issues concerning hydrogen storage are being addressed in a fundamental way - the science component is strong.
- Good mix of experimental and computational techniques. Went outside Univ. of Hawaii to get the job done when needed! Good! Both practical work (improved doping, cycling) and fundamental (mechanism, computation) were conducted. Not much said about safety. Assume that it is okay, but DOE needs to audit sometime during grant period.
- The group used a large array of solid state methods to apply to understanding alanate behavior.
- Assembled a good team of scientists with a diverse set of experimental skills and techniques.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- PI did not provide clear evidence that catalysis mechanism has been fully understood. Two year debates of mechanism remain other than rather obvious proposed phenomena of bulk substitution has been eliminated.
- Solid results were obtained that furthered the knowledge upon which we can now build.
- It was not clear if the PI answered the questions that the PI raised last year. The scientific conclusions appeared rudimentary. There is a higher expectation of the PI based on his previous work and accomplishments in the field. The conclusion of this project was disappointing. DOE should review the ways to increase benefits from projects that are expiring.
- The presentation shows significant progress (compared with 2004 results) in complex hydride development and experimental work.
- Although technology does not meet the current hydrogen storage goals, it had the capability of meeting the goals that existed when the project was started. Gained important knowledge of new classes of materials.
- Lots of data and a large amount of information have been collected in a cost effective manner, using different characterization techniques. As a result of this work there is now better understanding of the material behavior but rather slow progress toward a system engineering solution.
- Presentation emphasized results from prior year efforts shortchanging presentation of current efforts. This may be a miscalculation based on poor presentation choices by PI.
- Provided understanding and mechanism of the effects of catalytic doping of sodium alanate on structure and kinetics.
- Good progress in identifying state of titanium [catalyst]. Illustrating the fact the Ti changes state for several cycles is of significant interest. Essentially the fate of Ti is largely pinned down now. Effect of milling is more than size; it is defects. The analytic measurements are not very clear from the presentation but may be quite useful. No update on the advanced materials mentioned last year, had anticipated a year would be enough to reproduce that.
- Diffraction studies probed (1) lattice distortion due to ball milling and (2) pertinent structural transformations during cycling. The speaker had to rush through discussion of the most recent results, e.g., anelastic [relaxation spectroscopy] studies that reveal an interesting and possibly significant point defect structure.
- Improved doping methodology. Established long-term behavior.
- Outstanding progress development of mechanistic understandings of the doping process. Last year it was mentioned that the understandings derived from this project have resulted (theoretical or experimentally?) in a secret new 7 wt.% hydride. I would have liked to see a little more on this possibility this year.
- The group completed a large number of studies, but a model is still not defined.
- Progress made on elucidating where the majority of the Ti is in the microstructure. However, also showed that perhaps that is the wrong question to ask (i.e., that it may well be the minority Ti that is crucial). Disappointing that, despite many years' effort, and extensive list of collaborators, that the role of Ti in enhancing the kinetics of NaAlH<sub>4</sub> remains largely a mystery.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.9** for technology transfer and collaboration.

- PI is involved with all the appropriate partners and MHCoe. Evidence of PI involvement is obvious in many other presentations and posters in DOE programs.
- Excellent collaborations with a large number of partners.
- The PI has established a large network and collaborates with many groups.
- Apart from the consultation to other projects (UTRC and UOP) and national collaborations, the PI has created an outstanding network of active collaborations with Norway, Italy and Japan, which added, at no cost for the Sub-program, important experimental results.
- There is a broad network of collaborators; that is well respected.
- Excellent, highly effective collaboration record and great use of resources.

- Collaborations are incredibly strong on this effort both nationally and internationally. PI is to be complimented for his interactions around the world. PI also consults with two domestic commercial concerns and collaborates with a third.
- Excellent collaboration with academic and industrial partners around the world.
- A model of how collaboration can help a program.
- Many well-considered and substantive collaborations.
- Good work leveraging in areas where Univ. of Hawaii did not have the needed tools.
- Excellent national and international collaborations in a wide spectrum of scientific disciplines. There is probably no better example of this in the entire EERE storage program. Good opportunities for tech transfer.
- The group has put together a very good team of materials scientists from around the world.
- Excellent. Prof. Jensen is basically working with just about everyone in the field of sodium alanates, including collaborations in Europe and Japan.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- PI does not have any future work; involvement with COE is unclear at this point. [C. Jensen/Univ. of Hawaii is a member of the DOE Metal Hydride Center of Excellence; work has started in FY05.]
- The group will be continuing with the DOE Metal Hydride Center of Excellence.
- What has been learned? How can these learnings be applied to new alloys? Or can they at all? As part of the formal closure of this project, it would be imperative to do a comprehensive look-back and determine short-falls and strengths.
- The prosecution of work fully relies on previous results and aims at reducing key technical barriers. The new research work is already funded and started in 2005 on a reasonable timeframe and with acceptable objectives.
- Current project wrapping up. Future work part of the DOE metal hydride center of excellence.
- The experience gained in this project will be valuable for the tailored design of binary hydrides with improved hydrogen cycling kinetics able to meet the storage system requirements.
- PI gave short shrift to description of future plans in presentation preferring to emphasize prior year accomplishments.
- Future work under Center of Excellence will benefit from the results of this project.
- Generally good plans though it would be preferable to close out the NaAlH<sub>4</sub> work sooner and move on to more attractive systems.
- Future plans are extensive; for the most part they seem appropriate. Hawaii will become part of the DOE MHCoe [Metal Hydride Center of Excellence].
- This is not really relevant since the project is over [in FY05].
- Perhaps a little too much on tying up loose scientific details over applying what has been learned so far to new hydrides. The group should focus strongly on the 7% material.
- Still focused on alanate.
- Will be a good addition to the DOE Center on metal hydrides, which should be an excellent team.

### **Strengths and weaknesses**

#### Strengths

- PI seems to understand several metal hydride systems and progress of other PIs without being biased to his own work.
- The group had excellent scientific know-how. There was extensive collaboration even on an international level. The group effectively used their resources.
- Depth of experience and knowledge of the PI in the field.
- The prior work, the experimental results, and the strong research network with national and international partners are a patrimony that must be well integrated in the new project in the DOE MHCoe. The scientific and technical know-how and the resources are more than adequate to carry out the assigned work.
- Good findings regarding effects of titanium which can be applicable to other systems and projects. Appropriate characterization techniques have been found with convincing interpretation of the results.

- Great network effectively used to study the problem.
- The principal investigator has engaged in substantive collaborations to probe mechanisms using the most advanced/appropriate characterization methods available (in most cases). This particular group has lots of momentum in the hydrogen storage community; other projects have built upon findings/knowledge from the Hawaii effort.
- An excellent scientific basis to the project with equally excellent national and international collaborations. Impressive publication and presentation lists.
- Good fundamental approach. This was well executed. Leveraged through collaboration.

#### Weaknesses

- Continuation of effort to characterize materials that do not have the ability to meet DOE goals. PI was unable to elucidate how fundamental  $\text{TiCl}_3$  catalysts will transfer to future materials. It is not clear that  $\text{TiCl}_3$  or similar structured catalysts will become the catalyst of choice in future systems. PI must do more to convince community that this work has basis in future material systems (non alanate based).
- The biggest problem with sodium alanate is that the alloy can not meet the targets.
- Some collaboration is based on voluntary and scientific agreements, which may not be necessarily available in project planning and in future work.
- PI spent too much time early on in his presentation with background material (acknowledging collaborators, discussing approach, etc.) that left too little time for the important technical discussions later. PI had to rush through valuable technical details and never fully explained theory or results in latter slides. PI should be encouraged to exercise more discipline and to more thoroughly rehearse.
- There is no system-based data and no cost information available.
- The project was focused on the material that would not meet DOE targets. Still, a comprehensive concept of the catalytic effects has not been fully developed.
- Time to move on from the  $\text{NaAlH}_4$  work even if not every aspect is fully settled.
- The published results of decades of work on metal hydride systems tend to suggest that the material of choice for meeting 2015  $\text{H}_2$  storage system goals will not be a metal hydride. The presentation was not planned out very well for the time available; the speaker had to speed through portions of the talk near the end that I would like to have heard more about; over 30 slides for a 20 minute presentation is too many.
- Not always able to relate large number of experimental results to material performance. Lots of correlations, not sure which were really relevant (causes vs. effects).
- Practical implications for future hydride design (as derived from past results) not clear (or at least not disclosed). Are the industrial collaborations (UOP, GE, UT) inhibiting full and open disclosure?
- The research needs to extend beyond sodium alanate.
- PI wasted too much time on the names of collaborators. Missed too much technical content near end of presentation. Please have PI only touch on acknowledgements near end of presentation.

#### Specific recommendations and additions or deletions to the work scope

- The project is expiring but the lessons learned here must be applied in the future projects. Considering the resources, the PI has done an outstanding job.
- The indication of better quantified targets for materials in the new project would be functional in selecting materials and clarifying the real possibility for storage applications of alanates. The addition of longer cycle life test will allow for a more complete evaluation of the alanate and complex hydrides possibilities.
- Consider transferring material data and results to system level. That will be a valuable contribution to the Program. As a future undertaking and possibly under the Center of Excellence Project, investigate cost.
- Project is complete now.
- Optimally the  $\text{NaAlH}_4$  work would be moved to general catalysis of advanced hydrides under DOE BES [Basic Energy Sciences]. This would allow Dr. Jensen to use what he has learned here to create new higher capacity material. The center as a whole needs to move past sodium alanate. DOE BES could fund working out the last iota of understanding.

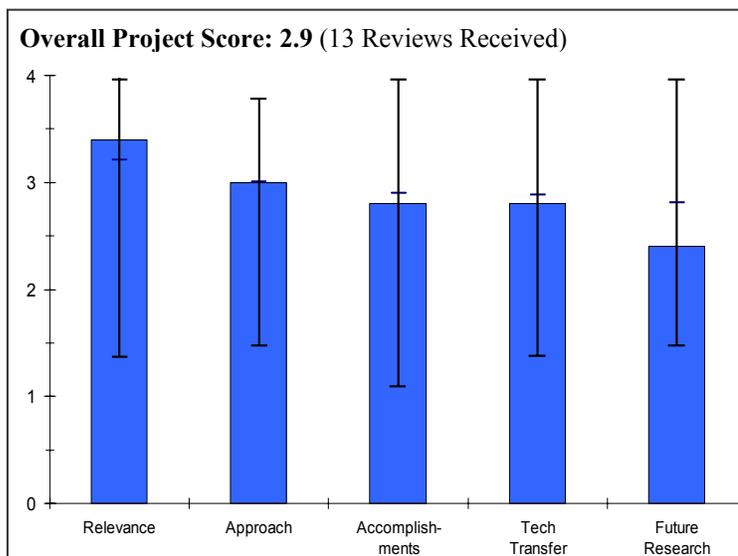
- For future reviews, prepare a prior year to current year progress comparison to help gauge performance in the budget year. Limit the slides to only the most compelling results; make sure to leave sufficient time for all compulsory details. I suggest to the DOE staff that they allow at least 10 minutes for discussion of individual project presentations in future reviews.
- Is there relevant information in the fundamental work on Ziegler-Natta catalysis done over the last 40 years?
- In the next year, project should develop matrix of likely systems to which sodium alanate results and principles may likely be extended (e.g., amides, borohydrides,  $\text{AlH}_3$ , others?). What are the possible materials and paths to get to the 2010 DOE targets by 2010?
- For future work, many of the proposed activities are very similar to the previous DOE project on  $\text{NaAlH}_4$  (e.g. location of Ti species, elucidation of role of Ti, determination of thermodynamics). These activities have been largely studied by Prof. Jensen over the past several years, and more work is unlikely to produce qualitatively new key insights. Recommend to remove these activities from the future plan in favor of the fourth bulleted item: to prepare new thermodynamically tuned materials.

## Project # ST-04: High Density Hydrogen Storage System Demonstration Using NaAlH<sub>4</sub> Complex Compound Hydrides

Anton, Don; United Technologies Research Center

### Brief Summary of Project

United Technologies Research Center (UTRC) is working to design, develop, and evaluate a prototype in-situ rechargeable hydrogen storage system initially employing NaAlH<sub>4</sub>-based complex hydrides, but capable of using any endothermically discharging hydride media. The hydrogen storage system performance will be suitable for a PEM fuel cell powered mid-size automobile application. UTRC's approach is to develop improved sodium alanate-based materials and to design and fabricate 1-kg hydrogen systems for initial testing. UTRC will attempt the following: to improve the hydrogen charging and discharging rates of the NaAlH<sub>4</sub>-based materials to meet steady-state PEM fuel cell demand; to increase the charging rates to achieve the five-minute refill requirement; and to increase the reversible weight fraction of hydrogen stored up to the theoretical maximum of 5.5%, through enhanced catalyst compositions and processing techniques. If other suitable high capacity hydride systems become available during this effort, every effort will be made to incorporate them into this prototype system. UTRC will also determine the safety and risk factors associated with the enhanced material compositions.



### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- At some point, real system tanks need to be built to truly understand the system requirements of metal hydride storage systems on vehicular levels.
- The relevance of this project should have been much higher, had the PI decided on a more effective approach. The value of this program is diminished primarily by the tank design.
- The system development is highly relevant to the DOE goals and the President's Initiative. The PI clearly presents the specific and general advantages to develop a flexible system design and a storage device applicable to any reversible material.
- Hydrogen storage is the highest priority research area supporting vision of hydrogen economy. This project explores an important technological approach that may prove to be a practical storage media, even if it does not meet all the targets.
- Work is of high relevance to objectives of the President's Hydrogen Fuel Initiative.
- Important research, focused on system level targets. While NaAlH<sub>4</sub> may not achieve goals, it is working towards system level targets.
- Objective is not directly associated with meeting DOE targets on storage system; it puts system design ahead of the development of basic storage medium. It can be considered as a model to elucidate potential barriers towards system development. The concept still supports the plan objectives.
- Objective is to build and analyze a flexible prototype low pressure/high density hydrogen storage system. Highly relevant to HFCIT hydrogen storage system development; much is getting learned about the development and testing of such systems that will benefit those who follow the storage system RD&D trail.
- Highly relevant as the tank would serve other metal hydrides, which have a chance to meet goals. Learn about making large batches of material and how it differs from the sub gram experience.

- First publicly accessible information on a practical complex hydride storage system. Identified problems going from gram to kilogram scale. Won't meet DOE goals.
- The project provides much needed engineering data on alanate beds, data obviously capable of extension to other (future) hydride systems. This approach is important to the HFCIT program and it fits very nicely within the plan.
- Important to study system issues related to fabricating solid state storage systems.
- This type of system design is very important to have in the DOE portfolio, as the lessons learned will be applicable to emerging materials classes. Currently, only project in DOE to focus on this type of system construction.

### **Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- PI has taken the appropriate steps in construction of the vessel and even left packing options open. The PI should have taken into consideration more of the [FreedomCAR and Fuel hydrogen storage] tech team requirements such as min/max flow rate of 1.6g/s. Failure to realize the sensitivity of this requirement will likely lead to an undersized system or lower than expected "usable" capacity of the system. PI should also pay more attention to manufacturing production techniques and attempt to address some of these issues such as [vessel?] structure and packing methods in this program.
- Identifying and documenting the technical barriers that have surfaced will be the greatest contribution of this project to the entire DOE storage program. Because of the proprietary issues, it is not clear how the information will be shared with rest of the scientific community. The specific design of the current tank is not scaleable.
- The approach is reasonable and adequate to face material, system and safety issues.
- Good solid technical approach recognizing that the technology is unlikely to meet the current hydrogen storage targets.
- Approach is generally well thought out however, the project could have looked at a broader array of potential designs for storage systems or presented results of decision analysis that led to this particular design.
- Project well conceived to achieve goals; though it is not clear if barriers can be overcome.
- Comprehensive approach including majority of potential issues in the design of storage vessel. May not be flexible enough to accommodate newest material developments.
- Use of theory and science to guide engineering is highly appropriate. The use of a large cap and then approximating the metrics of the 'real' system without that cap is sub-optimal for demonstration.
- Made some mistakes and some mid-course corrections; hindsight is 20-20. The overall approach is both pioneering and sensible.
- Good safety. Good systems modeling. The group addressed unanticipated problems well.
- The approach is sharply focused on engineering approaches and practical data generation. Logical and very well executed so far.
- The group focused on variations of basic design. It would be valuable to look at other designs.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- The tank is nearly complete. PI did not report actual final built specifications clearly. Estimated improvements in future systems that can be made by "minor tweaks" are unlikely; - often 3 to 4 times improvement is required which will not be achieved by minor tweaks or engineering solutions.
- The key factors here are: the gravimetric/volumetric storage of the system, heat and mass transfer, and pressure vessel stability. None is promising at this point. No innovative solution has been offered for powder packing and densification. Only when there is a viable engineering solution for removing the stainless steel end cap and the cooling/heating manifold, the cap's weight credit (i.e., reduction from the system weight) should be applied. If this is proprietary information, DOE should appropriately evaluate the technical feasibility.
- The progress of the project appears in line with the schedule and the expectations even if the experimental results are not completely presented. The PI does not specifically emphasize the development of specific test protocols.

- Project was initiated to meet old technical goals and has made good progress toward those goals, but cannot meet present goals. May be harder to ramp up and engineer the way from current status to the volumetric goals than the PI expects. Question viability of next generation prototype to meet targets -- conventional finned heat exchanger may add too much weight and volume, moving system even further from volumetric% and mass% targets.
- Progress has been quite reasonable.
- Although system can not meet targets with current material (NaAlH<sub>4</sub>), it is advancing system level understanding.
- Project appears to be aimed at identifying potential barriers of storage vessel design rather than at overcoming them. Upscale prototype system has been demonstrated, however, it did not get even close to meeting DOE targets (those are actually stated as technical barriers).
- Built and loaded the vessel. Learned many of the problems in creating material in bulk and loading a tank. Over optimistic on volume target being near.
- Much learned; gravimetric system metric is ca. 50% hydrogen; established many other useful metrics. The system projection chart has great utility; it should be treated as a work in progress and continuously updated. Good technical progress with system assembly and testing.
- Has shown likely parameters for real system: weight, volume, complexity. How about projected cost? Identified tradeoffs involved with charge time and system mass/volume.
- Plan followed very well. I would have liked to see a little more on the potential safety problems. Any new data since last year? Very good engineering data generated so far. Good scale-up data on various catalyst mixing techniques.
- Completed fabrication and made measurements on the bed. Made good progress on processing alanate material for packing into bed.
- Good progress and lessons learned through the course of putting together this project. Projections for future system design seem overly optimistic. Said that volumetric goals are easily achievable with small modifications; however, are currently a factor of 3 below the 2007 volumetric goal (11.7 vs. 36), and even the modified system #1.1 and #2 don't achieve the 2007 goal.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.8** for technology transfer and collaboration.

- PI is conducting project independently. More communication with ANL [Argonne National Laboratory] and TIAX LLC and their modeling work will substantially improve results of this project. Lack of collaboration is evident by lack of attention to resolve all of DOE targets and practical build techniques.
- There are little interactions on the key issues related to the vessel design and powder packing.
- The role of collaboration in the project is not well described. The interaction with the MHCoe may be usefully developed.
- Good mix of industry & academia. Seems to have the right collaborators.
- The level of technology transfer and details of collaborations could have been clearer. Impression left that coordination and collaboration could be improved.
- Stay connected with Metal Hydride CoE work.
- Working with several outside groups to enhance the program. They really need to publish more of the details to count as transfer.
- Well considered partners; collaborations seem to be effectively interfaced and coordinated.
- Good with partners. Not a lot outside of those. Partners appear to have been well selected for tasks.
- Many good collaborations, but more international connections might be advantageous. I get the feeling corporate IP concerns may be limiting collaboration and tech transfer a little.
- Assembled good team.
- Key to communicate lessons learned in this project to the external community; not clear that the communication to the community is open enough to enable all to learn from this work.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.4** for proposed future work.

- Not much time is left in this project. PI did not seem to address dynamic performance of this tank or how it will be integrated into a fuel cell system - if at all! [Integration of the storage tank with the fuel cell power plant was not part of the scope of work.] PI does not seem open to reveal testing results or list of build issues. [Some methods were considered proprietary, for example, material-fill methods. Only public information was presented at the Merit Review and Peer Evaluation Meeting.]
- It is not clear what the future steps are, especially in face of the significant technical barriers that the project has encountered. For example, the PI stated that the aluminum foam will be replaced by finned tubes. While this will solve some problems, the ANL analyses work showed a potential major heat transfer penalty. This may also adversely affect the powder densification and containment problem.
- The PI shows the expected design improvements and the future steps. There is no indication of a possible testing plan to be performed on the final prototype and their effective duration.
- Plans seem reasonable and a logical extension of past work. Will be interested to see how close the new design iteration comes to meeting program targets compared to current design.
- Good effort as far as it goes.
- Second prototype proposal to address cost and adaptability is good future approach.
- Future work is planned towards the improvements of primarily gravimetric characteristics of existing prototype without considering other potential storage media that would be closer to the targets.
- Improved heat transfer is good idea. Basically, on the right track. Need to do response work, how does the thing respond in transients.
- Sensible plan for future work that follows logically from what has been learned/achieved so far.
- Is manufacturing for double hemisphere tank simple enough to be realistic?
- PI admits the Na alanates will not meet the 2010 DOE goals. Maybe it is time to move beyond the alanates into newer systems with more potential (borohydrides,  $\text{AlH}_3$ , amides, etc.)? The engineering data thus far generated should apply to other systems?
- Relatively narrow extension of existing system design.
- The prospects for improving the system design and performance characteristics are not clearly explained, and the numbers seem overly optimistic. Really need to give actual numbers for the built system, rather than projections of the system. How much does the system weigh, how much volume does it take up and how much hydrogen comes out? Would be very valuable to give measured data of hydrogen output, i.e., rates of discharge and charge as a function of filling.

**Strengths and weaknesses****Strengths**

- Ability to build the system in a timely and safe manner. PI has exercised careful and diligent attention to safety.
- UTRC experience and knowledge. Capabilities and resources.
- The system engineering approach may be the reference point for the Subprogram for better addressing material requirement. The project has set up expertise and facility for complete system testing.
- Important component of the Initiative. This project is to be complimented as to begin to address scale-up problems early in the game even though final material is not known.
- Good presentation with fair portrayal of project's strengths and weaknesses. Focusing on system level targets is important.
- Identifying potential barriers towards the development of storage vessels based on metal hydrides, and generating knowledge and experience in this area. Good focus on safety issues.
- Learning what difficulties lay ahead for making large systems.
- A strong team with the right mix of capabilities. Producing results that give confidence of eventual success in meeting HFCIT H-storage system manufacturing goals (but not necessarily H-storage targets).
- Systems approach. Strong safety emphasis.
- A sound and excellent engineering approach this is much needed.

- Comprehensive project covering all aspects of solid state storage system fabrication. Good combination of modeling and hardware.

#### Weaknesses

- The project should share information generated publicly as much as possible (within the restrictions of company IP) to prevent unnecessary and expensive duplication. The reviewer's opinion is that this system likely has no chance of commercial success in the automotive industry and that this endeavor is not the first of its kind. The reviewer's opinion is that not all the challenges are resolvable with engineering solutions. The reviewer does not believe that resolving the poor flow rate issues of this system can be resolved with engineering solutions and still maintain adequate usable capacity or range in a vehicle; it is a materials characteristics issue.
- Lack of flexibility. Have not dealt well with the technical challenges.
- The collaboration with MHCoe and other projects should be enlarged to give better support and basic information to better define basic material requirements. The development of testing protocol may be made functional to develop standards and carry out prenormative research work on specific aspects: e.g. safety, sensors, and duty cycles.
- System Projections slide is overly optimistic that all the planets will align to achieve the system projections in right most column. All the listed actions are required to get there: not a trivial task.
- Could have looked at a broader range of systems. Could have explained design criteria better and rationales for choices.
- Current compound [NaAlH<sub>4</sub>] is not capable of meeting goals.
- Design is based on sodium alanate that will not meet DOE targets. Lack of projected cost estimates and comparative data with other developers.
- Plan did not allow for making the actual designed vessel (needed large heavy end). Density used was low, would have been better to figure out how to densify. Still have not given the simplest number, what they actually accomplished. They assume a lighter larger vessel in the calculations of mass and volume efficiency.
- I wish this team was working on a hydrogen storage material that was something other than a metal hydride.
- Focused on one bed design concept.

#### Specific recommendations and additions or deletions to the work scope

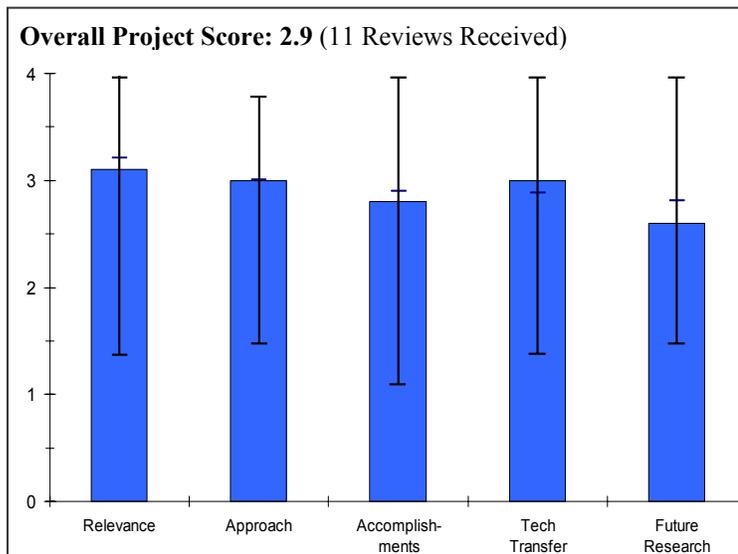
- Similar work could have perhaps been accomplished by integrating existing Ovonic metal hydride tank or approaching ChevronTexaco or DaimlerChrysler or SRNL [Savannah River National Laboratory] for a much cheaper rate. It is becoming evident that alanate systems will not perform any better than established and perhaps safer LaNi based systems such as Ovonic. It is reasonably safe to assume that all metal hydride systems will perform dynamically similar to each other, further efforts to build tanks is not necessary until a much improved capacity material is available.
- This is one of the most difficult engineering projects in the program. The team should be commended for their hard work and diligence. The current data indicate that the project will miss its target but there are valuable lessons in this work. An important task is to document the failures and lessons learned. It is highly recommended that DOE add a specific scope to quickly capture these items. There are tremendous values in these early experiences that can help the entire program.
- The addition of a preliminary testing protocol and its experimental validation would be beneficial and useful for the work in the Testing Group.
- Broader range of powders, catastrophic failures such that we are better aware of safety design issues.
- Put some focus on more promising storage materials in order to be closer to targets. Create more innovative engineering solutions such as main port design, etc.
- Again - publish details, this is unlikely to ever go on a vehicle in this form. Really, really, need to do transient testing and several different states of charge.
- Forget the 2010 targets for hydrogen storage, start working towards meeting the 2015 targets--the applicable storage system details could change considerably--it would be a shame to waste good engineering work on dead-end materials. For future reviews prepare a prior year to current year progress comparison to help gauge performance in the budget year.
- Might be useful to publish "lessons learned" explaining what the crucial parameters are for future workers, i.e., materials packing, changing rate tradeoffs, etc. Determine and report quantitative tradeoff between charge time and system weight/volume.

**Project # ST-05: Discovery of Novel Complex Metal Hydrides for Hydrogen Storage through Molecular Modeling and Combinatorial Methods**

*Lesch, David (PI); Sachtler, Adriaan presenting; UOP*

**Brief Summary of Project**

The objective of the UOP project is to discover novel complex metal hydrides to enable a hydrogen storage system that can reversibly desorb 6 wt.% or more of hydrogen between -30 and 100°C. UOP is applying methods of combinatorial chemistry and molecular modeling to discover materials with optimum thermodynamics and kinetics for on-board hydrogen storage. Virtual high-throughput screening will be used to screen complex hydrides to find materials which could meet the DOE system requirements and focus the synthesis effort on making the most promising materials. Even more importantly, the coupling of combinatorial experiments with molecular modeling of structural and thermodynamic properties will provide insights into the underlying mechanisms of action in these complex materials, permitting the design of hydrogen storage materials which would never have been envisioned otherwise.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- PI is investigating hybrid approach to ternary metal hydrides. Developing modeling techniques to identify potential good candidates.
- The project appears to fit well with DOE's goals and objectives.
- The project is relevant to the DOE Subprogram because it addresses specific requirements in the specific sector of complex hydrides.
- This is a good effort in its relevance. The work is a necessary component of the overall program considering systems that should be considered yet not highly likely to be strong candidates for actual application.
- Project scope and objectives fit well with the DOE vision and targets.
- Good set of materials with the possibility of meeting goals, if they work.
- This project does align with RD&D goals in the key area of hydrogen storage but seems locked into one storage material type [alanates].
- No materials close to targets. Relevance could rise if right material found.
- The effort actively seeks the new hydrides need for the HFCIT multiyear plan. It fits the goals and objectives of the plan.
- Materials being studied relevant to program targets.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- PI conducted modeling to quickly sweep combinations and eliminate poor candidates. PI started from hydrated and dehydrated states to evaluate if end products were the same – good. Why did PI synthesize some components that were thought to be uninteresting?

- The approach seems reasonable to achieve the project goals. It is highly focused on the material discovery process.
- It is not clear what elimination process was chosen to narrow down the field of search beyond the rudimentary storage capacity. For example, how do the PIs view the heat of formation effect? How about the packing properties? Or in general, system effects? There have been some well established criteria on what properties a workable metal hydride must have.
- The approach is interesting and reasonable because it combines theoretical analysis (modeling) and combinatorial methods to prepare and select new materials. The PI clearly presents the method applied for fast experimental screening of a variety of material compositions.
- Again, the approach would be better if there was a better explained theoretical basis for this choice of systems to be investigated. Appears to be a more brute force approach to the problem. A more intelligent or coupled theory approach might lead to the choice of other systems for investigation. Presumably with the collaborations with Ford and UCLA this should be present, yet it was not adequately presented.
- The approach involves systematic studies of alanate-based systems assisted with molecular modeling.
- Combinatorial approach is appropriate. Theory guidance will enhance chances of a discovery that meets goals. There is need for a wider scope however, while the 3 materials chosen are good ones, there is nowhere near the breadth of scope normally used in combinatorial tests by making many libraries. New approach with more elements is more appropriate. They have started with hydrided and dehydrided forms which is a good approach.
- The combinatorial/modeling approach is being applied in what seems to be an effective manner; FY 2005 results are encouraging in the sense of verifying the methodology.
- VHTS good approach. High level QM not fast enough for screening. Combisystem impressive.
- The approach is high throughput combinatorial modeling and experimental validation. It is an approach well worth trying, combining efficient experimentation strategies and predictive first principles.
- Rapid screening approach has some advantages over other methods.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Results have been disappointing - as predicted by modeling; at least modeling is partially validated. Potentially interesting compounds proved unfruitful- disappointing.
- Approach appears to be validated with the results obtained so far.
- Difficult to evaluate as it is started several months ago. [The project has been running since ~May, 2004.]
- The main achievements are well in line with the schedule. The screening protocol appears well designed and effective in selecting materials. The PI should give more details about the experimental results.
- Solid, significant progress is being made.
- Even if results are negative so far (in terms of finding a materials that meets DOE targets), the project still helps build a good knowledge database in the area of alanates, and helps move forward towards discoveries of novel systems in other areas of storage materials.
- Showed the reproducibility of method. Completed testing of Mg, Li Na system based on 3 substances chosen. Figured out what was forming and why the results were so much lower than expected. Started doing elemental (dehydrided) synthesis with a broader range of materials. Started virtual screening. Showed that they could measure multiple storage materials at once.
- FY 2005 results suggest that the project is capable of meeting its long term goals, i.e., identification/optimization/verification of H-storage material compositions in relation to HFCIT RD&D targets--the concern is about whether any metal hydrides can meet 2015 targets.
- Good work on Li, Na, and Mg phase diagram work. Systematic study was needed--even if it did not show great materials.
- A reasonable start for the first year, showing the basic utility of the combinatorial approach. But few unexpected or promising results. Give the effort its due course of time.
- Completed first matrix of material combinations. No winners found.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- Contributions by partners were not described in the presentation.
- There are adequate amount of interactions.
- The collaboration in the project is not well presented. The possibility of further collaborations with other projects and the MHCoe is not envisaged.
- Collaborations with prominent modelers briefly described. Individual contributions to collaborative effort could have been presented in greater detail.
- Already a collaborative team.
- I assume that all the listed team members are making contributions on a regular basis. However, it is not obvious from the presentation who is doing what, in all cases. The benefits of adopting H2C methods are apparent.
- Good interactions with partners.
- The collaborations seem to be more than good, and mix varied expertise quite well.
- Limited team assembled.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.6** for proposed future work.

- PI is working down list of heavier elements - seems desperate and lacks vision to move on to other systems - contractual obligations aside. Some of heavier elements may yet produce good results as they produce double the hydrogen bond sites.
- The approach encompasses the future research by ramping up the number of samples that are tested. This should result in an efficient process to identify promising materials.
- It is a mix of newer modeling work with more traditional approach.
- The description of the future activities is vague and uncertain even on the work on new materials (written "if needed").
- Expansion of approach to include work on amides & destabilization of hydrides is to be encouraged as appropriate.
- There is no technical justification provided for including additional elements (Ca, K) in the composition for future HT and modeling experiments.
- Broadened elemental scope and testing at higher rate, plus 1000 virtual tests/ month are all good ideas.
- The future plans follow the charter for this project and do make sense in the context of what has been accomplished/learned so far.
- Given lack of positive results in systems studied thus far, should work move to new systems? New HT system encouraging. What will new bottleneck be? Testing?
- Reasonable. Hard to call "outstanding" with pregnant potential. Obviously investigators need to get beyond Na-Li-Mg pseudo-ternary systems. Results so far are not very promising. Is there some possible overlap with ST6 (UTRC) that should be coordinated or avoided?
- Straightforward continuation of work.

**Strengths and weaknesses****Strengths**

- UOP is quickly eliminating poor candidates and working with OEM that understands true requirements of the system. PI developed consistent and effective method to test samples concurrently.
- Experienced and knowledgeable people. Access to resources. Good collaboration.
- The effective use of molecular modeling and combinatorial approach may be useful in accelerating synthesis and selection of a large variety of materials.
- Systematic approach to new materials discovery assisted with molecular modeling.
- Theory guided combinatorial testing.

- The combinatorial synthesis/characterization approach seems to work even though it has not pointed to a new/improved composition for the Li-Mg-Na/AlH<sub>4</sub> system (unfortunately, I suspect this will be the case for all the metal hydride systems).
- Strong synthesis/testing capabilities. High throughput screening methods.
- The first systematic modeling/combinatorial approach within the HFCIT program.

#### Weaknesses

- PI did not demonstrate how models will be improved from recent round of results.
- Unclear alloy vetting selection/rejection process. Need to start considering storage system needs when an alloy is being evaluated for further work.
- The PI does not show clear future work and adequate experimental activities. The collaborations are limited.
- Empirical addition of new elements in the matrix (K, Ca) that dramatically increases the number of experiments but does not increase probability of success overall.
- Restricted systems tested so far. Troubled by not revealing all materials, hard to appraise the work if we can not see it.
- This project seems to be locked into metal hydrides [current scope of work with DOE]; the combi/modeling effort might better serve other storage material types in the longer term.
- Relies too heavily on the overworked alanates, so far. Seems to have possible overlaps with ST6 (UTRC) relative to both techniques and materials.
- Rapid screening encompasses limited level of processing conditions. Although one looks at large number of material constituent contents, it does not look at processing variables or catalyst variables. Not clear how modeling folds into experimental work.

#### Specific recommendations and additions or deletions to the work scope

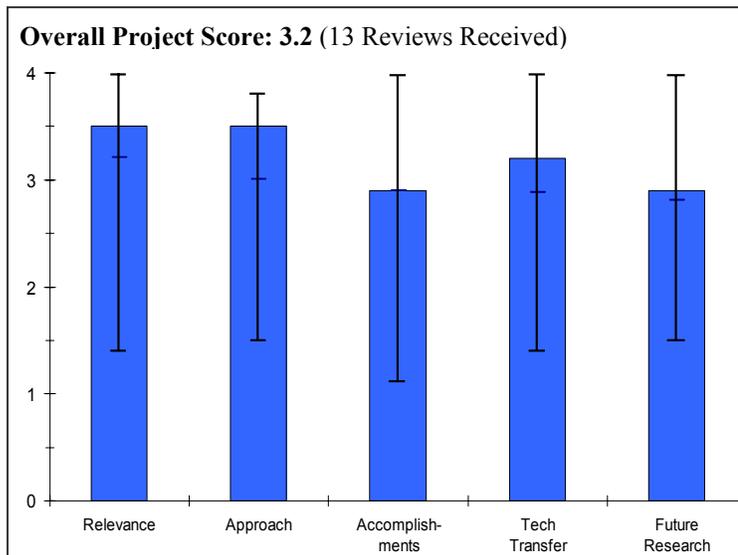
- PI should continue to refine model.
- There has been much work in the field thus the PIs are expected to use the lessons learned and effectively manage the project and re-align (with the DOE goals) when faced with technical challenges. Part of this must be measured (by the DOE and the reviewers) as indicated by the number of choices that are rejected before a candidate alloy is chosen for further studies. The program must maintain its goal-oriented focus.
- The project plan should contain more details about the future work. The experimental work and the development of the complete system require better specifications. Better collaboration with other projects and MHCoe is recommended.
- Wrap-up search in the alanate area. Expand the scope into other areas of storage materials.
- They should be freed to expand into materials other than alanates if they wish. Suggest that they confine to test points with materials 4% (for learning purposes) or more.
- Since the modeling of the Li-Mg-Na/AlH<sub>4</sub> confirmed the experimental findings, i.e., that no promising compositions were being missed, can we now assume that we can rely on the modeling to guide us to the systems we should study? -- If so, in principle we should be able to save lots of measurement time and resources by relying on the modeling supported by a few judiciously planned experiments? For future reviews prepare a prior year to current year progress comparison to help gauge performance in the budget year.
- As suggested by PI, move into newer systems: borohydrides, amides, etc. Can there be some coordination with ST6 (UTRC) to avoid duplications of effort? Will corporate IP issues prevent that?

**Project # ST-06: Complex Hydride Compounds with Enhanced Hydrogen Storage Capacity**

*Anton, Don (PI); Opalka, Susanne presenting; United Technologies Research Center*

**Brief Summary of Project**

United Technologies Research Center (UTRC) will develop new complex hydride compound(s) capable of achieving greater than 7.5 wt.% hydrogen capacities and 500-cycle reversibility with 100% efficiency. The focus will be on  $Ak_xAe_yM_{+iz}(AlH_4)(x+2y+iz)$  in the multi-dimensional phase spaces formed between alkali (Ak) and/or alkaline earth (Ae) hydrides, metals (M), alane ( $AlH_3$ ), and molecular hydrogen ( $H_2$ ). The team will utilize first principles modeling to guide and accelerate the discovery of new complex hydride compounds with solid-state, molten-state, and solution-based processing methods. The team will conduct three levels of performance evaluations to select compositions for further development, optimize dehydrogenation and hydrogenation catalysis with spectroscopic mechanistic studies and first-principles screening simulations, develop manufacturing processes to reduce cost and scale-up production, and develop business analyses for the commercialization of hydrogen storage systems integrated with fuel cell power plants.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.5** for its relevance to DOE objectives.

- PI project aims to expand beyond basic alanates.
- The project is in line with DOE goals and clearly states the main goals addressed.
- Hydrogen storage is a key enabling technology that is critical to the success of the hydrogen economy. This project supports the initiative through exploration of new materials for hydrogen storage.
- Project is addressing issues critical to the realization of the President's Hydrogen Fuel Initiative.
- Development of new compound to meet goals is important. Goals clearly identified.
- Aimed at improved alanates and thus build off the proven  $NaAlH_4$ , which is appropriate. Improved theoretical application would also directly address key questions.
- Clearly linked to goals and objectives of HFCIT RD&D program.
- Relevance will ultimately depend on results.
- Clearly looking to develop new materials to meet DOE storage targets.
- Materials under study important to meeting program targets.
- Focused on materials discovery of new high density hydrides.

**Question 2: Approach to performing the research and development**

This project was rated **3.5** on its approach.

- PI project aims to expand beyond basic alanates. Atomic modeling, molten solution processing are welcome alternatives to traditional ball milling techniques which will be difficult to scale up.
- The internal alloy selection process is not clear. As the PI has access to results from ST4 [The UTRC System Prototype Project], this would be a perfect opportunity to use the vessel design issues as part of the vetting process for alloy. However, this has not been addressed.

- The PI illustrates an acceptable approach with a combined use of modeling and synthesis methods. The approach also includes fast selection criteria of technical and economical nature. The approach does not give clear indication about the selection of materials really suitable for the DOE goals.
- Good, logical, sequential analytical, modeling, synthesis and experimental approach.
- Approach which consists of closely coupled theoretical and experimental components is sharply focused and a credit to the PIs and to the overall program.
- Approach is strong with ability to evaluate behaviors before experimentation, thereby not wasting effort on dead-ends.
- The approach has some unique aspects in comparison with other related projects sponsored by DOE. Computation and experiment are closely coordinated. Project is exploring some interesting processing options that have not been deeply studied in the past
- Broad but systematic approach. Predictive thermodynamic tools ensure a good materials selection process.
- Theory guided experimental tests is a good one. Exploring new technique to make material is appropriate as well. Looking at scale-up may be key in future, though of little use this year.
- Balanced approach between theory, synthesis, and characterization. Good variety of synthesis methods. ATM: how many candidates per day can be assessed? Is computational method faster than synthesis?
- An excellent combination of modeling and synthesis techniques ("processing"). The MSP [molten state processing] (Savannah River National Laboratory contribution) approach is innovative.
- Good approach to use different material processing methods to further study development of quaternary compounds. Coupled modeling to experiment. Validated model to experimental results.
- Interesting combination of modeling and processing approaches. Clarification is needed as to why these four specific approaches are combined together in this effort. Need more specifics about compositions/stoichiometries to be studied in each of the systems, as well as more details about the high-throughput experimentation.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.9** based on accomplishments.

- Poor candidates have been quickly eliminated. PI is showing reproducible results.
- Difficult to consider as this project started a few months ago. [The project has been running since ~May, 2004.]
- The technical achievements are consistent with the objectives expected for the period. There are no clear modalities for comparing synthesis methods, materials and validating models.
- Reasonable progress with concrete results during the past year.
- PIs are to be complimented on the theoretical screening of potential compounds prior to experimental preparation and characterization.
- Integrating experimentation with simulation. New materials discovery work progressing well.
- Developed several theory techniques for use in this field. The SRNL [Savannah River National Laboratory] work is not new so can not really be counted as progress. Albemarle's progress is of unclear value at present. Unclear how many points in each of the 7 systems were actually tested?
- Even if results are negative so far (in terms of meeting DOE targets), it still helps make definite conclusions on the systems investigated.
- Some success in achieving improved performance with molten state processing. Some interesting results from coupled reaction studies. Have not yet identified a reversible metal hydride storage material that approaches 2015 "system" targets.
- Good understanding of materials being studied. "Mapping" of new materials using experimental and predicted thermodynamic properties good approach. Will data be published? TiH<sub>2</sub> work encouraging.
- The use of predictive modeling is very nicely demonstrated. Nice study of the relative merits of three different synthesis techniques. The alanates are rather overworked. OK to show the value of modeling, but perhaps the time to move on.
- Extensive modeling and experimental studies have been completed to date.
- Until theory starts making tangible predictions of new compositions, the experimental effort is a bit of a "shot in the dark." The modeling effort needs to quickly start making predictions for the experimental effort to verify.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.2** for technology transfer and collaboration.

- PI should coordinate with UTRC tank project [ST-04 System Prototype Project] in order to better tailor research on metal hydride candidates. PI otherwise well coordinated with other labs and key researchers.
- There is adequate technical collaboration.
- The collaboration with the MHCoe and other projects should be more emphasized and made operative. The contribution of Norway is valuable and appropriate.
- Good mix of industry and research associates.
- Coordination appears in place and seems appropriate. PI could have spent slightly more time in presenting the contributions of the collaborators.
- Many capable partners contributing to this project.
- Multiple team program.
- A well organized, multi-institutional project; the presentation made clear what each participant is doing.
- Good partners for project.
- Excellent collaborations.
- Would be good to expand collaborations, particularly with CoE's.
- Though there are a large number of partners in this project, there does not appear to be any attempt to coordinate or interact with other projects.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- PI is pursuing materials past alanates however plan and strategy seems unconnected or weak. Original focus of systematic selection not evident in future work.
- The future work is well connected to the previous results. There is the need to focus more on the selected materials.
- Future plans seem reasonable and logical extensions of work done so far.
- Strong future plan building on current efforts.
- Continue close collaboration with DOE MHCoe.
- Not very well defined.
- Future plans are a logical extension of the presently established capabilities of this project and the findings from FY 2005 activities.
- Transition metal addition good direction.
- PI realizes the need to get to newer families of materials. Has identified a number of possibilities. Precise future directions and materials a bit vague sometimes, presumably because of IP considerations.
- Need to expand beyond alanates.
- Future plans are a bit vague at this point, because the modeling needs to make predictions of compositions to guide the experiments. Otherwise, the experimental effort will have to just pick a few representative stoichiometries. Since future plans involve addition of heavier elements (Ni, Co, Fe, etc.), the focus should be exclusively on compositions and systems where at least a theoretical density is higher than state-of-the-art.

**Strengths and weaknesses****Strengths**

- Non ball milling techniques are welcome. PI understands impracticality and limitations of ball milling. Solvent processing is generally more amenable to high volume manufacturing, molten process potential amenable to manufacturing if pressures remain modest.
- Organizational capabilities. Resources.
- The combined approach is a valuable method for rapidly developing and comparing materials.

- PI did an excellent job of presenting material in an unhurried, professional manner. Information was clearly presented with examples and sufficient data to illustrate accomplishments. This should be a model presentation for other PIs to emulate.
- Goal focused. Very good collaborative effort.
- Combined predictive methodologies. Broad approach still allowing thermodynamic productions of experimental results, reducing necessary experimental effort. Modeling compliments experiments, good match. Need to increase weight capacity search criterion to at least 9% (currently 7.5%).
- A lot of theory guiding things and checking against each other.
- A well organized/coordinated project. They have established a comprehensive capability to explore hydrogen storage material/concept options.
- The group has a balanced approach with good capabilities; combisynthesis.
- A very nice combination of modeling and synthesis optimization.

#### Weaknesses

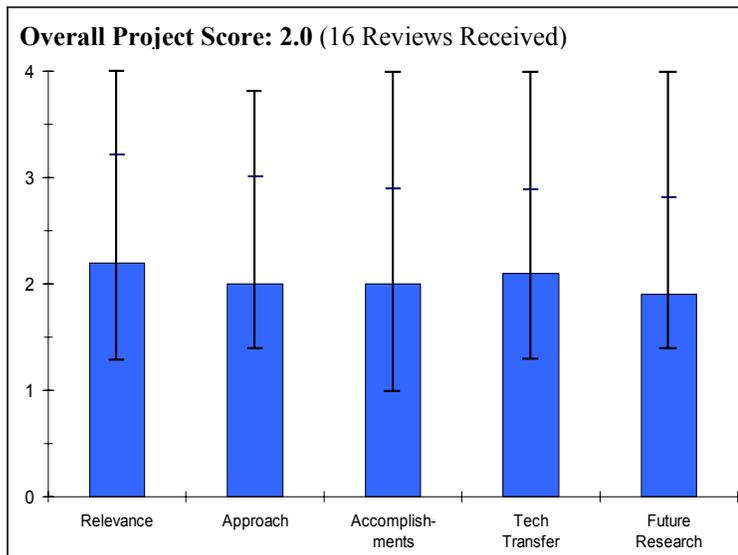
- Rapid elimination process may also miss a few good candidates, however at this stage, that is less a concern than cycling through all the possible permutations.
- There is no clear pathway to integrate lessons learned from other internal studies in the system development.
- The multiple approaches require clearer criteria to compare not only materials but also synthesis methods.
- Not much truly new coming out of the experiments. Need to give more data on what results for the 7 systems in high throughput were.
- Presently focused on metal hydrides.
- Relies too heavily on the overworked alanates, so far. Seems to have possible overlaps with ST5 (UOP) relative to both techniques and materials.

#### Specific recommendations and additions or deletions to the work scope

- Need to increase search criterion for new materials up to at least 9%wt (currently 7.5%). Focus on alanates decreases probability of success.
- It seems as though excessive ball milling in order to achieve nanoparticles is a misleading practice. Often, in a real tank system, nano particles will decrepitate after cycling and continued vibration and thus any advantages gained will be quickly lost. Most current systems find that due to packing factor and expansion issues, nano particle sizes may not be practical.
- There is a need for additional experimental work on the selected materials.
- Move away from alanates. Use a single preparative method (molten processing, etc) for model compounds as upon cycling the material will come to most thermodynamically stable state anyway.
- Limit the use of Co, Fe etc to amounts that will allow for at least 4%, preferably higher, storage.
- The project staff should consider how seamlessly they could transition their methodologies to other types of materials/concepts for H-storage, e.g., should major breakthroughs occur outside the metal hydride arena. For future reviews prepare a prior year to current year progress comparison to help gauge performance in the budget year.
- As indicated by PI, move into newer systems: borohydrides, amides, etc. Can there be some coordination with ST5 (UOP) to avoid duplications of effort? Will corporate IP issues prevent that?

**Project # ST-07: Sub-Nanostructured Non-Transition Metal Complex Grids for Hydrogen Storage***Talu, Orhan; Cleveland State University***Brief Summary of Project**

The objectives of this project are to grow sub-nanostructured metal grids (<1 nm thick) with about 50% microporosity (<1 nm wide) and measure hydrogen uptake/release on these novel metal grids for hydrogen storage applications. The premise is that the overall hydrogen dissociation reaction rate will be higher (because the external metal surface area is enhanced), and the diffusion time constants will be lower (because the diffusion path is greatly reduced). In addition, it is hypothesized that conduction in the highly interconnected metal grid and convection in the micropore space may enhance heat transfer. The nanostructured metal grids will be grown from pure and alloyed non-transition metals and the phase diagram is anticipated to be different from the bulk phase diagrams because of the quantum effects that may arise at these length scales.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.2** for its relevance to DOE objectives.

- This is an interesting approach to synthesize new materials; however the likelihood that this can achieve any appreciable hydrogen storage capacity is very low. This material may however have application in micro channel heat exchangers or gas diffusion layers if metals other than Fe are used.
- The project is obviously relevant if it works and can meet the cost targets.
- Fast kinetics is crucial to metal hydride storage.
- The project is relevant to the DOE objectives.
- This was a concept that was worth investigating to see if it could meet the storage goals, but it does not appear to be making sufficient progress.
- Materials development work based on a new concept that could support the Hydrogen Initiative.
- This effort is reasonably aligned with the goals of the President's Hydrogen Initiative. There are also potential contributions of this work to the field of catalysis which are also highly relevant to energy consumption but less relevant to this particular initiative. A higher risk, potentially higher payoff set of objectives.
- Novel concept with new approach. Not much hope of meeting goals even with other materials.
- This project does address specific critical goals of the HFCIT program in the storage area; it just does not do so in a very compelling or convincing way.
- Interesting idea. Questionable economics. Difficult experimental challenge. Path to large scale production?
- The project does not seem to quantitatively address many of the DOE targets, in particular gravimetric and volumetric energy densities.
- Project does not address program targets.
- Topic is largely irrelevant to DOE objectives. The topic is high-risk and no real foreseeable payoff for hydrogen storage. Even if these materials could be made (which would be an extremely major accomplishment) they simply will not enable high densities, and will not survive repeated cycling. Thus, the approach is of limited/no value to this DOE program. Probably should not mention "quantum effects" unless there is some real evidence or reason to suspect they will increase capacity. To date, there seems to be no evidence.

- There is potential for great relevance, however, there are several barriers which must be addressed (e.g. mold removal, loss in volumetric capacity, cycleability, deposition techniques, etc.) before this will be fully relevant to DOE.

### **Question 2: Approach to performing the research and development**

This project was rated **2.0** on its approach.

- The electrodeposited materials that the PI intends to use will hydrate! This will eventually break down the structure of the material after a few cycles. It seems unlikely that significant cycling capability will ever be demonstrated even if acceptable capacity is initially demonstrated. All materials that can be electrodeposited have some capacity to hydrate hydrogen. It would be difficult to see how homogenous alloy layers can be deposited due to the different electropotentials of each metal. Otherwise the approach is very interesting in terms of using simple and cheap zeolite materials to form a "negative" mold. This is certainly valuable work for undoubtedly many other applications.
- The approach is clear and the project seems well designed, but as the project is high-risk and exploratory, it is not clear at this time that it is feasible. But, of course, that is the nature of good, high-risk, exploratory work.
- The proposed approach is very innovative. May not be applicable to metal hydrides of practical interest, namely complex metal hydrides.
- The approach identifies some key issues. More focus and justification are required for the research choices.
- Tried several novel approaches to develop hydrogen storage media, but none seem to be yielding results.
- Novel, interesting approach but not enough evidence about the feasibility of this work program and how the targets are actually addressed.
- Generally well thought out and appropriate approach.
- Good approach given the objective to make a high surface area material of metal for use in storage. However the sought material is highly unlikely to be stable at relevant temperatures and under the stress of hydrogen insertion and removal, so the goal is unlikely to be met. And it can not make the goals.
- Creating nano-porous structures for hydrogen storage is a good idea in a general sense; however, there must be better approaches than what this project proposes (see Recommendations below).
- Are there examples of anyone creating these metal structures from zeolite templates? Hydrogen behavior on small metals is well known. Copper is known to be a very good metal for plating/electrochemistry. Other metals may not work as well. Simple gas adsorption techniques needed to characterize microporous materials. Should consider mesoporous materials like MCM-41 as additional transition to zeolites. Pore blocking by initial deposits is likely to be a problem.
- The whole approach is doubtful to this reviewer. While heat transfer and gas impedance might be improved, one would think gravimetric and volumetric densities would be decreased. Repeating my unanswered question of last year, can PI make any calculation that would suggest that the volumetric and gravimetric DOE targets could be theoretically achieved?
- Only addresses kinetic properties. No capability to synthesis high capacity compounds. Only addresses metal systems which are known to be too heavy.
- Does this procedure work for anything other than metals? Most hydrogen storage materials under consideration today (if not all) are not classical metal hydrides (e.g.,  $\text{NaAlH}_4$ ,  $\text{LiBH}_4$ ,  $\text{LiNH}_2$ , etc.) So, the utility of this procedure is of significantly limited importance for the DOE objectives. Also, the very large surface areas of this approach will also translate into an effectively large volumetric penalty of the hydrogen density (compared, say, to the single crystal density). Gravimetric density is not the single controlling factor behind solid-state storage materials. Volumetric density is, in fact, the whole reason why solid-state materials are considered at all.
- Issues were well explained. Nothing specifically about metal hydride work; is this going to be part of the project? Possibilities for increased hydrogen storage are great.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.0** based on accomplishments.

- PI has made good progress in synthesizing the material. PI has demonstrated good control in modifying the characteristics of the material.
- Still more exploration must be done before one can say it is going to be feasible.
- The project is exploratory and timely progress is difficult to predict.
- The PI's presentation gives a limited overview of the major results, showing the achievement of the proposed objectives.
- Most technical approaches reported have not been successful. Results of research so far are not meeting objectives. Several approaches have been tried without success. It is unlikely this avenue of research will result in technology that can meet the storage goals.
- May need to speed up the characterization part of the work.
- The rate of progress towards the objectives has been somewhat slower than might be expected given the size of the project and financial support provided.
- Inserted copper in zeolite and started removal. The key will be next year's progress. Have not done any useful metals yet.
- Progress to date is not impressive and seems peripheral to the main goals for the project. The current effort is more about finding ways to make the originally conceived project actually work at some level than about being at the stage of making something to begin testing.
- Good progress on growing films. Real problem will be metal grids. How much copper is getting deposited on zeolite films? Should be able to calculate whether pores are being filled.
- Some modest progress in doing what PI wants, but almost no indication that work can overcome any storage barriers.
- The group has only attempted nonhydride forming material depositions.
- The group did not answer the issues/questions raised by the reviewers from last year.
- Spent lots of time that was wasted due to microcrystal growth closing off electrolyte solution during plating. Nothing stated about milestones.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.1** for technology transfer and collaboration.

- PI is working independently. Given that the work is unique, many collaborators in manufacturing of zeolites or electrodeposition experts could be consulted for help. PI should look to suppliers and manufacturers outside the hydrogen storage community to determine if interest exists for collaboration.
- Most outside contacts are with other researchers at this time. But, given the high-risk exploratory nature of the work, significant involvement of potential implementers is premature at this stage.
- Not applicable due to the novelty of the proposed technique. The PI could envisage some sort of collaboration with the DOE Metal Hydride Center of Excellence. They are planning some overlapping activities in this area.
- The collaborations are limited but appropriate.
- PI is working with respected technical collaborators, although, from the presentation, it is unclear what their contributions have been.
- The project could benefit from more extended collaboration with other institutions. No evidence of technology. To the defense of the program, is this really applicable?
- Coordination and collaborations were less apparent in this project. At this stage in the project collaborations may be less necessary.
- Appropriate outside academic collaboration. No industrial input.
- This project desperately needs some strong collaboration that can send it in a more promising direction (see Recommendations below). It is not clear that the listed collaborators have been or currently are engaged in the project.
- Partners with expertise in zeolites/catalysis would be good addition.
- Minimal collaborations. No experienced hydride people? Tech transfer possibilities not very clear at all.

- Does not appear coupled to rest of program PIs.
- Very little talk about outside work. Some collaboration could be possible for help with metal hydride work, when it starts.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **1.9** for proposed future work.

- Looks fine. Logical progression.
- The work is not completely clear and does require more experimental work using hydrogen to start the experimental verification of the claimed advantages.
- Question whether future research along these lines will come any closer to meeting the FreedomCAR goals.
- Not entirely convinced future plans can provide the required results.
- Future research plans appear reasonable.
- Can not really be suitable because it just will not work.
- Directions for future work sort of make sense in the context of the present approach but I am not optimistic that results from this particular project will ever lead to a functional, cost effective, durable hydrogen storage/delivery system.
- Need to answer question of metal growth in zeolites sooner rather than later. Real question is whether grid can be made.
- Pd and Mg will not lead very well in the direction of eliminating barriers. Should get to more practical H-storage alloys as soon as possible.
- Proposed metal depositions not consistent with program goals.
- Issues are well known and pathways were explained to overcome these issues. Lots of ideas expressed during presentation but need to focus-in on ideas. Nothing explained about actual metal hydride work.

#### **Strengths and weaknesses**

##### Strengths

- Extremely interesting material research, material synthesis seemingly fits all criteria for economical scale-up and production - cheap, proven base (zeolite) material available which already has many other applications. Could this material also be used as a membrane or filter?
- The PIs are experts in their field of zeolite and related catalysis.
- Good idea.
- Novel way of making nanoporous metal structures that is potentially useful in other applications.
- The preparation techniques of nanoscale grids may be of wide benefit to the Sub-program.
- Innovative approach.
- High risk project that may, if successful have broader impacts beyond hydrogen issues.
- Innovative out-of-box thinking, nice-looking idea.
- High [surface?] area and simple concepts.
- The approach is very much different from that of other HCFIT storage projects, so, in a sense, it represents an alternative to the more conventional hydrogen storage approaches taken by the larger family of HFCIT storage projects.
- Hard to identify any. Might be more appropriate to carbon as hydrogen storage medium.
- Possibilities of this approach are unlimited. May help get the metal hydride area of research over the "hump" and achieve the 2015 DOE goal of 9 wt.%-- a goal conventional metal hydrides have trouble overcoming.

##### Weaknesses

- Material has no chance of being a practical hydrogen storage material with cycling capability. Unlikely to be cheap enough to remanufacture several times to be used as a chemical hydride type of material.
- None apparent at this time, but could do a better job of presenting concept of electrodeposition; hard to visualize.
- The PI did not properly address the drawbacks of his approach, namely the loss in storage capacity and how to avoid decrepitation of the nanoporous structure.

- The advantages on hydrogen storage systems of the developed grids are not yet verified.
- Rather high risk project that does not seem to appropriately address the targets.
- Probability of significant contribution to Hydrogen Fuel Initiative is less than other projects reviewed thus far. This is not a criticism of the project relevance only an assessment of probability of successful contributions to the Initiative. Perhaps this effort got off to a slow start.
- Idea is irrelevant to hydrogen storage applications.
- Still feel the structure will be unstable and the program has almost no chance of success.
- To appreciate the possibilities of success for this project, one must recognize that it is at an early stage of progress and that something exciting could come from the research over the next year or so--personally, I am not optimistic. The basic idea of creating nano grids is a reasonable one, but molecular sieve-type templates may not be the best choice; templates that can be formed in a truly contiguous architecture would work much better.
- Investigators need to look at existing catalysis literature. Doubtful that quantum effects occur. Should increase kinetics, but not capacity. Difficulty of making grids is probably underestimated.
- Of highly doubtful value to eliminating barriers, compared to DOE money spent.
- The fundamental approach of the project does not appear to be applicable to the development of lighter weight, high density hydrogen storage materials.
- Lots of barriers before results can be seen. Weakness of scale-up. Still same issue with 50% loss of volumetric capacity; presenter said "No way to prevent this."

### **Specific recommendations and additions or deletions to the work scope**

- The project should have go/no-go milestones.
- Future work will begin to explore H<sub>2</sub> storage capable materials. PI should shift focus to find materials suitable for heat exchange materials. Could this material be suitable as a heat exchanger for new fuel cell coolants using Teflon based materials? The corrosion to the metal would no longer be an issue.
- This is excellent research despite the poor ratings. This research should continue, however applications with the FreedomCAR body materials group or fuel cell tech team should be investigated. PI should contact manufacturers of micro channel heat exchangers to determine if his research has potential for their application.
- While this is an interesting material development technique, it is significantly out of the focus area of the DOE hydrogen storage work. It is not clear how the successful completion of the preliminary tasks will help DOE's storage targets. As PI stated, in some respects such as volumetric storage it will have the opposite effect. It is recommended to phase this program out of the "Grand Challenge."
- None.
- Need to determine at an early stage the family of metal hydride that could be prepared via this technique.
- The addition of specific experimental work with hydrogen will accrue the achievements of the project.
- Consider ending project or moving it to DOE BES.
- Need to interface with other institutions that can give a 'boost' to the research work with their related experience.
- Recommend looking at uncosted balances for the project and if large, consider stretching out budget and project periods accordingly.
- Consider to change scope of the project completely for relevance to DOE targets.
- This program might have much more application in other fields, or in unknown applications that do not require the metal to ingest hydrogen. This program would be much more appropriate in DOE BES and if a way could be arranged to hand this off to that office it would be more appropriate there. If moved, it should not be a hydrogen project anymore but general material generation.
- I recommend that the project staff arrange visits to one or more of the DOE/BES Nano-Science Centers to explore alternative options for the template structure-type and architecture, e.g., anodized, atomically ordered arrays, deep x-ray lithography, there are others. I have a sense that in the next year or so materials concepts emanating from the nanoscale activities in other HFCIT storage projects, particularly the Centers of Excellence, will overwhelm what this project is trying to accomplish.
- Need to consult with zeolite experts.
- Recommend discontinuing project unless some theoretical calculation is made that shows any hope of reaching DOE gravimetric and volumetric target energy densities.

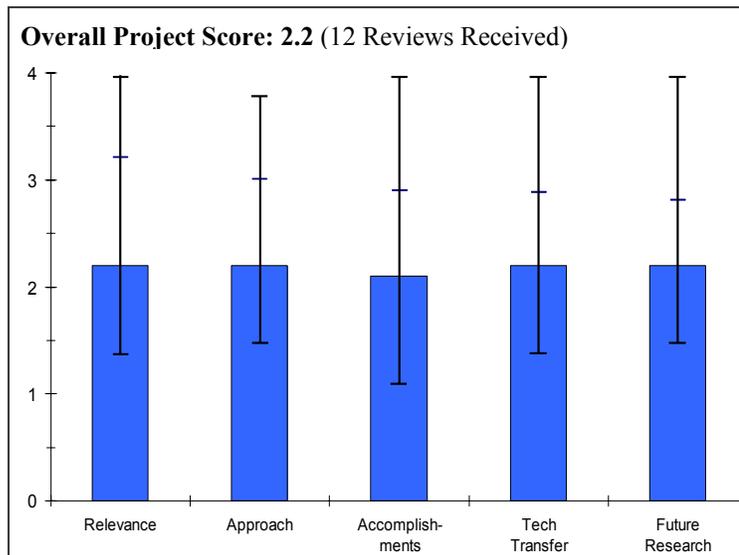
**Project # ST-09: Clean Energy Research at the University of South Carolina**

*White, Ralph (PI); Ritter, Jim presenting; University of South Carolina*

**Brief Summary of Project**

The University of South Carolina Clean Energy Project addresses research for hydrogen production, storage, and use. Currently, 5 tasks make up the Clean Energy Research Program initiated in FY04. Hydrogen Production: Low Temperature Electrolytic Production – This task will focus on production by electrolysis of anhydrous gaseous HCl and by the electrolysis of gaseous SO<sub>2</sub>. Both of these electrolysis processes are steps in proposed thermochemical processes. Hydrogen Storage: Development of Complex Metal Hydrides. This task will focus on the storage and retrieval of hydrogen in metal doped complex metal hydrides (alanates). Hydrogen Storage: Chemical Hydrides.

The possibility of using sodium borohydride to store and release hydrogen will be investigated. Fuel Cell MEAs: Diagnostic Tools for Understanding Chemical Stresses and MEA Durability Resulting from Hydrogen Impurities. Fuel Cell MEAs: Durability Study of the Cathode of a Polymer Electrolyte Membrane Fuel Cell. This is a cross-cutting, congressionally directed project started in 2004.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.2** for its relevance to DOE objectives.

- The study of co-dopant is a welcome change from the traditional Ti based dopants. Investigating steam hydrolysis of borohydrides will never be a practical automotive system. Work presented by Dr Michael Matthews was conducted in collaboration with DaimlerChrysler almost two years ago. DaimlerChrysler abandoned this effort due to the unmanageable complexity of a steam based NaBH<sub>4</sub>.
- A number of research areas are redundant, and covered by other programs. It is not clear how this project will be serving the objectives effectively.
- Hydrogen storage is a key enabler to the success of a hydrogen transportation system. This project has several parts all of which may be able to further the knowledge base; some parts more so than others.
- Goals are reasonable but the diversity of the goals and lack of cohesiveness of the goals of the overall project is a detriment to the potential contributions of the project. The goals of this task (Project II: Development of Complex Metal Hydride Hydrogen Storage Materials) are not particularly novel.
- Several types of projects using this budget. Although the targets are identified, the performance to the targets is not.
- Some of this work applies to storage but the majority is not storage work. That work does not apply to this important task though it does potentially aid the overall goal.
- Materials are not going to meet DOE goals, but good models. Dry steam work interesting, but real problem is regeneration.
- The H<sub>2</sub> storage tasks are relevant to the DOE storage program. The other tasks may have relevance to the other DOE H<sub>2</sub> program areas.
- Note: There are 5 projects covered in the contract. This reviewer covered only the two storage projects (II & III).
- Both projects are reasonably well oriented toward DOE vehicular storage targets.

- Portions of the work appear to be high quality, and well focused on DOE objectives. Combination of work on enhanced kinetics (e.g., carbon catalyst) and high capacity (e.g.,  $\text{LiAlH}_4$ ) could prove fruitful in the future. Task II (complex hydrides) appears to be very competent, well-aligned, and focused on DOE objectives. Other portions of this project do not appear to be supporting DOE objectives.
- Too much emphasis on sodium alanate, which we know will not meet targets.

### **Question 2: Approach to performing the research and development**

This project was rated **2.2** on its approach.

- Carbon and iron and possible Zr based dopant may be cheaper than Ti dopants. Use of these dopants seems to be more flexible than Ti-based and may have uses beyond alanates (always a bonus). DaimlerChrysler investigated steam hydrolysis and determined that the energy load required to dry  $\text{NaBH}_4$  in order to move it as a powder is prohibitive; steam-based systems had a tendency to plug and form "cakes." Moving powders is much more difficult than liquid or gas in an automotive system - Creating a thin layer powder (coating on a glass bead was meant to determine monolayer kinetics of the system only.  $\text{NaBH}_4$ , once reacted with water, will form a  $\text{NaBO}_2$  shell which is impervious to water and thus the reaction rate decreases dramatically. Attempts to portray this work as a "breakthrough" in improving kinetics is highly misleading.
- The alloy vetting process (with respect to system development) was not presented.
- Technical approaches of most aspects of the research seem competent and logical.
- The breadth of efforts in this project is a detriment and severely limits its potential contributions. The approach followed under this task (Project II: Development of Complex Metal ..., which entails the consideration of dopants in traditional metal hydride systems,) has some aspects that may lead to progress in overcoming barriers but largely is behind the field.
- Although the approach is okay, it appears duplicative of other work going on in the program that is further ahead – the group even admitted as much during its presentation. No funding breakdown for each "mini-project"
- Synergy work is appropriate but needs to be moved to making better systems. Graphite work is interesting though not improvement. The  $\text{MgAlH}_4$  work is of dubious value as it is irreversible thermodynamically. Hydrolysis work does not approach the key problem which is recycling. But much of the work does little to advance storage.
- Materials being targeted are still at 3-4% wt capacity. Alanates have been extensively studied by others and results have been reported. Dry steam hydrolysis approach for chemical hydrides is interesting to make some improvements in kinetics but does not help in solving principal problems such as storage capacity, regeneration issues, etc.
- Co-dopant approach fairly unique. Carbon doping work promising. Mechanistic work would be good addition.
- The approach is to look at combinations of dopants to enhance hydrogen absorption and desorption in alanates. The novel aspect of the approach is to use sonochemical pretreatment prior to ball milling. The chemical hydride approach is looking at the dehydrogenation of the hydride using steam rather than liquid water to produce a dry product. The objective of the research is to understand the reaction mechanisms to fully utilize the steam and maximize the  $\text{H}_2$  delivery rate.
- Combination of dopants with Ti may lead to improvements in kinetics and capacity relative to doping with Ti only. Not attempting to understand the underlying mechanisms of the doping process. Li alanate is fully reversible (only 5% capacity below about 120 C) but not likely to be done at a gas station. Thin films of sodium borohydride.
- Project II is oriented toward catalyzed alanates. Although there is some innovation (e.g., combined carbon-metal catalysts), it seems to significantly duplicate other alanate activities funded by DOE. Project III is oriented toward chemical hydrides, in particular the borohydrides. While the steam reaction approach is innovative, the practicality will be dictated by the difficult challenge of borohydride regeneration costs.
- Much overlap with other projects in program. Only focused on sodium alanate. Dry steam approach not applicable to onboard storage because system parameters would not meet targets.
- Interesting approach to new catalyst materials, and distinct from others in the field (Task II - complex hydrides.) Other Tasks are not as well designed.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.1** based on accomplishments.

- Alanate work seems to be progressing at an acceptable rate. Sodium borohydride work: This is not novel work. This work was conducted almost two years ago for DaimlerChrysler and verified by DCX researchers.
- It is difficult to gauge as most of the work were redundant.
- I could give a better assessment if each technical sub-project were able to be rated separately. The Ritter storage work is novel and overall very interesting. Work with carbon is very interesting; a possible use of low cost materials that can help address the cost targets of the program. The NaBH<sub>4</sub> work is neither new nor innovative.
- Accomplishments are at best fair given the resources applied and not a credit to the overall Initiative. There is no evidence of collaboration between the PIs within the project as evidenced by publications thus far. Accomplishments and progress under task II are more substantial than the rest of the project and are good.
- Observed variation from simple mixtures of dopants. This is not fully new, though cheaper catalysts will be of use. Faster desorption with carbon added or with sonication which pointed to mechanical size reduction. Claim LiAlH<sub>4</sub> at 5% at 150C but no data or proof. And it is only reversible under severe conditions so this may not be an accomplishment. Understanding of dry hydrogen is scientifically interesting but ignores the main problem of recycle.
- Studying materials, but results do not appear well documented. Reversible lithium hydride system interesting, but not enough information provided.
- Good progress for first year on doping work.
- Sonochemical pretreatment showed improved uptake kinetics for sodium alanate with 2% Ti dopant. Some preliminary data reported on dehydrogenation kinetics of recrystallized thin films of NaBH<sub>4</sub>. Initial rates were 2-3 times faster than slurry reactions. However, yields were less than 100%.
- Reasonable and interesting progress on both projects. DOE targets cannot be met with the alanates. Only marginal improvements shown in this project.
- Not competitive with other projects in program that are attempting to determine mechanisms in sodium alanate.
- Good progress on enhanced catalysts in complex hydrides. Rating could potentially be "outstanding" depending on the results of the LiAlH<sub>4</sub> reversibility, which were not shown due to IP issues.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.2** for technology transfer and collaboration.

- USC is working closely with SRNL [Savannah River National Lab] which is strong in this type of research.
- Some portions of the project have reasonable levels of collaboration. One aspect has none. Collaboration by other researchers is not reported.
- Outside collaborators exist but their contributions were poorly described.
- Limited collaboration with others. Might be worth trying to incorporate into DOE MHCoe [metal hydride center of excellence] activities.
- Broad team. Adequate collaborators.
- Limited collaborations outside of immediate partners.
- Some collaboration was reported. A means of integrating this work into the CoEs should be explored.
- Reasonable collaborations, but not extensive. Would be good to join MHCoe and CHCoE [DOE Metal Hydride and Chemical Hydrogen Centers of Excellence] to enhance possibilities for tech transfer to industry. Is SRNL collaborating on melt processing with USC and UT (ST6)?
- Only limited interactions with others.
- Storage work is closely connected with external researchers and other DOE projects. Other work seems to be independent and somewhat disconnected.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.2** for proposed future work.

- Good plans for alanate and co dopant work. Borohydride work: It is highly unlikely that realistic improved kinetics will be achieved for steam hydrolysis. This system may only be practical in stationary applications where excess steam is available; however, the overall system efficiency will likely not exceed traditional cogeneration techniques.
- Ritter future plans are good and could provide valuable information. Mathew's proposals for NaBH<sub>4</sub> do not appear to be breaking any new ground. I question need for prototype systems when there are already industrial companies fielding prototype systems. Weidner plans really need to be assessed in comparison with other hydrogen production projects to evaluate value and direction.
- It is difficult to envisage this project as making significant contributions to the President's Hydrogen Fuel Initiative.
- Future work may yield improvements, but would be much better if this project worked more closely with DOE and the FreedomCAR & Fuel Partnership.
- LiAlH<sub>4</sub> is appropriate if onboard reversible but less so if really a chemical processing method. The NaAlH<sub>4</sub> probably is not, as it is only showing what is known, that size and dislocations help.
- NaBH<sub>4</sub> work: Economics need to include reprocessing!
- The proposed alanate research could lead to improvements but the alanate system is not likely to meet the DOE goals.
- Continues to work on alanate. Proposed methods of study do not appear to have the potential to contribute to greater understanding or to enhance the performance of the alanate. Chemical hydride work is not well defined.

**Strengths and weaknesses**Strengths

- The project is in reasonable alignment with the needs of the program and progress is good (NaBH<sub>4</sub> work aside).
- The enthusiasm of the PIs. Willingness to change course and flexibility.
- University of SC has strong capabilities. Experience working with DOD.
- Dry steam hydrolysis approach.
- If LiAlH<sub>4</sub> is reversed then that would be a strength. Need to address the difference from the expected amount. Seems that it is not actually reversible on-board.
- Steam reaction with NaBH<sub>4</sub> is an interesting new approach.

Weaknesses

- NaBH<sub>4</sub> work has been evaluated before. The PI does not offer any new expertise or revelations.
- The project is not effectively using the wealth of information already available. The alloy vetting process must be clarified and periodically re-calibrated using system analyses projects
- Too many technical areas in one project to evaluate properly. There are such different technologies being pursued to such different levels of success that evaluating it as a whole is very difficult. Some of the work is really novel and could be beneficial, but the remainder of the project work drags down the evaluations through the need to find an average.
- Project alignment to DOE goals seems to be weak.
- Focusing on well known materials such as alanates, boron hydrides, etc will most likely NOT help in meeting the DOE principal targets.
- Need to address: Is the catalyst work truly learning anything new, is this really just dislocation and size reduction? Does not address the key problem of hydrolysis (recycle); seems to ignore the difficulty of fueling and especially defueling solids.
- Steam work looks at the "easy" part of the problem. The real killer is regeneration of [spent, the oxide] NaBH<sub>4</sub>.
- Not well coordinated with the CoEs. Only a portion of the funding is being used for H<sub>2</sub> storage research.
- Alanate work (P.II) somewhat duplicative and limited in potential. NaBH<sub>4</sub>-steam process (P.III) will have the usual borate regeneration cost problems.

- Not in step with DOE program, other constituents (e.g., auto companies), other PIs in program. Most of proposed work does not appear to be relevant to program.
- An earmarked [congressionally directed] project is always going to be a weakness, simply because it does not undergo the rigors of peer-review. In this case, some of the work (specifically the storage work) seems to be well-aligned and of high quality, but for earmarks that is really the exception rather than the rule.

#### **Specific recommendations and additions or deletions to the work scope**

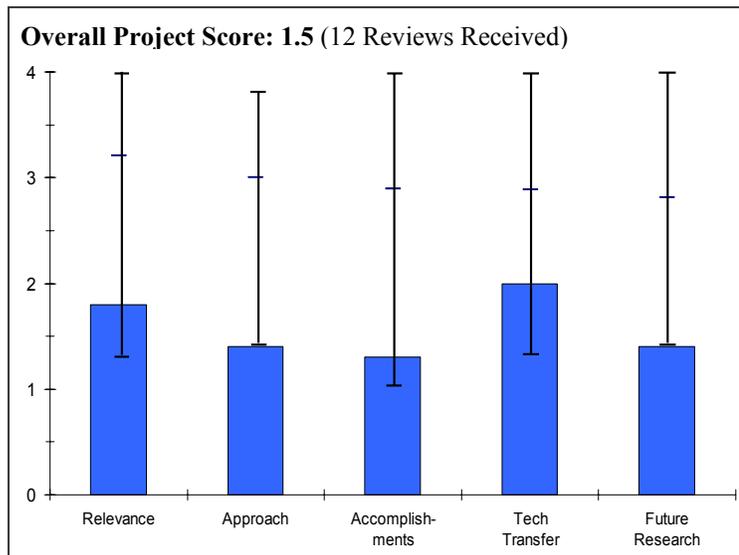
- For Project II, I suggest moving out of alanates into other more advanced materials. Work is duplicative of others and cannot likely meet DOE targets.
- Work on the  $\text{NABH}_4$  system is not novel, it has been evaluated as impractical before by more than one automaker. Stationary applications are unlikely. Regeneration of the  $\text{NaBO}_2$  would still be an issue which will also never be economical to regenerate due to the large thermodynamic well of B-O bonds.
- The technical approach is disengaged from onboard storage end product development. Specifically, one of the proposed systems required steam to facilitate hydrogen release. There was no clarification or further explanation where the energy for steam and/or water source will come from onboard the vehicle. The program scopes and focus are not appropriate to stay within the Grand Challenge.
- This project really needs to be separated into its parts for individual review.
- Reduce scope to increase focus, adjust project funding downward accordingly.
- Do not present non-storage projects in Storage review session. Work with DOE and the FreedomCAR & Fuel Partnership to get better alignment to goals.
- Redirect storage project scope towards materials potentially capable of meeting capacity targets. Collaboration with DOE Chemical Hydride Center of Excellence on the steam hydrolysis topic would be very useful.
- Move fuel cell and production work to the appropriate budgets. We saw very little about the other 3 areas and were not really competent to review it, all the more reason to split up the program between budgets. It is nice that the DOE team was able to shape this program to actually be of some value when it did not go through the technical review.
- Coordinate work with the CoEs.
- Project II: Suggest discontinuation of work on alanates. Project III: Coordinate with Millennium Cell on cost problems. Cease work if no hope of substantial cost reduction.

**Project # ST-10: Fuel Cell and Hydrogen Research University of South Florida***Stefanakos, Lee; University of South Florida***Brief Summary of Project**

This multi-faceted University of South Florida project will investigate several hydrogen production techniques; hydrogen storage in the areas of transition metal hydrides, nano-structured materials (nano-composite conducting polymers), and components designed for manufacturability; electrode improvements; water and thermal management; and a testing facility for fuel cells. This is a cross-cutting, congressionally directed project started in 2004.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **1.8** for its relevance to DOE objectives.



- The goals of the project are reasonably aligned with the President's Hydrogen Initiative.
- DOE targets (system basis) are stated, however, characteristics of materials being investigated are far below those requirements.
- Some relevance to H<sub>2</sub> storage program is evident.
- Three tasks related to storage: Transition Metal Hydrides, nano-structured Materials, and Hydrogen Storage Components.
- The project scopes are diverging from the DOE's grand challenge framework and goals.
- A cross-cutting project including conducting polymers, nanoscale transition hydride materials as potential storage materials. Just started a study of a manufacturing process based on nanostructured film approach. Starting three "new" tasks - geologic storage of hydrogen, new materials and advance thermal compression of hydrogen.
- Team lacks experience and data does not uniformly seem accurate.
- Materials under study not relevant to program. Researchers are not focused on DOE objectives, and have not answered criticisms from last year's review about analyzing even the theoretical limits of their approaches.

**Question 2: Approach to performing the research and development**

This project was rated **1.4** on its approach.

- Some of the approach may be OK but other parts lack viability.
- Little conceptual or theoretical approach.
- The approach is limited with respect to materials studied and methods, processes.
- Materials under study have wrong thermodynamics for storage application without possibility of changing them significantly.
- It is unclear if this technical approach will result in any new knowledge or add any significant value.
- The diffuse nature of the project limits potential for meaningful impact on the goals of the President's Hydrogen Initiative. Given the size of the project a more meaningful coordination of the approach is imperative.
- Oxidized catalyst unlikely to survive in hydrogen atmosphere. PI has not identified any metal hydride type material that has potential to reach 2007 or 2010 targets. The PI is not conducting any basic research on these materials that may translate to higher capacity materials.

- One novel approach that is being investigated is the use of electrical charge to desorb hydrogen from the carbon nanocomposites. The second approach is to investigate nanoscale transition metal hydride systems. The third approach with thin films does not appear to present a path to a system with high enough storage capacity to meet the DOE targets. The TGA data seems to indicate 15 wt.% storage capacity.
- Conducting membrane approach is interesting.
- Some of the alloys for hydrogen storage start at very low storage capacities, well below system goals of the program. It is not clear how the PIs will be closing the gap. There are no internal vetting mechanisms.
- Three empirically-selected approaches have been demonstrated without presenting evidences that those can potentially meet targets.
- The use of voltage to maintain capacity seems certain to have excess parasitic loss.
- MgFe is well understood and will not meet goals.
- Why would alignment increase adsorption? Low fields wouldn't ionize or align polymer
- What is path for thin films to be commercialized?
- Materials seem to have low capacities and high cost.
- Electrical process is not clearly on plan. Hydrides with appropriate capacity are not defined.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **1.3** based on accomplishments.

- No significant results that indicate research direction or results could be capable of meeting storage goals.
- Progress has been slow thus far and is addressing issues largely previously resolved by the community.
- Limited new information/data.
- Slide 12 indicates storage capacities of 8 and 15 percent. This is not possible when the maximum theoretical capacity of  $\text{Mg}_2\text{FeH}_6$  is only 5.5%.
- Only about 3% wt capacity has been demonstrated in relatively mild conditions for the approach 1.
- Deviation in adsorption and desorption points toward a measurement problem by people new to the technique.
- 5% in  $\text{Mg}_2\text{Fe}$  system at 300°C does not seem relevant to goals nor is it very new, plus only about 2% is really viable.
- Experimental results seem questionable.  $\text{H}_2$  capacity is not a simple measurement. 15%  $\text{H}_2$  on  $\text{LiMgFeH}_6$  which should contain max of 6% $\text{H}_2$ .
- Hydride material has demonstrated only 5.0 wt.% storage capacity.
- No viable storage media has been identified. Conducting polymer show low hydrogen absorption and even lower desorption. Cannot meet capacity targets.
- Too early to study manufacturing processes on these unacceptable materials.
- New Materials discovery not discussed in any detail.
- Thermal compression has been studied several years ago.
- There has not been a great deal of progress over the past year.
- Volumetric storage density of the proposed materials was not presented.
- The results from the carbon-doped nanocomposite work showed that the  $\text{H}_2$  capacity is only about 3%.
- TGA data for Li-modified  $\text{Mg}_2\text{FeH}_6$  indicates about 15% weight percent hydrogen released from the material at a temperature of about 300°C. Data needs to be confirmed.
- The hydrogen storage measurements (e.g., from TGA) look to be done incorrectly. Data is inconsistent with even the theoretical maximum density for this material.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.0** for technology transfer and collaboration.

- Collaboration among several Florida Universities but no industrial and/or commercial participation noted.
- Speaker mentioned that they are in the process of identifying additional potential collaborators.
- The team is diverse and well connected.
- Interaction with a number of collaborators is evident. Interaction with Hy-Energy should improve the analysis capabilities of the project team.

- Good to see Hawaii, NREL, and SWRI (experts in hydrogen storage) involved as partners in this project. These partners should help guide this effort towards more relevant research activities.
- PI has not collaborated with any established players in hydrogen storage.
- The PI lists many activities and personnel in his "partnership" but it is unclear from the presentation exactly what any of them are contributing.
- Research apparently mostly being done by three Florida universities. Role of other partners not clear.
- Need to make contacts with people who can help you to do the right experiments correctly. Collaborators should be used to examine validity of assumptions involved in polymer work (field alignment, etc.)
- Little apparent interactions with other labs.
- 

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **1.4** for proposed future work.

- PI needs to understand 2010 targets and propose realistic mechanisms which may allow them to achieve this goal.
- It is still not clear that a pathway to higher storage capacity has been identified. A clear indication of the science behind the work on destabilized materials is not evident.
- Seems to be just a collection of "ideas" related to hydrogen storage and fuel cells lacking a coherent development plan.
- It is unclear from the presentation comments by the PI that he has a clear plan for next steps in the transition hydrides area.
- Hydrogen compressor work would seem to be better aligned to Production or Delivery. (Note: this is a cross-cut project and the compressor task is aligned under the hydrogen production and delivery work)
- Effect of potential is interesting but ignores the effect maintaining a field will have on net storage.
- LiN system has been well studied; no clear point here. 8% hydride would be more interesting if there was more detail on what it was but based on what was presented this team is not likely to understand the material.
- Need mechanistic work: compressor using electrical discharge very inefficient: better sources of thermal energy. Work with Hera.

### **Strengths and weaknesses**

#### Strengths

- PIs have more extensive background in electrical engineering. Suggest that PI continue work on novel electro activated composites- these materials have potential for success in a system.
- USF does appear to have some capabilities in hydrogen research.

#### Weaknesses

- Lacks understanding of definitions of 2010 targets and the demands of automotive or stationary systems put on these storage materials.
- Unfocused activities without clear direction or potential to achieve worthwhile results.
- Though there were slides for previously identified issues, no discussion for them was given.
- Few empirically-selected well known-systems will provide very little probability of success to meet the targets.
- Not clear storage measurements are being made correctly. Needs verification by SwRI. Little understanding of the field or what has been done.
- Experimental approach seems fragmented. Serious questions about experimental results.
- An integrated project plan is not evident. The approaches look to be only loosely coordinated.
- Very large number of participants, but split among different unrelated projects.

**Specific recommendations and additions or deletions to the work scope**

- PI should terminate work on  $Mg_2FeH_6$  as it has been researched extensively for many years and concentrate on the conducting polymers which may be more conducive to their expertise as electrical engineers.
- Nanoscale  $Mg_2FeH_6$  has been investigated for several years by Dr Varin Univ. of Waterloo in Canada (mechanical engineering department) please contact him for collaboration.
- Encourage PI to continue in amides where potential for higher storage exists - PI also is encouraged to collaborate with many other PIs on this subject.
- Address previous questions regarding volume density of films and thermodynamics of hydrides.
- PI is highly encouraged to team up with established experts in the storage field.
- Project would be improved if efforts were better aligned to DOE and the FreedomCAR & Fuel Partnership goals.
- Need innovative ideas to generate novel approaches. Conduct go/no-go assessment soon.
- The manufacturing of nanostructured film work (Approach 3) should have a go/no-go decision. The approach does not show much promise for hydrogen storage.

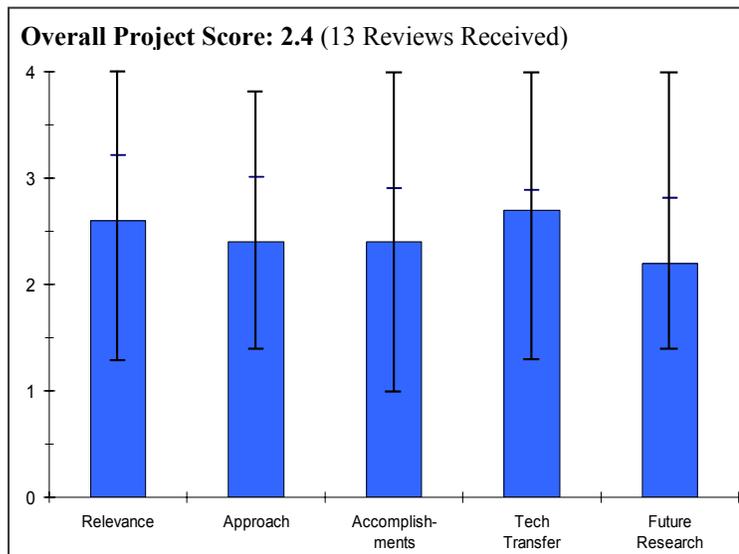
## Project # ST-12: Process for the Regeneration of Sodium Borate to Sodium Borohydride for Use as a Hydrogen Storage Source

Wu, Ying; Millennium Cell

### Brief Summary of Project

Millennium Cell's project is focused on the development of a reliable low cost regeneration process for sodium borate to sodium borohydride that meets DOE cost targets. The technical approach is to identify electrolytic processes that improve efficiency and reduce cost. It considers both the traditional Schlesinger route utilizing a lower cost sodium source from a novel electrochemical process and direct borate reduction. A key tool is to use hydrogen gas to reduce cell voltage and improve overall regeneration efficiency. This project started in 2004.

### Question 1: Relevance to overall DOE objectives



This project earned a score of **2.6** for its relevance to DOE objectives.

- Off-board regeneration of sodium borate to sodium borohydride at acceptable costs is a requirement for this storage technique to be viable.
- Obviously relevant if it works to the extent that the cost targets can be achieved. Borohydride is a major option being considered for hydrogen storage.
- Electrochemical regeneration of a material is the only process identified here that has promise or may translate to other materials. All other process mentioned here are not relevant since the starting materials do not make sense. NaOH is not a trivial material to generate.
- NaBH<sub>4</sub> will only have practical application in premium backup power applications.
- Hydrogen storage is a vital technology necessary for the achievement of the goals of the hydrogen program. This research when initiated seemed promising but now appears unable to support a technology which can meet the 2010 or 2015 goals.
- Issue of regeneration is very important to the needs of the President's hydrogen fuel initiative.
- The work is in the area of storage which is important, but the project aims at goals below the 2010 targets, which is troubling.
- The project has failed previously to perform the basic calculations of feasibility that would show if it can be viable, thus the alignment is not clearly good.
- NaBH<sub>4</sub> system problems seem to preclude it as transportation storage medium, but any progress in borate regeneration should affect other hydride systems.
- The project is relevant to the DOE Hydrogen Program objectives. Onboard systems based on Millennium Cell technology have been done. Millennium Cell focused on critical step in making the technology viable.
- This technology (the Millennium Cell approach) is not a new approach. It has been extensively evaluated previously by many auto companies, and largely rejected as impractical for a wide variety of reasons, only some of which have to do with regeneration costs. The proposed work seems very unlikely to significantly advance the field or the technology forward.
- Chemical storage is one of several possible storage technologies to meet DOE goals. Cost goals seem to be a major challenge.

**Question 2: Approach to performing the research and development**

This project was rated **2.4** on its approach.

- The approach to looking at the regeneration of the borate stream in response to past reviewer comments is the critical step in demonstrating the technical and economic feasibility of the sodium borohydride fuel cycle.
- The technical approach is looking at new processes for reducing the cost and increasing the energy efficiency of the full fuel cycle--both on-board and off-board the vehicle.
- Approaches are based on direct borate reduction, reduced cost for Na production, and co-production of sodium and boric acid.
- Multi-tier approach with timely down selects and go/ no-go decision points.
- Electrochemical approach is unlikely to address energy concern.
- PI does not indicate cost of starting material of NaOH to manufacture NaBH<sub>4</sub>. This is not trivial and will likely erase any gains made over NaCl as a starting point. This approach does not address the point that if a NaBH<sub>4</sub> economy is to happen with their system, the raw material starting point must be NaBO<sub>2</sub>.
- Thermodynamic energy to break B-O bond will always be too steep to be economical.
- Issues were well explained. Possibilities for increased hydrogen storage are great.
- Considering the thermodynamic barriers, the approach is reasonable. While it is important to try harder to solve these problems, it is not clear what criteria are used to decide on a go-no go on the approach. One suggestion is for the PI to voluntarily re-scope the project as some pathways are failing.
- Logical, reasonable approach based on three identified pathways for regeneration with a down select to the most viable approach. High cost element (Na) identified and focused on to reduce costs.
- The approach is clear and the project seems well designed and focused. A high degree of understanding of the chemical systems being researched is evident.
- It is unlikely that this technology can achieve the technical goals of the DOE storage program. This research is relatively high risk and significant funds are being devoted to it. Despite the unlikelihood that the technology can meet the targets, the research work is addressing commercialization issues like lower cost materials, well to tank efficiency analyses, etc. This line of research seems inappropriate given the technical shortcomings.
- Approach is well focused.
- Have failed to do the basic energy calculation to see what the total energy cost is.
- Improvements of one step process are appropriate.
- Organic solvent has economic incentive but is much more challenging.
- Electrochemical regeneration seems to be a nonstarter for transportation fuels. Inefficiency of electrical generation compounded to process energy normally makes it energetically and economically unsuitable for bulk fuels.
- Labor cost seemed to be larger than DOE target, so how would cost goal ever be met? How three main research areas, but never said which looked most promising.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.4** based on accomplishments.

- There has been some progress but this project requires a major breakthrough.
- A one step electrical synthesis of the borohydride was demonstrated but the yield of the process is less than 10%. An alternative hydride transfer electrocatalyst for conversion of B-O to B-H has not been found. Concluded that the most promising approach is to reduce the cost of manufacturing Na and therefore NaBH<sub>4</sub>. Even though the results have not been too encouraging, there is evidence of significant effort toward the objectives.
- The PI hasn't proven that the first two approaches have made significant progress, even if progress was made, the overall impact on NaBH<sub>4</sub> cycle is not significantly impacted.
- PI has quickly abandoned electrochemical approach of B-O to B-H work due to low yield. This should have been an intuitive assumption prior to starting work.
- Good progress made with cost of regenerated NaBH<sub>4</sub> lowered by a factor of three.
- Very good; Narrowing down to the best routes.

- PI reports that feasibility of hydride transfer catalyst has not been established. This is disappointing considering the investment in the project over the past year. Is this an indication of infeasibility of the technology?
- The bulk of the technical accomplishments seem focused on improving materials processing, reducing the cost of materials and recycling materials. This would be fine except for the fact that the technology has not been proven capable of meeting the goals of the storage program. This kind of work ought to follow once the feasibility of meeting the volumetric and gravimetric goals has been established.
- Nice result on the one pot synthesis of  $\text{NaBH}_4$ .
- 8.3% yield of  $\text{BH}_4^-$  in one reactor; No success to date on alternate solvent to molten hydroxide.
- Lower energy of formation for Na is an improvement but does not include hydrogen used. It is also based on limitless NaOH at a low price which is not so.
- One-pot synthesis encouraging? How much improvement possible in yield? How much energy required? Any way to recycle  $\text{Br}_2$  and recover energy?
- The well-to-tank efficiency slide is almost impossible to understand. This analysis needs to be consistent with the protocol developed under the H2A effort.
- The group has made some improvements in the overall cost.
- The group has explored a number of options.
- Achieved some improvements in efficiency.
- Cost reduction of Na metal compared to current process seems to be not an apples-to-apples comparison. In the end, one will start with borate and regenerate (not hydroxide or chloride) and need to compare various alternatives from the same starting point.
- Cost reduction by co-production of Na and  $\text{H}_2\text{BO}_3$ .  $\text{NaBH}_4 \rightarrow 4\text{H}_2$  gave 94% mos yield- seems to show they are on right track. No hydride transfer agent found yet?

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

- Has a separate project from center work.
- Look for opportunities for greater collaborations.
- Have initiated discussion for collaboration with Rohm and Hass. Millennium Cell indicated that they are collaborating with the Center of Excellence on a separate effort although there is little evidence of this in the presentation.
- Good partners now and will be incorporated into chemical hydride center on a separate effort.
- Continuing collaboration with Air Products.
- Why is PI not collaborating with the biggest producer of  $\text{NaBH}_4$  Rohm & Hass? (Note: Millennium Cell is actively collaborating with Rohn & Haas through their project with the Chemical Center of Excellence)
- There is very little talk about outside work.
- Fairly limited area.
- Involvement in the Chemical Hydrogen Center on a separate effort as a full partner is very positive.
- Built-in. MCEL and APC would be the potential implementers.
- Industry and academic partners identified.
- Coordination between Millennium Cell and Air Products appears good. Would be nice to broaden collaborations as recommended by previous peer review.
- Well connected to other partners.
- Air Products is good partner with process expertise that's needed here.
- Core business partner in  $\text{NaBH}_4$  regeneration/production may help project. Air Products only collaborator.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.2** for proposed future work.

- Plans are appropriate for this project, but again, it is not clear that the total energy is feasible and that total energy and hydrogen consumption calculation is needed.

- The work plan is appropriate and eventually should lead to a realistic determination of the economic feasibility of the borohydride system.
- The one project worth working on -electrochemical regeneration was abandoned early due to poor yield. PI should investigate dissolving  $\text{NaBH}_4$  in non aqueous media in order to improve recycling yield. This will eliminate the NaOH stabilizing agent and reduce the excessive bonded water molecules to the borate. PI should investigate the work of Dr Boyd Davis at Queen's University Kingston, Ontario, Canada.
- Issues are well known and pathways were explained to overcome these issues. Lots of ideas express during presentation, but need to focus in on ideas.
- This is no reflection on the PI work but rather the difficulties that they are facing. The thermodynamic energy barriers require new chemistry breakthroughs. It is not clear if the current approach is adequately addressing them.
- Good plan for future research direction.
- Continued well-to-tank efficiency and cost analysis is essential.
- Possibility of co-production of Na and  $\text{B(OH)}_3$  is positive.
- Looks fine. Logical progression.
- Engineering feasibility and further cost reduction work is unnecessary until capability of technology to even approach the DOE goals has been proven and verified.
- Have outlined a reasonable plan for future research.
- Continue on track already developed.
- Project needs to determine which area it wants to focus on.

### **Strengths and weaknesses**

#### Strengths

- Millennium Cell has experience in building and operating sodium borohydride based system
- The PI's have long-standing experience in the field. Strong incentive for the success.
- Millennium Cell has initiated this storage approach and thus built up a focused technology base with experience and expertise.
- Strong companies with extensive knowledge in the field.
- Tremendous amount of useful data/knowledge regarding potential regeneration options has been accumulated that can complement future research in this area. In the future, depending upon the situation with materials and energy costs the electrochemical regeneration option may become economically feasible.
- Company expertise with  $\text{NaBH}_4$ ; Collaboration with Air Products.
- The team is striving to answer the critical questions related to the energy efficiency and costs of the regeneration of dehydrogenated fuel.
- New approaches given to low cost for borohydride regeneration/production.

#### Weaknesses

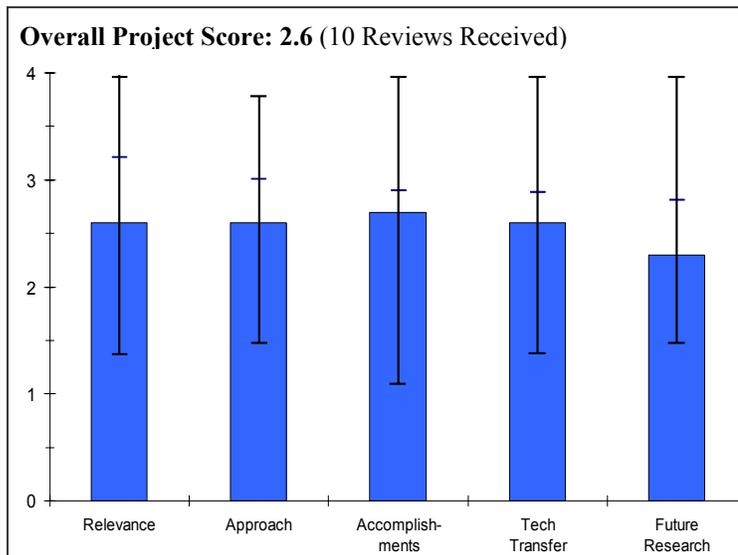
- PI needs to be more forthcoming in revealing the true system operation and the full energy cycle to DOE which will reduce the appeal of their work.
- Millennium cell is not a materials company. Regeneration techniques should be transferred to members of the Chemical Hydride Center of Excellence.
- Basic thermodynamic barriers.
- The regeneration processes are complex and complicated.
- None apparent at this time.
- It can be disputed whether or not the team has actually achieved the  $\text{NaBH}_4$  cost reduction goals as claimed in side 18. More details are needed to evaluate.
- The sodium borohydride system does not appear to be a solution for on-board storage applications at present due to overall energy efficiency (cost) barriers.
- Consistently avoids true cost evaluations; always leaves out the hydrogen value.
- Electrochemical route will always suffer vs. primary energy route.
- Somewhat confusing presentation.
- Project seems to be too broad at this stage.

**Specific recommendations and additions or deletions to the work scope**

- Solid-state material storage level of 21% assumes that the water is available for free. This is not the case and is misleading. PI strongly encouraged to not reporting storage values this way. (Note: PI also reported NaBH<sub>4</sub> solution values and system level capacities)
- It is recommended to bring up the go/no-go decision point once the system analyses work is completed.
- It is also recommended to give the system analyses work on this concept a higher priority to accelerate the decision point.
- Cost of NaOH and impurities in NaOH should be considered.
- Investigate possible effects of impurities in NaOH. May not be as "inexpensive" as first thought.
- Complete the project scope as stated, especially economic feasibility study relevant to the processes developed.
- They need to make a system and run it using waste products and show us the full scope of energy and materials added. Then we will have evidence of progress.
- Determine total energy required for "one-pot" synthesis. Any use for Br?
- Still need to correct well-to-tank slide. Feel like last year's suggestion was ignored. Suggest using overall US mix for electrical generation efficiency/CO<sub>2</sub>.
- Even though the energy and economic analysis was reported out to DOE, a summary of that analysis should be included in future presentations.
- Need to downselect on best method for borohydride production to best use funding still remaining on project.

**Project # ST-13: Chemical Hydride Slurry for Hydrogen Production and Storage***McClaine, Andy; Safe Hydrogen***Brief Summary of Project**

The objective of Safe Hydrogen's project is to demonstrate the viability of magnesium hydride slurry as a cost effective, safe, and high-density hydrogen storage medium. The pumpable, high-density slurry offers infrastructure advantages, and high system energy density with high vehicle range. The focus of the project will be on regeneration of the spent slurry and conversion of magnesium hydroxide to magnesium hydride to meet DOE cost targets for off-board regeneration. Work will also be done on mixer, slurry, and system development to meet DOE capacity targets. During the past 11 months of performance, the researchers have increased the stability of a slurry to a week; they have shown that the reaction rate of the slurry is fast enough to allow a small, lightweight mixer; and they have nearly completed the initial cost and efficiency analyses. In addition, significant progress was made in the solid-oxide oxygen-ion-conducting membrane (SOM) process development: the operating temperature was reduced to 1,150 C and the membrane showed little wear (promising low costs).

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **2.6** for its relevance to DOE objectives.

- Obviously relevant if it works to the extent that the cost targets can be achieved. Slurry idea is excellent in that it may provide an option that mimics current liquid fuels.
- This is a novel proposal of a method of hydrogen storage that needs to be evaluated to determine if it can meet the DOE goals.
- This project is relevant to the DOE program.
- There is partial support of the objectives of this project to the goals of the President's hydrogen fuel initiative. There are other mechanisms for the transport of fuel.
- Irreversible technique that could support both on-board and off-board hydrogen storage.
- The project is in the right directions but can not meet the 2010 system goals so they can not be said to be likely to move us toward the vision. It is an especially safe system which is in line with the vision. Cheaper  $MgH_2$  could be useful if  $MgH_2$  plays a role in other systems.
- On-board system could meet DOE targets. Most expensive part of process is reduction of  $MgO$  to  $Mg$ .
- Project focused on development of a chemical hydride system that has been tested, but with a different material.
- This project has no potential for automotive or stationary applications. This system uses water which will freeze (unacceptable for automotive) and provides humid  $H_2$  stream which is not required for state of the art high temp low humidity fuel cells currently available. Note most stationary applications have switched to a PBI - Imidazole based membrane (low humidity) and has eliminated condensers and humidifiers. Note this system may be used at forecourt stations however the overall efficiency is unlikely to beat ammonia or liquid hydrogen delivery
- Internal combustion engines are likely better suited to tolerate some level of humidity in the combustion chamber

**Question 2: Approach to performing the research and development**

This project was rated **2.6** on its approach.

- The approach is clear and the project seems well designed, well-defined, and well laid-out plan. A high degree of understanding of the chemical systems being researched is evident. Excellent understanding and analyses of the economics of the process.
- Approach seems reasonable.
- Approach is reasonable; project relies on collaborations with other efforts to achieve results on regeneration.
- MgH has high energy density supporting on-board storage.
- PI does not resolve the issue of water in the system- freeze issue. When approached, the PI explained that this was an engineering issue that is solved with using antifreeze instead such as water/glycol. this approach is impractical since it will 1- reduce the system density by water displacement of the alcohol. 2- the antifreeze will have a high vapor pressure which will show up in the H<sub>2</sub> stream, 3- the vaporization of the vapor will have cooling effect and reduce kinetics, 4- if the alcohol reacts, methane and other hydrocarbons could be formed or more damaging aldehydes will form.
- Use of bladder system is completely impractical for any system that generates H<sub>2</sub> based on heat without catalysis. Waste product will always return hot to the fuel tank. Heat will conduct through a membrane and cause premature H<sub>2</sub> evolution on the fuel side that must be contained or purged. How will PI address this issue?
- The main task here is testing various Mg recycling schemes.
- Compares favorably to compressed and liquid hydrogen storage in life cycle efficiency (although this comparison may be optimistic).
- Making slurry stable is well approached. Making MgH<sub>2</sub> is an area where study should help either here or in other Mg systems. Unfortunately the base system can not make the goals so the whole program approach is not sound.
- Some new information has surfaced for carbothermal reduction that shows promise. Regeneration of the MgO by a carbothermal process rather than an electrolytic process could lead to lower cost methods for regeneration.
- Developing a system to meet the 2010 weight targets.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- PI has investigated many regeneration techniques.
- PI finally demonstrated system with Mg, all previous work was based on Lithium experiments.
- The PI's have been delivering their milestones so far. They have been very responsive to comments and directions provided by DOE and the tech team. They have also provided consistently system based analyses.
- Good progress has been made in this project. Cost estimates at large scale production are encouraging. However, the requirement to recycle 95% of the by-product is challenging.
- Very good. Making good progress.
- Progress appears to have been good over the past year. Study of regeneration processes should be complete next year. Analysis shows promise for meeting the DOE H<sub>2</sub> cost target. Addressed reviewer comments from last year very well.
- PI has shown some good results and provided back up data supporting graphs showing that the technology can almost meet the DOE goals. However the back up analyses supporting the graphs will need to be carefully studied. It appears the PI has been optimistic about some of the cost elements which may explain the good results.
- Progress is modest to reasonable thus far. Will the oil used need to be recycled/cleaned-up in some way after use? Wear on the pipeline and pumping systems was not presented nor was it discussed and may be an important component of the economics of a slurry system.
- Energy efficiency calculation looks like it may unfairly penalize the reference systems based on the recycle process chosen. This needs to be checked. None the less, the efficiency is much higher than might be expected and, if proven, is a step forward for this system.

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.6** for technology transfer and collaboration.

- Sufficient academic collaboration seems evident; however, PI has no industrial support.
- It would be helpful to have partnership with one of the Mg producing company or even vertically integrated collaboration through the Mg cycle.
- Significant collaborations are impressive.
- Addition of slurry expert is a positive development.
- Built-in, Safe Hydrogen could be a potential implementer. Good to see Prof. Uday Pal at Boston University involved as he knows the SOM MgO reduction well.
- Some partners are listed, mostly from industry, but it is unclear what their roles have been.
- Mention was made of collaborators but no meaningful detail was presented regarding coordination and technology transfer.
- Appropriate slurry experts enlisted. Good contacts with others in the MgH<sub>2</sub> formation field.
- The project has a number of partners.
- Good use of H<sub>2</sub>A protocols/models.
- Only limited collaborations/interactions.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **2.3** for proposed future work.

- Has the purity of the H<sub>2</sub> stream been evaluated? This stream comes out fully humidified which is not required for future low humidity membranes. Stationary high temp PEM cells are already operating on low humidity which will render PI system incompatible.
- PI underestimates the size of heat condensers required. Most automotive systems have low temp coolant loop at around 50C which reduces the delta temp and thus increase the condenser size. PI is assuming ambient temp condenser. In either case PI does not account for the increased size in heat exchanger required.
- Proposed future activities logical and straightforward. Looks fine, logical progression. Future plans seem reasonable, especially plans to do scale up experiments. Future research plans appear in-line with project goals. Plans are appropriate.
- Future research should lead to determination of the feasibility of the system both on-board the vehicle and on a life-cycle basis. Need to focus on building system, and demonstrate whether proposed energy densities are really feasible or not. This should be the top priority.

**Strengths and weaknesses****Strengths**

- Good management: flexibilities in their approach open to suggestions and easy to understand.
- Good to see the system-level calculation so explicitly spelled out.
- Strong team approach, building a strong base for future development of MgH storage materials including regeneration.
- Strong company with extensive knowledge in the field.
- May be making progress on Mg generation.
- Brought in slurry experts to aid in choosing dispersants to make slurry stable for months at a time. Very good presentation that is easy to follow. The energy analysis was done according to the methodology developed by the H<sub>2</sub>A group.
- Project may have application in marine applications where salt water can be achieved for free.

### Weaknesses

- The biggest problem is the enormity of the tasks: onboard heat management, Mg recycling infrastructure development.
- Unlikely to meet goals. Excess water to keep the byproduct liquid so it can return to the waste bladder is not counted in the mass calculation.
- Methods and equipment used to determine yield are crude. At reaction temperatures suggested by PI, the mineral oil used in the slurry will have a vapor pressure with hydrocarbons in it that the PI has not accounted for. Suggest PI have H<sub>2</sub> stream evaluated for Purity. Suggest that PI evaluate sample with SWRI.
- PI neglected to mention that at least 20% excess water is required in the mixer to ensure kinetics and acceptable viscosity of waste product. PI does not account for this in the bladder design or the fact that the waste product has larger volume than the two reagents. This again will increase the tank size and reduce storage density. Use of bladders is not practical for reasons mentioned above and also that slurry will have a coarse texture which will quickly deteriorate any bladder membrane.
- If hydroxide forms these calculations will not hold, and that needs to be proven not assumed.
- Mass and volume number need vetting, but seem better than might be anticipated. Not at all clear the gravimetric and density calculations are based on numbers that can be truly achieved, condenser for exhaust and tank of only 3 pounds for example.
- There are concerns about his analysis results. They seem to be inconsistent with other analyses.
- For system calculations, several assumptions are made that are not realistic: 1) flow rate is only about half of what is needed; for a more realistic flow, heat exchangers, condensers, etc. will be heavier and take more volume; 2) Fuel tank seems unrealistically light; 3) May need extra water (other than what's used in hydrolysis) to keep system fluid.
- PI is assuming that the removal and re-introduction of the mineral oil will be accomplished for free in calculations (i.e. no loss in yield or energy required) this is impossible.

### Specific recommendations and additions or deletions to the work scope

- Need to focus on constructing system to prove that it has the predicted characteristics (or prove that it doesn't). Progress along these lines needs to be significantly accelerated.
- PI needs to build a system to prove out the estimated system efficiency and cost projections shown in the presentation. The technology seems to be promising, but it is unclear if it is because of its actual feasibility/capability or because of optimistic projections for system efficiency and cost.
- This project will never achieve the 2007 targets. PI should not assume any water will be available from the fuel cell. Future fuel cells will have even less water available than current systems. PI must incorporate FULL thermal management load, condensers, heat exchangers etc.
- System likely to form hydroxides which will significantly decrease the densities of the system. Need to build system and demonstrate that it has the attributes claimed.
- Energy efficiency calculation looks like it may unfairly penalize the reference systems based on the recycle process chosen. This needs to be checked.
- What water displacement method is being used? Unless the hydrogen is extremely dry, h<sub>2</sub> flow meters or mass flow meters will have significant measurement error.
- Recommend to have one of the system analyses teams verify Safe Hydrogen system analyses. This is the key to the go/no-go decision.
- Should be rerouted to delivery where it has more chance. Really they need to make one of these slurry systems as calculated and justify the calculations to show the vehicle based system is viable.
- None. An interesting synergy might be the use of SOM for production of magnesium for this and other purposes such as lightweight automotive structures, which (synergy) could help lower costs due to economies of scale. Suggest talking to FreedomCAR Automotive Lightweighting Materials about possible co-funding of the SOM work.

## Project # ST-14: Development of New Carbon-Based Sorbent Systems for an Effective Containment of Hydrogen

Cooper, Alan; Air Products

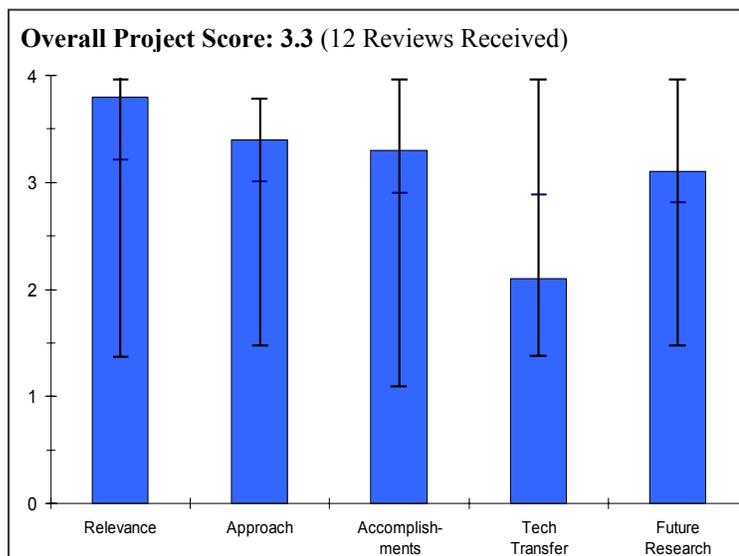
### Brief Summary of Project

Novel hydrogen storage systems are being developed which depend on a facile, reversible catalytic hydrogenation of highly conjugated organic molecule substrates. Current focus is on devising liquid-phase organic carriers that can store and supply hydrogen for both on-board vehicular and stationary applications.

### Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Very interesting project - only one to date that beneficially captures the exothermic reaction of the regeneration process.
- May prove to be a feasible proposal to meet 2010 storage goals. If so, it will fully support hydrogen initiative.
- Work is highly relevant and critical to the issues of hydrogen storage transportation generation and regeneration.
- Goals identified and well defined.
- Process takes advantage of existing industrial practices and uses familiar liquid handling techniques to transport the hydrogen. Air Product is a very capable company in understanding manufacturing and shipping of fuels and gases
- A reversible storage technique using available waste heat.
- Has potential for 6.9 wt-% storage capacity.
- Obviously relevant if the ideas work to the extent that the cost targets can be achieved. Provides an option that mimics current liquid fuels.
- Liquid materials have significant advantage in fuel/refuel and thus align well. Room for improved systems to meet goals.
- Also may make good use of "waste heat", and helps on transport costs.
- Conformable system which is very good.
- Very relevant to the DOE program.
- This concept looks very promising for meeting program targets.
- Good focus on high density reversible liquid carriers. Have the potential certainly to push the state-of-the-art, and possibly even to achieve the 2010 goals.
- What is the volumetric density of hydrogen in these liquids?
- Very innovative new approach (liquid carrier recharged off-board) to the storage problem, which also has implications for infrastructure and production.



### Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- The approach is clear and the project seems well designed. The plan is not articulated, but seems obvious: cut-and-try based on accumulated knowledge. Use of the waste heat is good.
- Target of research takes advantage of utilizing existing or similar infrastructure. Public acceptance of this product will be much easier compared to other storage methods.

- Process to capture regeneration heat will improve well to wheels efficiency dramatically.
- Focused on narrow field of materials - may be limiting on the flip side though.
- There are some under estimations on the difficulties facing this project, namely, a significant progress on the catalyst (lower precious metal loading, with higher activity), new molecule synthesis (with around 100C dehydrogenation), and significant improvement in onboard reformer design and associated balance of plant.
- A methodical, systematic approach.
- Novel approach to meeting storage goals especially addressing regeneration of storage media and dealing with waste materials.
- Approach appears quite reasonable to the goals of the project.
- Approach strong, planned results being achieved, and new carriers identified.
- Suitable overall approach.
- Use of waste heat is a good target.
- Screening many catalysts to get improved rates is appropriate.
- Checking impurities is a good practice.
- New carriers sought with lower temperature of dehydrogenation.
- Focused on carbazole and similar compounds that have low dehydrogenation energy and clean hydrogen separation.
- Secondary focus on porous ionic solids.
- Liquid approach has significant advantages over other approaches.
- Conformable tank design capability.
- Exothermic off board regeneration suggests overall energy efficiency should be good.
- Need to lower temperature of desorption to be consistent with fuel cell vehicles. What are the prospects for doing so?

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.3** based on accomplishments.

- Significant progress in candidate carrier and catalyst identification has been made and verification and validation is underway.
- Very good. Seems to be making good progress especially in the liquid-phase materials. The solid materials are only based on theoretical computations so far, and this work on the ionic solids should not be allowed to affect the work on the organics.
- Kinetics and temperature still unsuitable for automotive applications.
- May already be suitable for home heating or power applications. Since home gas units have consistent pilot burner on for safety purposes, the pilot burner could be used to keep reactor hot to ensure fast startup.
- Interesting approach turning disadvantages of metal hydrides into advantages.
- Conformable storage system is an advantage.
- Data seems to indicate cycling stability but only over 3 cycles.
- Pleased that more technical details are now being shared by PI.
- Capability for high throughput screening of catalysts is to be complimented.
- Met year 1 performance milestone for dehydrogenation (3wt%@150 C).
- New liquid carriers show promise, but lower hydrogen capacity may limit further progress.
- New high gravimetric and volumetric carrier identified.
- Five to six percent delivery in 5 hours at 200C (slightly slow but close to need), rehydrogenation in a few minutes.
- Fourteen hour desorb at 150C. New catalyst has doubled the rate. New isolated material with 6.9% that may cycle.
- Have identified some compounds that look promising, 6.9% demonstrated. High hydrogen quality. Performance of these compounds under hydrogenation-dehydrogenation cycling needs to be verified through more demonstration. Data on possible long-term degradation of the compounds needs to be acquired.
- Have found some promising systems.
- So far purity of output stream looks good.
- Thermodynamics look good in these materials.

- Excellent progress in discovering several new liquid carriers in the range of 5-7 wt.% and with operating temperature of 150-250C.
- Volumetric densities of these liquids should be considered. (Particularly so, since these liquids could have conformable tanks, and therefore could benefit from a "bonus" due to conformability).

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.1** for technology transfer and collaboration.

- Air Products is a reputable company with extensive experience in producing and delivering hydrogen and many other fuels or gases. Air products have excellent understanding of economics and life cycling of equipment etc.
- Air Products could benefit from some more coordination with OEMs in order to fully understand system requirements and practical engineering solutions.
- There doesn't appear to be any external collaboration at the present time.
- Apparently some interaction with outside storage community but no direct involvement.
- Built-in. APC could be a potential implementer. Other collaborators could be the Chemical Hydride Center of Excellence.
- PI has been very vague about outside collaboration.
- There is little outside interaction however, I am not sure that further collaboration would add much to this project. I was informed in private conversation with the PI that other aspects of this project (to be reviewed in another session) have substantial external collaboration.
- Some collaboration with OEMs, but nothing formal.
- Air Products project only.
- Not a great deal of collaboration.
- Going forward Air Products could collaborate with CoE, but it is not a part of a center.
- Partnerships/collaborations not mentioned.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.1** for proposed future work.

- Reasonable plans for future - the project seems to be headed in the right direction.
- Looks fine. Logical progression.
- Looking forward to further confirmation of good results presented here.
- Future plans seem reasonable. It would have been nice to hear more details as to plans for finding new carriers.
- Future activities planned to further year one's work.
- Plans are not very precise, but the route and direction are correct.
- PI is focused well on the remaining barriers of reducing temperature and catalyst loading. PI is using a very high concentration of noble metals at the moment and reducing this may be difficult.
- PI needs to work with materials in the 10kcal/mol dehydrogenation range (limited materials) for this business model to work.
- Environmental assessments will be done when a suitable candidate is found.
- Straightforward continuation of current work.
- Not clear why the ionic solids work has been delayed. If there is no time or incentive to work on this prediction, should disclose the compound so that others might test the idea.
- Future work should be directed at even lower temperatures of operation than currently stated (6 wt.% and 200C for Year 2), and/or higher densities.
- If densities could be significantly improved (i.e., H:C ratios higher than one) with the thermodynamics sufficiently tuned, it might be possible to consider burning some H<sub>2</sub> to heat the liquid to the desorption temperature.

### Strengths and weaknesses

#### Strengths

- This is perhaps the only project in which the fuel is returned to the factory and regenerated exothermically in a manner which the heat can be captured for practical use. This significantly improves the overall system efficiency and integration with other industrial processes.
- Overall, this has been the most promising presentation in the merit review. PI has well thought out the entire process, and recent revelations of materials and progress has done much to provide credibility to project
- Pumping a gasoline like fluid is desirable and understood by the industrial community. This non abrasive fluid has a much better chance of success to work in a bladder based system.
- Since the fluid requires a catalyst to evolve the hydrogen (presumably non temperature dependent in the 0-200C range) the risk of hydrogen evolution in the fuel tank due to hot waste should be minimized.
- Water is not required - big plus!
- Safety of this fluid seems to be better than an ammonia based system- leaks seem containable.
- One of few systems that are conformable and operate at low pressures.
- Competent PIs and has good resources.
- Strong, innovative concept based on Air Product experience and expertise.
- Strong company with apparently extensive knowledge in the field.
- Well organized, with methodical approach, and focused on goals and performance.
- The approach of liquid hydrogen carriers covers several areas such as hydrogen transportation, delivery as well as off- and on-board storage. The project is critical to potentially achieving the DOE targets in multiple areas.
- Clearly see need to stay as liquid; only cycle hydrogen (no cleavage); low volatility; and right range of heat of dehydrogenation; low cost.
- Most completely innovative program we have right now.
- Working with liquids that look a lot like transportation fuels.
- Very innovative and exciting new idea about the combined approach to hydrogen storage/infrastructure/production via liquid carriers. A very important program in the DOE portfolio.

#### Weaknesses

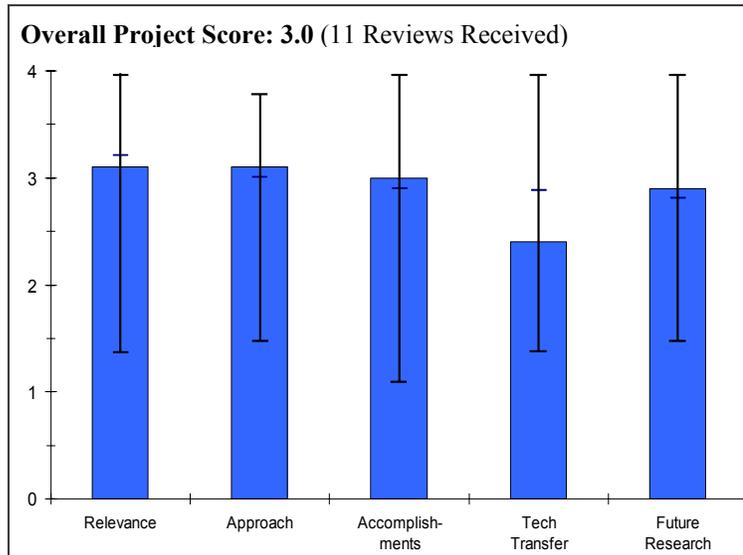
- Could PI indicate what the volatile components that are released in the reaction are? Even though volatility is low. VOCs must still be present to some degree.
- Reducing catalyst loading is going to be difficult.
- Window of opportunity ( $\Delta H$ ) is very narrow for the concept of infrastructure to work.
- What is the viscosity and volatility of the waste fluid? Please reveal more characteristics. Are there several reaction paths that lead to several different waste streams?
- Volumetric density is still low, however conformability of fluid and low pressure will partially compensate for this weakness.
- Would prefer more openness regarding partners and technical details of process.
- PI should present ALL data and details in each presentation. I understand that the presentation in Hydrogen Production and Delivery session was more detailed, but I was unable to attend it because of other meeting/review commitments. Reviewers should not have to base their evaluations on incomplete information.
- Not much collaboration.
- No significant "show-stoppers" have been revealed so far.
- Need to regard low temp operation (will it freeze). Temps remain too high to use the free heat of the fuel cell.
- Carriers' capacities are still a little too low.. Will need to discover new carriers to reach DOE ultimate targets.
- Slow hydrogen release kinetics in material to date.
- Materials with greater hydrogen capacity are needed.

**Specific recommendations and additions or deletions to the work scope**

- Please have PI present the Production and Delivery presentation to the H<sub>2</sub> Storage tech team. Apparently that presentation addressed some of the onboard system design which was lacking in this presentation.
- This is one of the projects which is ideal for system analyses work. While it is asymptotically clear that a new molecule with lower dehydrogenation temperature and much higher activity catalyst are required, an early system analyses could reveal other hidden factors that are needed to be addressed. For example, what is the minimum material-based hydrogen capacity which can yield a 6 wt% (system basis) capacity? Can the PEM fuel cell exhaust adequately provide enough heat? Do we need to burn some of the hydrogen? What is the round-trip energy efficiency? In short, it is recommended to establish the minimum molecular target requirements for this kind of approach.
- Look at potential health effects of new liquid carriers to see if there could be any show-stoppers like there was with MTBE. Make sure the work on the ionic solids does not detract from the work on the organics.
- Would like to see many more cycles run to confirm preliminary results of cycling stability.
- Consider benefits of opening up to more collaboration.
- More focus on critical issues such as catalyst development for dehydrogenation and continuous search for the carrier molecules with improved thermodynamics.

**Project # ST-15: Low Cost, High Efficiency, High Pressure Hydrogen Storage***Ko, Jui; Quantum***Brief Summary of Project**

Quantum Technologies' project goal is to deliver a cost-effective and safe high-pressure hydrogen storage system that will meet DOE targets. The technical plan entails a three-pronged approach: lowering the cost and weight of the storage system (via material optimization, process evaluation and use of lower cost carbon fibers); reducing the amount of material required through the use of sensor technology to monitor storage system health; and increasing the density of hydrogen by filling and storing at lower temperatures.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.1** for its relevance to DOE objectives.

- Although compressed hydrogen storage may not be able to achieve the 2010 DOE goals, it is a technology that is feasible today (only) in prototype use in fuel cell and H<sub>2</sub> ICE vehicles. However, more development of the technology is needed before it can move from the research and development phase and into product engineering phase; thus, continued federal funding is justified.
- Obviously relevant if the ideas work to the extent that the cost targets can be achieved.
- Work addresses compressed storage needs in general.
- Will address short term needs and potentially future systems. Can PI indicate what relevance this project has to stationary cost, weight etc requirements?
- The project is relevant to DOE'S near-term storage goals.
- Obviously relevant if the ideas work to the extent that the cost targets can be achieved.
- This is an important component of efforts to meet the storage requirements necessary for the President's Hydrogen Fuel Initiative. However, it will be difficult for 10ksi H<sub>2</sub> to be able to meet the 2010 goals for H<sub>2</sub> storage.
- Likely to be launched for many vehicles if nothing better comes about. This is aligned with the president's vision. May be useful to other solid material systems.
- Unlikely to meet goals.
- Quantum is seeking to improve compressed storage and thereby lengthen what is considered the short term viability of for compressed storage.
- Good relevance to the DOE program for systems that can meet the 2005 gravimetric targets but not volumetric targets.
- Composite tank development is relevant to a number of different storage technologies besides compressed gas
- Needed for short term applications.
- One of "commercially available" storage components.
- Claimed that objective is to try and enable 2010 targets, but volumetric density of 10000psi hydrogen is already below the 2010 target. Is cool-fuel going to be able to achieve 2010 volumetric target (particularly at 5000psi)?

**Question 2: Approach to performing the research and development**

This project was rated **3.1** on its approach.

- Reasonable approach addressing various aspects of compressed tank R&D necessary for advancing the technology as far as possible
- Approach to the problem is realistic and sharply focused to try and meet storage requirement goals and is a credit to the project and the program.
- The approach appears sound and capable of meeting the project and DOE goals
- The general approaches are clear and logical: minimize the amount of carbon fiber or use less costly carbon fiber by substituting efficient process design ("Cool Fuel") and sensors.
- Compressed hydrogen tanks can only meet near-term goals.
- Reducing fiber cost is right direction. Use of sensors to reduce over design is right direction.
- Increase hydrogen loading by cooling is a possibly useful approach.
- State-of-the-art compressed storage systems that can be integrated into fuel cell vehicles. If volumetric requirements could be relaxed, maybe could satisfy the range requirement of FCVs.
- Good approach to developing a smart tank. Addressing questions of how to do a smart tank by studying damaged tanks by Cool fuel looks promising to achieve full fill.
- Sensor approach should help reduce amount of fiber needed which will help weight, volume and cost.
- Cool fuel approach may result in improved energy density for compressed gas storage systems.
- For cool-fuel, "dormancy" (in terms of temperature) of the fuel should be considered. If one fuels the tank, then parks the vehicle for an extended time, does the system vent hydrogen, or allow the pressure to rise?
- Wasn't explicitly stated, but this cool-fuel system is at 10000psi?
- What are the safety implications that the fuel should heat up?

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- The project made good progress and is accomplishing its objectives. The use of commercial grade carbon fibers has made significant improvements in meeting cost targets.
- Very good. Seems to be making good progress. Has reduced potential cost from \$18/kWh to \$10/kWh. Still long way to go to \$4 and \$2.
- Interesting to see that small damage to the tank had minimal impact on burst pressure.
- Cool Fuel system needs to well to wheel efficiency predictions validated.
- Could system be cooled a little further for cool activated carbon applications? What is the well to wheel efficiency of this system?
- Quantum continues to make progress improving the volumetric and gravimetric efficiencies of tanks.
- They are now assessing the total system, an improvement over last year.
- Progress has been quite good in terms of tank building, testing, the incorporation of sensors and strain evaluations.
- Improved the capacity while switching to lower cost fiber.
- Strain monitor allows damage detection. Thermal model developed to evaluate temperature in fill and operation.
- Unclear the cool fuel will be viable, seems to discount the idea people fill before the weekend and then sit there over the weekend fairly often.
- Very good progress on a number of fronts.
- Demonstrated sensor application to tanks and studied sensitivity of sensors to help determine number of sensors needed.
- Cost analysis of tanks for 3 tracks followed in program.
- Not very much progress has been made, despite the fact that the project appears to have been going on for a year, and that some of the objectives (composite optimization) appear to be quite similar to previous work by these PIs. Need to show more progress more quickly.

- Marginal cost improvements are being made; more effort should be made in order to achieve conformable systems. Cool fuel technology could be interesting if cooling costs and system fill specs drawbacks can still result in overall system improvement.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.4** for technology transfer and collaboration.

- Quantum is working with GM and other suppliers to develop tanks. Manufacturing costs still need to be addressed for practicality of these systems.
- The collaborative effort as discussed in the project presentation is mostly with car manufacturer OEMs to determine customer requirements.
- Fine. Quantum could be a potential implementer, so technology transfer is essentially built-in. Working with GM.
- Although not extensive, collaborations seem appropriate for the technology R&D program.
- Quantum cited work with major OEM manufacturers. No details were provided.
- It would be beneficial to have broader collaboration with developers and manufacturers of carbon fibers.
- Suitable transfer and collaboration.
- Works with major OEMs on tank development. Possible collaboration with solid storage concepts should be encouraged.
- Only limited partnerships/interactions, not defined.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.9** for proposed future work.

- Future plans are incorporating lessons learned thus far and appears focused on the key technical barriers.
- Work on replacing fibers with sensors would continue.
- More effort in general is required to reduce carbon fiber costs - this would have advantages for all hydrogen applications - Quantum should not necessarily conduct this work.
- Looks fine. Logical progression.
- Future plans seem reasonable and logical extensions of prior research.
- Future plans appear to reasonably build on past work.
- The approach is appropriate for their goals.
- System validation is expected in 2006.
- Results will build on current results.
- Would have expected some of the items listed in future plans to have been done already; need to accelerate the effort.

### **Strengths and weaknesses**

#### Strengths

- Quantum has experience in building high pressure tanks.
- Strong company with extensive knowledge in the field.
- Good near-term solution for on-board storage. Concepts are applicable to storage vessels for "chemical" storage applications as well.
- Making progress on fiber use.
- Cost share is above average for a demo project. State-of-the-art for Type IV all-composite tanks.
- System values include balance of plant. One of the few realistic system values presented at the review

Weaknesses

- Quantum has experience in building high pressure tanks but is system designed to get max fill with cool gas? Does this mean that slight increases in temperature necessitate purging? It is not practical to expect that cool temperatures can be maintained simply by driving the vehicle and discharging the tank. This is practical for stationary applications where the discharge rates are more predictable though.
- None apparent at this time.
- Compressed hydrogen will not meet 2010 and 2015 targets.
- Cool fuel system was not very fully elucidated, so it is hard to evaluate if it can work in real use.
- Even with improvements, may not be able to meet DOE volumetric targets.
- Cost higher for cool fuel concept, so goals of higher energy density and lower cost are counter to one another.

Specific recommendations and additions or deletions to the work scope

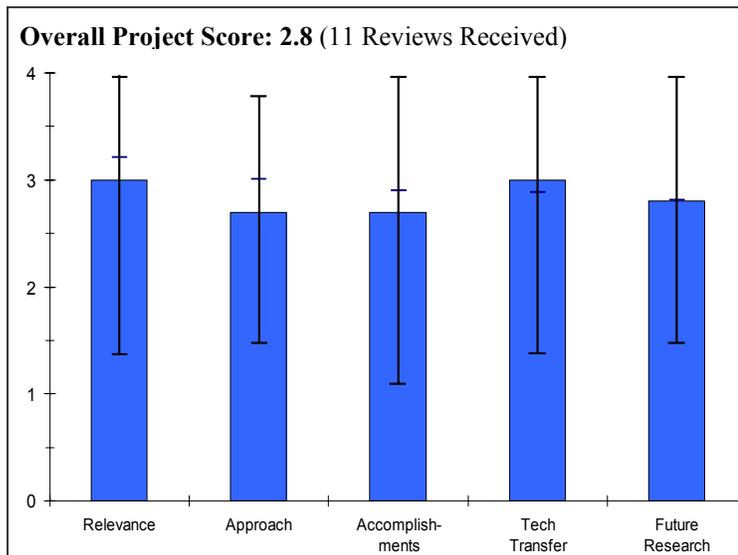
- Would be interesting to have PI perform evaluation of cool fuel tank design for low temperature activated carbons at ~150K and 100bar (system). How thick is the liner with insulation and carbon fiber for these conditions?
- Need to re-evaluate this project and quickly reach a go/no-go point.
- Many of the critical tasks here could be delegated to other groups in LLNL or ORNL.
- Look at possible effects of DOE's low-cost carbon fiber efforts and emerging long-fiber (chopped) technologies.
- Need to find a way for tank developers to work with materials developers to identify lower cost materials.
- Need to work with codes and standards setting organizations to explain value and feasibility of sensors in assessing strength and fatigue of compressed gaseous hydrogen tank systems to avoid establishment of unnecessarily stringent standards.
- Need to run the cool fuel concept through some typical fueling cycles to see if it will work.
- Consider how these tanks could be applied to solid storage systems or how this technology could be adapted for insulated pressure vessels.
- For cool-fuel, "dormancy" (in terms of temperature) of the fuel should be considered. If one fuels the tank, then parks the vehicle for an extended time, does the system vent hydrogen, or allow the pressure to rise?
- Wasn't explicitly stated, but this cool-fuel system is at 10000psi?
- What are the safety implications that the fuel should heat up?

**Project # ST-16: Advanced Concepts for Containment of Hydrogen and Hydrogen Storage Materials***Aceves, Salvador; Lawrence Livermore National Laboratory***Brief Summary of Project**

Lawrence Livermore National Laboratory's (LLNL) project goal is to develop conformable hydrogen tanks and advanced high pressure/cryogenic tank concepts to meet DOE targets. Conformable tanks have the potential to optimally utilize available space in a vehicle and thus greatly improve volumetric efficiency. Concepts developed by LLNL may also be applicable to long-term materials based technologies for hydrogen storage.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.



- The program provides a critical support to the transition as well as long-term solutions to the storage problem. It is the common denominator for nearly all the ongoing projects.
- Obviously relevant if the ideas work to the extent that the cost targets can be achieved.
- Hydrogen storage is critical to the success of the hydrogen program, so need to evaluate various approaches to try to find one that can meet the DOE targets. This project looks at several possibilities.
- The goals of this effort are laudable and one aspect of efforts that are critical to meeting the storage goals of the President's hydrogen initiative.
- Projects don't offer significant breakthroughs in development. Approaches will likely not achieve DOE targets.
- Liquid hydrogen tank and H<sub>2</sub> in N<sub>2</sub> systems aren't clear. Better definition of these systems could result in higher grade.
- Addressing many DOE storage issues.
- If successful, this work could be valuable to OEM's.
- Multiple projects including conformable tanks, insulated pressure vessels and H<sub>2</sub> absorption in LN<sub>2</sub>.
- Well aligned in that the goal is to get conformable vessels which is a step toward the vision.
- Very relevant to DOE H<sub>2</sub> program.
- Most aspects of the project relevant to storage program.

**Question 2: Approach to performing the research and development**

This project was rated **2.7** on its approach.

- This is an innovative approach.
- The general approaches are clear and logical. The dual-use tank idea is neat.
- "Squished" balloon tank - same results as last year, where is the new direction, stress areas are obvious- why is this work continuing PI unlikely to achieve any interesting shapes with this method that significantly improve volumetric density for automotive or stationary applications.
- Cube tank - a cube or rectangle is almost as difficult to implement in a vehicle as cylindrical - perhaps this has a better footprint for stationary applications - although the support rods required will likely diminish gains made
- Liquid H<sub>2</sub> tank - not sure what is different compared to other systems? Is purge H<sub>2</sub> regulated to the outer shell? Large improvements in density seem unlikely; PI must show calculations and assumptions. If it is to be used with cryogenic carbon materials, a heat leak would need to be incorporated into the system.

- H<sub>2</sub> absorbed into liquid N<sub>2</sub> - how much reduction in density with liquid N<sub>2</sub>? How much N<sub>2</sub> is lost in the H<sub>2</sub> stream to the fuel cell? Suspect it would be significant enough to seriously alter fuel cell performance or purge protocol.
- Supercritical hydrogen requires high pressure and cold temperature. Energies and wall thickness will be greater than current pressurized system. Seems unlikely that any DOE goals can be achieved even if materials can be found.
- Project contains a number of independent sub-projects that seem to be a scattered approach. Initially the conformable tank research seemed promising, but the direction of the research project continues to move away from this to other radical and not-so-radical concepts.
- Approach is reasonable. Both components of the two pronged approach are to be complemented.
- While compressed storage is not the long term solution, this project is focused on optimizing the packaging of compressed systems for the nearer term and ultimately may be used for other types of storage.
- Use of struts for thermal management is a good step.
- Conformable containers need to be demonstrated.
- Cryotank approach can limit dormancy losses.
- Approach to meeting the 2015 storage targets.
- Impact of macrolattice approach not clear. Do we need this?
- Given the size of the budget/personnel involved in this project, five separate ideas and thrusts seems to be too much for the PIs to adequately explore. The PIs should downselect the most promising one or two ideas and really focus on trying to make them work.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.7** based on accomplishments.

- Appears to making excellent progress towards project goals. Second generation tank is a significant improvement. Problem -- haven't yet tested the second generation tank.
- Very good. Seems to be making good progress. Really pushing limits of knowledge.
- Only item built is the cube which is not an impressive breakthrough in technology. Gasket used seams very prone to imperfections in manufacturing and installation is no trivial task, likely not amenable to high volume manufacturing.
- No proof of other systems having been built to validate claims is evident.
- The PIs had significant progress in the last 12 months.
- Macrolattice pressure vessel: nice to see the model, but what are the plans to test something to see if there is any real potential there?
- Insulated pressure vessel: not clear that there are any significant advantages over a traditional liquid storage vessel. It appears to be overly complex and could be very expensive. Need to see what testing with BMW will yield.
- H<sub>2</sub> absorption in N<sub>2</sub>: unclear with info presented if there is any real value in this line of research.
- Have chosen design and have built a prototype with high volumetric efficiency.
- Insulated pressure vessel demonstrated proof of concept with Sun Line.
- Insulated pressure vessel meets 2005 DOE targets.
- Did analysis of semiconformable continuous fiber tank and developed test configuration.
- Made test sample of square pressure vessel with struts. Mass and volume numbers are impressive but do not seem to include the full system. No tests of strut vessel yet.
- Not clear how the insulated pressure vessel does better on mass and volume than a dedicated liquid tank - this was accomplished using assumptions.
- Capacity claims are not proven and assume complete fill which has risk if the tank warms.
- Major accomplishment was to turn the cryotank on its side by working with the level sensor (capacitance) manufacturer.
- Demonstrated a working prototype of macrolattice concept.
- Completed design of second generation cryogenic high pressure tank.
- Measured hydrogen absorption in liquid nitrogen.
- Good to see that prototype of macrolattice idea has finally been built!

- Thermal management via these struts is an interesting idea.
- Supercritical hydrogen seems quite unrealistic; if these PIs are serious about this option; they at least need to consider the energetic cost of getting the fuel to these ultra low temperatures and ultrahigh pressures. Will any materials be able to survive these conditions?
- Considering the relatively small funding, it is not too surprising that there seems to be modest progress.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.0** for technology transfer and collaboration.

- PI seems to have sufficient connections with academia and industry.
- Building tanks for BMW is interesting. BMW continues to support liquid based systems.
- PI might benefit to collaborate with tank builders for future work.
- It is somewhat limited but there are good reasons for this.
- Excellent. Lot of partners including potential implementers.
- Some collaboration exists, but beyond 3 industrial partners, presentation is unclear with whom ("many universities") and doing what.
- Stated existence of collaborations with universities and a number of companies provided some details, could have provided more detail.
- Very strong collaboration with industry, universities and other National Labs.
- Suitably connected.
- SNL works with major OEMs and tank developers to understand vehicle requirements.
- Partnerships with tank manufacturers.
- Good to see they are working with an automotive company, at least on one of the activities. Will be very interested to hear about the testing of the cryo-compressed tank in collaboration with BMW.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Future research plans are reasonable.
- Should continue to build the pressure and liquid tanks to validate claims
- PI needs to address the N<sub>2</sub> release from tank to fuel cell, can both N<sub>2</sub> and H<sub>2</sub> be filled from the same port? In what ratios? How often? etc.
- The project looks fine and has made logical progress.
- OK plan, but I really want to see where the conformable tank research is going.
- Future research plans are reasonable.
- Future work is ambitious with well thought out and focused goals.
- If accomplished these would be good plans, but I do not see that many of these items can realistically be approached.
- Have identified pathway to meeting 2010 and 2015 targets.
- Insulated tanks can meet 2010 targets.
- Much lighter tank concepts are required for 2015 targets.
- Fabrication of second generation cryogenic tank will validate current estimates on weight and volume.
- Too many disparate ideas; need to focus on the most promising ones.

### **Strengths and weaknesses**

#### Strengths

- PI is knowledgeable in hydrogen characteristics in the low temperature regime. H<sub>2</sub> in N<sub>2</sub> may be interesting if more characteristics are revealed.
- The project is very innovative.
- Extensive experience in the field.
- The group is very flexible.

- Strong R&D organization with apparently extensive knowledge in the field and well partnered.
- Taking on several storage challenges.
- Prototype testing being initiated.
- If successful, it can be a near-medium term solution for on-board storage. Concepts developed here can contribute to other projects potentially utilizing pressure vessels at low temperatures (such as chemical storage sorbents having low binding energies of hydrogen).
- Clever concepts out of the box thinking.
- Near-term solution of the storage problem. Can meet 2005 and 2010 targets and have developed some thoughts on paths to the 2015 targets.

#### Weaknesses

- Supercritical hydrogen tank likely will never be practical due to excessive energy required to achieve those conditions. Finding a material that can handle those extremes will likely not come cheap either.
- PI does not have experience in tank building. PI should partner with a tank company.
- None apparent at this time.
- A lot of work is being undertaken for the current level of funding.
- The approach is limited by low density of liquid hydrogen to meet 2015 targets and by potentially high system costs.
- 80K and 1000bar is not very realistic thinking.
- Testing results are not presented yet. Promised for later this year.
- This was a very confusing presentation, how many projects is PI working on and how many are interrelated? PI needs to clearly define separation of projects.

#### Specific recommendations and additions or deletions to the work scope

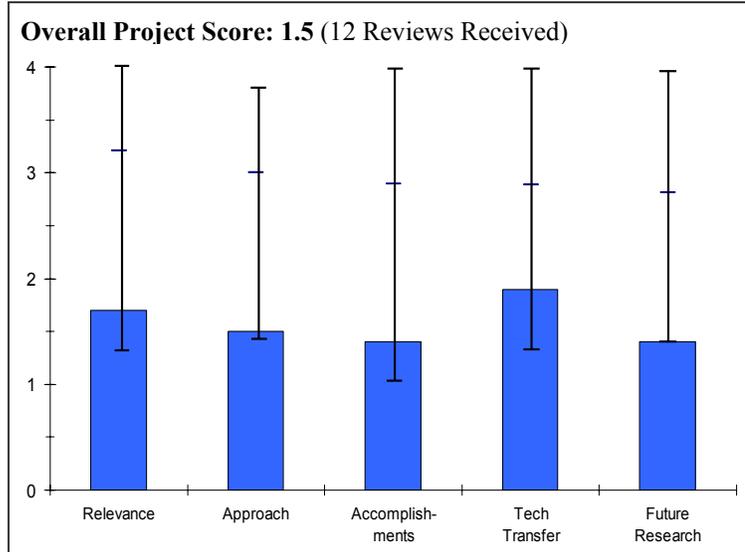
- Rational behind the energy release as a function of temperature and pressure is not clear. Even if the nitrogen is liquefied, will all the hydrogen be dissolved? Where is the pressure coming from? Is PI suggesting that the dissolved H<sub>2</sub> will be slow to desorb from the liquid N<sub>2</sub> in the case of a leak? Systems that leak aren't adiabatic in real life, heat will always be absorbed.
- There have been several significant steps accomplished this year but more importantly this momentum must be maintained.
- If the pace of the progress in this area is maintained, the status of the program should be extended to a full center.
- Look at emerging chopped long-fiber technologies to see if they have any chance.
- LLNL ought to try to narrow down the number of alternatives being evaluated; eliminate those with no likelihood of meeting cost, feasibility or DOE goals; and focus on those with some hope.
- Detailed cost analysis considerations for each approach are recommended to be included in the project scope.
- Test something other than the old existing system. Need real numbers, not estimated numbers.
- Work with Quantum to define pathway to meeting the 2015 targets.

**Project # ST-17: Advanced Manufacturing Technologies for Renewable Energy Applications**

*Ryan, Chuck; National Center for Manufacturing Sciences (NCMS)*

**Brief Summary of Project**

Working with DOE and the private sector, the National Center for Manufacturing Sciences (NCMS) will identify and develop manufacturing processes for the affordable manufacturing of hydrogen and fuel cell technologies, and will leverage manufacturing expertise from other industrial sectors. They will conduct workshops and solicitations and assess the feasibility of manufacturing technologies identified as key to cost reduction. This Congressionally-directed project started in 2004 and received an additional earmark in mid-2005.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **1.7** for its relevance to DOE objectives.

- While the ability to manufacture hydrogen enabling technologies is critical to the federal hydrogen initiative, it is unclear if this project will significantly contribute to the goals of this program.
- While activities may support the President's Hydrogen initiative, alignment to DOE Storage targets is not clear. In theory, this is not a bad idea; however fuel cell and hydrogen storage technologies have not advanced to the point where volume manufacturing should start to be considered. This forum is particularly premature for any hydrogen storage systems since no system has demonstrated practical performance at this point.
- These funds are best used for educating researchers that the materials and processes they are working on need to be amenable to manufacturing techniques, and to eliminate research options and materials that have no practical scale-up opportunities. Perhaps the DOE can conduct their own workshop with all the PIs in conjunction with the end user OEMs to discuss manufacturing options and requirements in order to better direct PI research.
- There is no clear indication as to how this center is calibrating their work versus DOE storage goals.
- Unable to judge until the proposals are selected.
- Project assumes that the private sector is unmotivated and incapable to respond to motivation of the initiative itself and that the PI's organization is more capable than the balance of the private sector in finding and coordinating manufacturing research and development efforts. Both assumptions are questionable.
- Basically only held a workshop and that is not part of the vision.
- Potential to be meaningful, but need to actually do something.
- The project nominally supports the hydrogen initiative as evidenced in its objective/mission statements. However, until the projects are fully defined, it is not possible to determine if this is so.
- Project selection process at NCMS is not conducive to choosing projects that best meet goals and objectives set by DOE and the President's Initiative.
- Projects chosen could be completely outside the critical needs of the program.
- Appears to be in conflict with the funding agency (DOE).
- Program is not focused on DOE objectives, does not support the President's Hydrogen Fuel Initiative.

**Question 2: Approach to performing the research and development**

This project was rated **1.5** on its approach.

- The general approach to developing the collaborations is obvious, but the approaches to the specific proposals remain to be seen.
- Approach seems reasonable, but after 7 months there is no significant progress to show.
- The approach is reasonable.
- The approach is poorly designed, and not well integrated with other research in the DOE portfolio. Underway for 6 months, the technical approach is not defined.
- Ideas were biased toward pre-chosen presentations/proposals by members.
- NCMS being heavily based on automotive manufacturing, is completely ignoring the guidance of the OEMs. DCX, Ford, GM, and Toyota were all present at the workshop.
- PI has no practical experience with fuel cells or hydrogen storage and thus has no way to determine the level of technology and what issues require attention. A one day workshop attended will not suffice to learn the issues and thus their funding decisions will be gravely misguided.
- This is obviously a “money grab” since any participant who has been awarded a project will need to start paying dues to NCMS. This is not in the spirit of DOE funding (although it can be assumed every tax payer pays dues to the DOE through taxes).
- Limited discussions on the barriers and how they were addressed.
- The project selection process appears to be somewhat closed. Not sure how much input DOE will have.
- The only items of value are the projects selected which may or may not be relevant to DOE Program needs. DOE must have the final approval on which projects go forward.
- The only value added by NCMS is project management.
- Appears to be in conflict with the funding agency (DOE).

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **1.4** based on accomplishments.

- NCMS has conducted one workshop. Results were confusing since most attendants agreed that the level of technology was advancing too rapidly to discuss manufacturing of already obsolete components. Why should anyone fund a cheaper humidifier when the aim is to eliminate them with low humidity membranes?
- Most of the topics they highlighted are still basic materials research which has nothing to do with manufacturing at this point.
- PI states that this project is 23% complete but they have nothing to show for this other than a report of a workshop and a list of participants providing "preliminary program inputs".
- Presentation was perfunctory; no valuable information was presented and no progress or accomplishments reported.
- The accomplishments thus far are modest and could have been achieved through other means.
- Only workshops have taken place with proposals solicited.
- While NCMS is collecting proposals, no proposal details or technical accomplishments mentioned.
- Project has recently started. No technical accomplishments have been demonstrated.
- Virtually no meaningful progress.
- Not much to report for \$3 million in FY 2004.
- Workshop appears to be the major accomplishment.
- Two workshops and a website with project proposal forms do not constitute progress.
- Should have shown all the project proposals received, which were rejected, and why.
- The group has made no technical progress. .

**Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **1.9** for technology transfer and collaboration.

- Technology transfer and collaboration have yet to be seen.
- PI listed many company names but gave no indication if any of them will actually be participating in federally funded research.
- NCMS is not strongly supported by the OEMS. DCX is not a member.
- This project will do little to educate the participants on manufacturing issues. This is best left to the normal business practice of OEMs specifying their requirements to researchers. NCMS is a redundant entity.
- The type of information to be gained and shared by this project could be done through other means without the need for the support of a separate project.
- Many participants involved in project.
- Excellent connections.
- Each project could collaborate with the others but the projects have not been selected yet. It is unclear if any storage-related work will result. This is a potential strength that NCMS could bring to the table.

**Question 5: Approach to and relevance of proposed future research**

This project was rated **1.4** for proposed future work.

- The proposed research may lead to improvements but it was quite difficult to tell based on the information provided.
- Have had workshops to initiate project solicitations, so all work is "future" work.
- Proposed scope appears too broad. Focusing on critical few aspects would ensure better progress towards objectives.
- Can't say, they really were not shown.
- Projects have not been defined yet.
- The proposed future research depends on which projects are selected.
- The proposed future work as currently stated is unlikely to change the relevance or progress of this activity.
- Perhaps the single most obvious "low hanging fruit" project that NCMS could have funded was not selected. [A project submitted by a rubber hose maker to manufacture.]
- Wait and see.
- Want to see what the proposals are first. Disappointed that the PI did not provide the opportunity to review the kinds of manufacturing projects suggested for future expenditure of federal funds - if only from the broadest perspective.
- Strong lobbying committee that knows how to solicit funds.

**Strengths and weaknesses****Strengths**

- None apparent until the proposals are seen.
- Many participants involved in collaboration.
- Concept of the project is expected to address critical manufacturing issues that are vital for implementation of new hydrogen technologies.
- Significant cost share [to be provided by proposers (not by NCMS)]
- NCMS could bring together a diverse industry group to address manufacturing issues, if properly utilized.

**Weaknesses**

- NCMS is a redundant and unnecessary entity. The OEMs are capable of addressing their own manufacturing requirements with suppliers.
- Difficult to assess this project.
- None apparent at this time.

- The presentation was superficial and lackadaisical, almost as if NCMS does not value their participation in the process or the input received. This is truly disappointing considering that almost \$3 million of taxpayer dollars are about to be expended on research projects funneled through NCMS.
- No mechanism discussed or otherwise presented for developing a ranking and prioritization of manufacturing needs or differentiating between that which is possible now and that which will need further development. Project was poorly motivated by speaker and in overheads provided both of which did not make a strong case for the need of this work.
- Project, as presented, doesn't identify any technical goals, progress or approach. While it is understood that this project has not been running for long and therefore may not have much in terms of accomplishments, technical goals and approach should be defined.
- 23% task completion has been stated, however, no new concepts of ideas have been reported so far.
- This program was given a large list of valuable projects prior to the workshop. These were ignored when the workshop was held. It is unclear what they will actually do.
- Storage work will be only a portion of the available funding.
- No guarantee that projects will be selected that address the technical barriers and goals of the President's Initiative.
- Too much of the monies are going directly to NCMS, which does not have the expertise in-house to provide a significant contribution to the advancement of the Hydrogen Economy.
- High NCMS structural cost overhead.
- Having NCMS going around the country talking to fuel cell/hydrogen storage developers/etc to explain the work and gather work is a waste of funding, since DOE has already done that.
- Difficult to make constructive criticisms on such a project. Don't see a purpose for the project.
- This program is extremely weak; it is poorly connected with DOE objectives and other research in the DOE portfolio.
- No real attempt to even address the goals or further the vision.

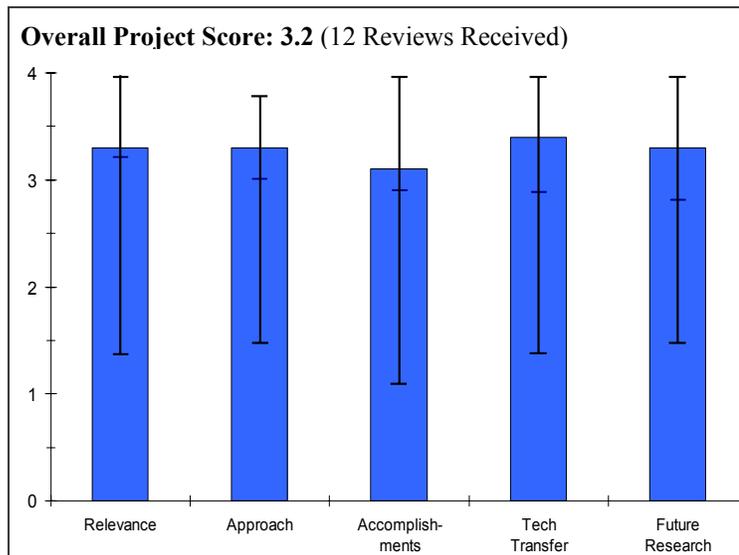
#### **Specific recommendations and additions or deletions to the work scope**

- Project team should spend time with DOE to focus on and establish goals and then identify an appropriate technical approach for accomplishing those goals. A milestone chart with timing and deliverables as addition to the project plan can be recommended.
- Try to steer storage work to address manufacturing issues with high-pressure and possibly cryogenic storage containers.
- Delete the task to provide a clearinghouse of information to promote technology utilization; this is a cleverly disguised support activity for the library staff at NCMS.
- Delete the task on development of the website <http://hydrogen.ncms.org>. It is a duplication of information that can be found on the DOE website.
- Delete the roadmap development task led by NCMS. FreedomCAR and Fuels Partnership Fuel Cell and H<sub>2</sub> Storage Tech teams (industry and DOE members) should offer advice and consent to the project portfolio to ensure alignment with the President's Initiative.
- Do a benchmark on the NCMS project management fees relative to other organizations to ensure they are competitive.
- Keep on working the proposals.
- Presentation of non-Storage activities should be withheld from Storage review sessions.

**Project # ST-18: DOE Carbon-based Materials Center of Excellence: NREL Activities and Overview**  
*Heben, Mike; National Renewable Energy Laboratory (NREL)*

**Brief Summary of Project**

The focus of the National Renewable Energy Laboratory's work is on hydrogen storage in carbon-based materials in conjunction with the DOE Center of Excellence (CoE) on Carbon-based Hydrogen Storage materials. The objectives are to determine the extent to which metal-carbon hybrid materials can reversibly store hydrogen, to tailor the mechanism of hydrogen storage through nanostructural control, and to develop low cost, reproducible, and potentially scalable processes for production. The main focus in 2005 was on producing materials that reproducibly store hydrogen with capacities greater than 4 wt% at room temperature and pressure.



**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.3** for its relevance to DOE objectives.

- Hydrogen storage is the highest priority research area supporting the vision of the hydrogen economy.
- Centers of excellence are important initiatives supporting development of hydrogen storage technologies.
- In line with the program objectives.
- It is likely that most of the novel material breakthroughs will come out of this area of research. It currently seems that the most efficient systems will be achieved with materials in this 10 to 50kJ/mol range. Center of Excellence should remain open to all materials (not just carbon) in this range.
- These materials don't seem to have many of the hazards associated with metal hydrides (pyrophoric, etc) and don't require as much rare earth components.
- The Center of Excellence addresses a variety of DOE plan objectives and is relevant to the President's Initiative.
- The PI clearly presents the objectives and the goals of the Center of Excellence and the related projects.
- Good science; thorough investigation of carbon-based materials potential; it has moved beyond SWNTS.
- This project is one aspect of efforts that are critical to the achievement of the goals of the President's hydrogen fuel initiative.
- Goals identified with strong alignment to the project.
- Can carbon be a cost effective solution for H<sub>2</sub> storage?
- A light material that has a moderate strength bond is well in the scope. However the goals are highly unlikely to be met with normal nanotubes based on current understanding of physics. Metalized carbon materials have potential to meet goals if light metals will work. So the program has had mixed relevance but is moving in the right direction.
- Very relevant to the objectives of the DOE H<sub>2</sub> storage program. Originally only appeared to have a chance to meet 2005 targets but have shown pathways to engineer materials with up to 8-9 wt. percent.
- Generally relevant to program, but many of the materials under study will not meet volumetric targets.
- Good to see focus on new ideas, potential higher-density materials, etc.
- The newly proposed doped-C60 materials have the potential to meet the 2010 gravimetric goal, though volumetric densities are less clear.

**Question 2: Approach to performing the research and development**

This project was rated **3.3** on its approach.

- The project adopts the acceptable approach to focus on a variety of technical issues to investigate alternative and innovative solutions.
- PI has broadened the R&D approach beyond carbon nanotubes to other carbon based storage technologies increasing the chance of success.
- The taken approach of reproducible activation and rational design of adsorbents brought a breakthrough and moved the work a step forwards. Very promising work.
- Approach is quite reasonable. There is a nice coupling of theory with experiment.
- Project is well organized and strongly focused.
- Project is integrated with other research including new Carbon CoE.
- PI has assembled a strong team of industry and academia.
- PI has expanded scope beyond SWNT.
- PI is beginning to focus activities using modeling to predict stable materials and, as appropriate, equipment in order to synthesize materials.
- PI has done a good job in addressing measuring techniques of these materials which to date have been difficult and sensitive.
- Need to tie in the material development work with the final storage system requirements.
- Develop a clear material vetting process for down-selecting the candidate.
- No clear pathway is given for the synthesis of the molecular modeling work.
- The metalized work makes sense to follow through on.
- The work on simple nanotubes was less likely to yield functional compounds.
- Use of theory to guide experiments is good (generalized gaussian DFT).
- Approach to materials other than SWNTs gives NREL hope to achieve higher wt. percents that have a chance to meet the 2010 targets.
- The rational design of adsorbents appears to be a good approach and one that is necessary to move beyond the SWNT work. A better approach than some form of combinatorial investigation.
- Using modeling, different synthesis techniques, different carbon structures; attempts to look at many aspects of absorption process for hydrogen storage.
- The main idea on which the majority of the work is based is theoretical; need much more information as quickly as possible about the experimental viability of such an idea: how can (large quantities of) these materials be made, will they be stable, and of course will they store the amount of H<sub>2</sub> predicted?

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.1** based on accomplishments.

- The highlight of the last year is the portfolio diversification of the possible carbon-based storage molecules. It is critical to continue this pathway and create a well-balanced program with proper risk mitigation.
- The results well support the progress also in consideration of the effort to have the CoE starting with the related project operative.
- Good work beyond CNT. Many research paths being followed by technically competent researchers resulting in very interesting progress.
- Modeling of higher capacity materials has been synthesis of these materials has not been demonstrated yet. These materials could be extremely difficult to manufacture at first. If manufacturable, it will take some time before the processes are robust and efficient.
- Advances in material development via reproducible processing.
- Promise of high reversible storage with carbon-based adsorbents.
- Advances in measurement techniques for materials and accurate sample screening.
- Accomplishments have been quite substantial; in many ways leads the CoEs in accomplishments relative to funds expended.
- Significant accomplishments, making progress towards goals.

- Since the Center was formed, the NREL project scope has been broadened significantly so that a number of innovative ideas and approaches have been generated targeting new materials discovery.
- Calculated binding energies in various carbon metal complexes. Challenged for volume goal but perhaps other materials of the same sort will yield better density.
- Apparently show that simple nanotubes are not holding much more than what the metals bind.
- Made BN single wall nanotubes. Built multisample test station.
- Not a lot of lab movement but good theory progress.
- Excellent progress in past year on a number of fronts. Understood the effect of metal introduction into the SWNT on uptake of H<sub>2</sub>. Developed materials that show reversible 6-7 wt. percent capacity.
- Experimental results have been verified by others. Addition of CoE partners offers good prospects for achieving higher weight percents.
- Appears to have validated measurement techniques.
- Has improved understanding of source of earlier variability in measurements.
- Should give more attention to the projected volumetric H<sub>2</sub> density of these modified C60 structures. In a relatively optimistic case, the projected density is 43 kgH<sub>2</sub>/m<sup>3</sup>; do these materials have (even theoretically) a chance to meet the 2010 or 2015 goals?
- Showed binding energy for single metal atom on a single pentagonal ring. However, is there metal-metal interaction (i.e., is the binding still strong for a fully covered C60 molecule with 12 Sc atoms?). Is the fully-doped system stable with respect to decomposition into C60 + metal or C60 + metal hydride?
- The desirable H<sub>2</sub> binding energies were calculated with GGA, but later it was stated that LDA is generally closer to experiment. This raises the obvious question: what are the LDA binding energies for H<sub>2</sub> onto these metal-modified C60 molecules? Are they still in the "desirable" range?
- Assuming the best-case scenario (full implementation of the H<sub>2</sub> economy), what is the total amount of Sc that would be needed? Is there that much Sc in the world?

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.4** for technology transfer and collaboration.

- The Center of Excellence has a well structured network of internal and external contacts, with appropriate connections with some independent project, such as SwRI testing and Argonne system analysis.
- PI has assembled a strong team of industry and academia.
- PI is using tank modeling to understand material requirements in a viable automotive system.
- The direct technology transfer to industry requires more effort.
- Broad and well respected collaborations. Only possible concern is that there may be too many institutions working on too many things to be able to adequately manage and direct.
- Very good collaboration record.
- An extensive list of publications.
- Good record of conferences organization.
- Work is well coordinated with external partners. Developments from the partners and external community are incorporated where appropriate into Center efforts.
- Very strong collaborative effort, including several universities, other National Labs and industry members
- They are well connected. They did point out the size and diversity of the team. Little industrial collaboration, but they are far enough from production that is not problematic.
- Collaboration has increased over the past several years as NREL has interacted with other organizations attempting to duplicate their results. Addition of Center of Excellence partners will only increase the collaboration in the future.
- Collaborations include universities, industry and staff at NREL

**Question 5: Approach to and relevance of proposed future research**

This project was rated **3.3** for proposed future work.

- The Center of Excellence is the most appropriate mechanism for integrating knowledge, expertise and for pooling resources in a range of research areas.
- The future work plan is to be complemented on the detail with which it was presented and the degree of incorporation of other organizations (i.e., Air Products & Rice) on the steering committee.
- Future work directed to support goals and accommodate previous review comments.
- Expanding beyond SWNT is critical.
- Revisiting the pseudo cold/pressure region is recommended, this may be the "sweet spot" or at least the happy medium where overall system efficiencies can be acceptable in terms of compression/cooling energies and transfer from forecourts to vehicle tanks - especially if bulk transport of hydrogen will continue to favor liquid hydrogen.
- Difficult to manage breakthrough. However a key metrics is how many materials are rejected. Optimal use of the resources will be a critical issue.
- The future activities require more specifications.
- The work appears based on experimental results and progress.
- Future plans to roll research into the center of excellence make sense.
- Need to continue on path away from carbon nanotubes to evaluate other alternatives.
- The future plans described here are building on past experience making appropriate steps forward.
- The group is encouraged to examine work beyond nanotubes.
- Interesting plans but they are really for the new center program so it is hard to evaluate.
- Work plans at NREL build on past work and really move off the SWNT path.
- Addition of CoE partners really broadens the work front and gives the carbon-based approach a chance to meet the 2010 goals and position the group to propose pathways to reach up to 8-9 wt. percent material.
- Will fold into CoE.

**Strengths and weaknesses**Strengths

- Center has aligned itself with the appropriate partners and is learning what potential systems may look like.
- Systems in the 100bar, 100K range seem to have good potential. The usable capacity of the materials exceeds any metal hydride systems.
- The materials come from cheap sources- time will only tell if synthesis of the large carbon structures will be cost effective.
- Excellent resources.
- Outstanding personnel with superb scientific background in the field.
- The integration of expertise, equipment and know how's in the CoE may be an accelerating factor in reaching the proposed objectives.
- The CoE has developed instrumental resources of valuable and general interest.
- Strong collaborations with key organizations.
- Strong team delivering very good science.
- The group is very well organized.
- Significant collaboration with industry, universities and other labs.
- Broadening scope of the project towards generating novel concepts and new materials discovery, focus on fundamental understanding as well as systematic approach (modeling) increases overall probability of success.
- Theory to guide experiments is a good improvement. Move to metal doping gives a possible success route that does not need new physics. Adding low temp work is a good move.
- Partners bring wealth of experience and new ideas to the field of C-based H<sub>2</sub> adsorbents. CoE appears to be off to a solid start.

### Weaknesses

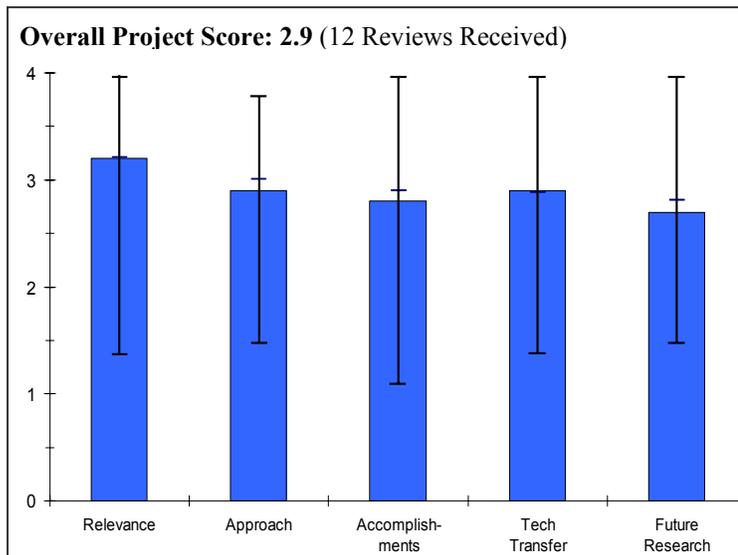
- Should increase flexibility.
- Difficult but try to find the optimum balance.
- Need to establish the internal material selection process/criteria.
- The start of the CoE and the establishment of defined projects may reduce the flexibility of small research groups to freely establish collaborations (outside the CoE).
- Still a risk area that may not deliver.
- With all of the parties involved coordination could be very challenging.
- Still some approaches consider 5-6%wt storage capacity (material basis). In addition, volumetric and cost targets aren't always given a priority.
- Still a very difficult thing to accomplish. Metals may not stay put. Density is too low but they may be able to find a solution.

### Specific recommendations and additions or deletions to the work scope

- Center should continue to expand activities beyond carbon work. It seems that all materials with low bonding energy 10 to 50kJ/mol would be appropriate for this center and the systems would be similar.
- The system analyses work on SWCNT should be given a high priority to establish the minimum baseline requirements for the material.
- The key issue with these materials is the volumetric storage. Powder packing and densification (as shown in metal hydride) is one of the important parameters. Need to address the structural vulnerability of these materials early on.
- The future work plan has to include better specification on a complete characterization (including cycleability) of the selected materials with protocols agreed to with other CoEs and with SwRI.
- DOE ought to consider a go/no go decision regarding single wall carbon nanotubes as it is clear that early promise has not been repeated or confirmed and likelihood of meeting program goals is slim.
- Carefully follow the planned milestones.
- Carry on with the work on a wider variety of carbon-based materials.
- Ensure an appropriate mechanism is put in place for the effective management of the Center of Excellence; this could be challenging in view of the size of the consortium and the diversity of the expertise there.
- Continue with the forward plan with an addition of go/no-go decision points for every approach, having in mind meeting all the targets (system basis) as a top priority.
- Should try to verify that metals on nanotubes do not move. This would best be done with single atoms but one may well get the answer with patches.
- Synthesis of these advanced carbon materials seem difficult to manufacture cheaply. Could PI present more information on general production methods and economies of scale?
- Should start narrowing the gap between molecular engineering work and macro system requirements.

**Project # ST-19: Analyses of Hydrogen Storage Materials and On-Board Systems***Lasher, Stephen; TIAX LLC***Brief Summary of Project**

TIAX will evaluate the projected manufactured cost and performance of four broad categories of on-board hydrogen storage options: baseline (compressed hydrogen), reversible on-board (e.g., metal hydrides), high surface area sorbents (e.g., carbon-based materials), and regenerable off-board (e.g., chemical hydrides). System-level conceptual designs, process models, activities-based cost models, and lifecycle performance/cost predictions will be developed for each system based on developers' on-going research, input from DOE and key stakeholders, in-house experience, and input from material experts. This will be an on-going and iterative process so that DOE and its contractors can increasingly focus their efforts on the most promising technology options.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.2** for its relevance to DOE objectives.

- This type of modeling is crucial in order to provide guidance to material researchers as to the true requirements of the materials they are developing. This information needs to be consistently relayed to all other PI researchers.
- Good to see where we currently stand with cost, performance and overall model refinement.
- One of the most critical projects. The main criticism is why DOE did not start this type of work much earlier.
- This project provides analysis and validation of fuel cell system performance, and projects cost factors and life cycle analysis based on current state-of-the-art inputs from suppliers.
- Recognize need for independent financial analysis of hydrogen storage systems.
- A critical component of the initiative. It will help assure viable pathways are identified and followed for economic onboard storage systems. Wish they were designing for DOE storage rate, volume goals -- hence a slight downgrade on relevance.
- Idea is well aligned.
- Alanate is probably the best material to use at the moment though it will not meet goals it is likely to be similar in many regards to "the material" and so will be a suitable surrogate. Model is probably only the first cut.
- Very relevant to the objectives of the DOE H<sub>2</sub> storage program. Materials developers need the benefits of a systems approach to understand the implications of BOP components on the characteristics of the storage system. DOE needs the ability to compare storage options on a consistent basis.
- Very relevant to R&D plan objectives. Analysis of all storage options on a self-consistent basis very important to understanding where DOE should put its emphasis.
- Supports program and program participants by modeling projected costs of storage system types.
- An important program in the DOE portfolio. Important for not only DOE, but generally for all of the PIs to be aware of these sort of system-level issues, and will help guide new and existing projects.

**Question 2: Approach to performing the research and development**

This project was rated **2.9** on its approach.

- PI did good job of accumulating much data from reliable sources.
- Modeling is based on current technology without being overly optimistic about novel approaches.
- Well thought out with many factors incorporated. The effects of cycling/lifetimes should be integrated into the results.
- The rating could have been 4 if the mid-point estimate would have been re-calibrated to a more realistic case; and the most optimistic case and pessimistic case would be given some probabilistic quantity.
- It is imperative to develop a rigorous model as the results may have profound implications on future directions of the DOE's grand challenge.
- Thorough, systematic approach back on realistic input from suppliers and potential users.
- Approach is logical and reasonable, but question whether or not there is sufficient technical progress and information in the various technology areas to begin making financial assessments at this early stage of the program.
- The approach is reasonable and generally well thought out.
- Not very detailed model technically but that may be OK for the moment. An assumption of current assembly process is disturbing if this is ever used for cost prediction. Cost model is adequate though not complete. Sensitivity analysis is a key point.
- Approach is to develop a generic system design that is based on available literature, information from developers, and theoretical analysis where data are not available. The cost of manufacturing this system is then estimated and the energy efficiency and well-to-wheels efficiency can then be estimated. This approach allows a consistent comparison across the various storage options. It gives materials developers a sense of the complexity involved in designing a realistic storage system.
- Have all appropriate components.
- Not adequate consideration of various system designs.
- Limited scope to date.
- Doesn't provide information that PIs or program managers can use to direct projects toward better storage systems.
- The approach seems sound. There are many assumptions involved in any such analysis, but these assumptions are clearly stated; the method needs to be flexible enough to be able to easily react to changes in the assumed input parameters as new data is generated and new materials are discovered.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- The project is showing significant progress towards meeting goals.
- Sobering results reveal extremely heavy systems
- Results are exhaustive and realistic given current data available.
- Achieving results will be more complicated with chemical hydrides as the potential amount of systems permutations will be much larger.
- Continue work for cooled activated carbon like materials.
- Used lots of design work from UTRC's project and lots of the numbers used (60% packing) are very optimistic based on the actual progress of the UTRC project.
- Very good start.
- Significant progress - compressed gas and metal hydride storage analysis completed.
- It seems to be too early in the development process of a NaAlH system to exercise the amount of rigor necessary for financial analysis. It is too early in the program to expect any directionally correct results.
- Gathered input data.
- Model based on current UOP assembly process which is very suboptimal.
- Model constructed to test this.
- Have looked at some sensitivities.

- Properly finds this system will not meet goals.
- The results are surely in the right direction but the answer was known beforehand.
- Value is in sensitivity identification and generalization (which is not clearly present).
- Results for a sodium alanate system were presented. The assumptions used in developing the analysis were conservative. Sensitivity analysis can lead to alternative designs and point out areas needing further development. This analysis represents the base case which will be updated as advanced materials are developed.
- A good start for the first year.
- Good to use the Na-alanate for the first base-case study. Pretty much shows what we all would expect.
- Completed most of analysis for specific design.
- Has done limited sensitivity analyses.
- Has not considered many of the aspects of the design considered.
- Good progress on the alanate system design. The results show the serious challenges involved in using this material in a system.

#### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.9** for technology transfer and collaboration.

- Collaboration with academia is very good in order to define material characteristics.
- More coordination is required with tank manufactures to determine practical tank building techniques; current schemes are not amenable to mass production.
- Lots of data used is based on UTRC goals which they have had problems meeting.
- Active team approach includes university partners. Also receives feedback from noted labs, developers and other stakeholders.
- Are the collaborators chosen sufficiently expert in the fields of engineering and manufacturing to contribute to cost assessments?
- The project has not provided significant evidence of working with equipment manufacturers regarding developments in the industry. This question was adequately addressed in the Q&A time period.
- Suitably connected.
- Collaboration with other organizations is good. It is particularly strong with developers as each system is developed.
- Urge that close connections remain with national labs and centers of excellence.
- Might wish to expand collaborations to industry projects (e.g., UT, P.S4). Would help to reduce any possible duplication of effort.
- Clearly has good potential for tech transfer to industry and others.
- Consistently references work/individuals providing input to model.

#### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.7** for proposed future work.

- Active plans to complete analytical tool for chemical hydrogen and carbon-based storage systems to allow "level playing field" comparisons and the leading storage technologies.
- Thermal integration to the stack will be important next step to evaluate if any system mass reduction is possible and effect of slow kinetics from the fuel cell coolant loop on hydrogen demand.
- Continue to coordinate with ANL tank modeling and industry; will be crucial to refine data.
- Will be interesting to see results on chemical hydrides and activated carbon. There might exist several model cases for chemical hydrides which will make it difficult to dedicate sufficient time to each one.
- Vehicle integration. Work with Millennium Cell for work beyond alanates.
- The project needs to do more at a much faster pace. The urgency for these analyses is acute. However, this urgency is not reflected in the future work.
- Here again, while the need for cost and WTW analyses are recognized, it seems premature to begin to do so until there are more fully developed systems to base the analysis on. Can the process be delayed until there is credible information that can be used?

- Future research plans are reasonable.
- Incorporation of storage materials that won't meet targets.
- Logical further work, but again this will show that these materials will not work. Also concerned about improperly optimistic supplier numbers twisting the analysis as TIAX is not informed enough to know when they are being led.
- Work plans call for each class of system to be analyzed. Vehicle integration issues need to be considered and could impact the system design.
- Baseline designs for all the storage systems need to be established early on. This may be difficult if the developers make major changes in their system designs. Some means should be developed to keep the baseline. This is a good project; it will last five years.
- Will properly look at all the basic forms of hydrogen storage on a self-consistent basis.
- Topics are right, i.e., doing analyses on other storage technologies.
- How good the future work will be depends on how the analyses are performed.
- Value of WTW analysis will depend on how well it's done and how the information is used by constituency.

### **Strengths and weaknesses**

#### Strengths

- TIAX has a strong history in modeling systems. The level of detail and completeness is better than most models. TIAX consistently seeks the inputs from its current and potential clients and will model many systems to determine feasibility.
- Good overall understanding of issues. Working well with various people to have accurate model.
- The project has good approach and methodology.
- Generating practical data for storage systems using existing materials and feeding R&D with input parameters for designing of new materials.
- One strength is that it is being done at all.
- Experience in developing cost estimates based on referenceable system designs. Rational system designs for hydrogen storage systems can be fed into integrated vehicle designs/analysis. DOE needs this type of comparison to make decisions regarding future direction of storage program.
- Capable independent analysis shop.

#### Weaknesses

- TIAX may not necessarily have all the technical background required to model these systems. It is important that they continuously seek and solicit knowledge from the appropriate sources.
- The values used in analysis vary from the actual values achieved in storage projects.
- Need more frequent update and coordination with the Tech team.
- Faster turn around.
- Using data obtained in R&D labs for system design that may not be accurate enough.
- Based on the current low volume process which is not reasonable. Based on materials known not to meet goals so has limited value. Concerned the wheels will come out saying that this is representative of what these sorts of systems can do and it is not, it is a snapshot in time.
- Am I correct in sensing some overlap with Project ST20 (ANL)? If so I suggest better coordination.

### **Specific recommendations and additions or deletions to the work scope**

- Continue work on metal hydrides with thermal integration from a high temp fuel cell (120C).
- Work on the activated carbon tank and coordinate with ANL prior to more complex chemical hydride system.
- The analyses projects in the storage area are critical to the success of the entire program. Their scopes and resources should be expanded. The analyses groups should be protected from external pressures. Their assumptions (in details) have to be reviewed in detail often.
- It is important to have concurrent projects in the area to further validate the results.
- It is recommended to change the work outline from a sequential process to a multi-task parallel work group.
- The early and extra investment in this area will invariably yield short and long-term dividends for the DOE.

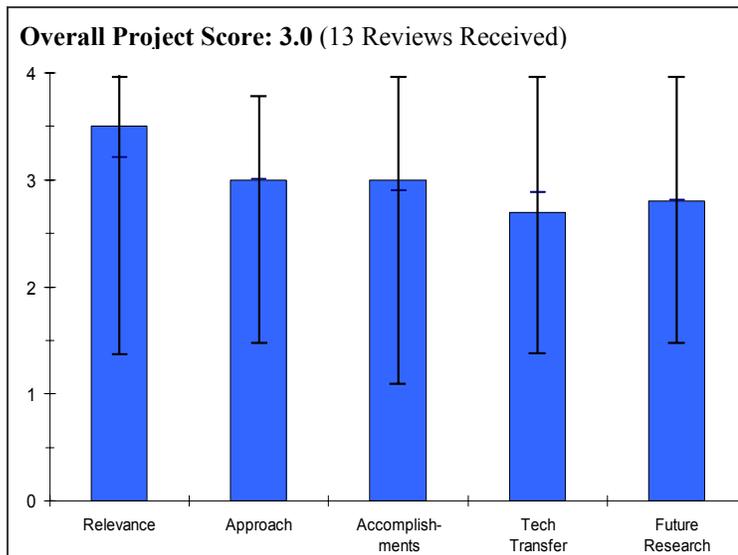
- It will be key for the DOE to capture the source code for this model so that it can be updated as needed for better refinement, and so new data can be "dropped in" to look at new materials.
- General recommendation to DOE: establish a more visible (Center of Excellence) system design team to establish baseline designs and rapidly incorporate latest designs that are being proposed by the storage system developers.
- Continue into new storage media as they are discovered. Evaluate amides at once. Maybe  $\text{AlH}_3$  soon.
- Expand collaborations with hands-on storage researchers.
- Need to constantly work towards keeping all of the PIs of the other DOE projects "in the loop" on their work. (They appear to be doing this currently).
- The UTRC results seem to show even significantly worse performance characteristics than proposed from this model; the PIs should work to identify whether this discrepancy is due to unrealistic assumptions in their model, or represent an opportunity to improve the UTRC design.

**Project # ST-21: Standardized Testing Program for Chemical Hydride and Carbon Storage Technologies**  
*Page, Richard; Southwest Research Institute (SwRI)*

**Brief Summary of Project**

In this project, Southwest Research Institute (SwRI) will develop and operate a standard testing laboratory aimed at assessing the performance, safety, and cycle life of emergent solid state materials (e.g., metal hydride, complex hydride and carbon) and systems for the storage of hydrogen. As part of this program, SwRI will work with industry, DOE and other stakeholders to develop an accepted set of performance and safety evaluation standards. Once fully operational, SwRI will apply those standards to provide analytical and R&D services at a national level.

**Question 1: Relevance to overall DOE objectives**



This project earned a score of **3.5** for its relevance to DOE objectives.

- The project provides DOE with facilities to independently assess the performance of solid state storage materials.
- It fully supports the RD&D plan.
- The project is highly relevant to the DOE's objectives, because it accomplishes the role of independent testing institute.
- Need to have an unbiased and reliable testing facility to evaluate performance of storage materials developed under the DOE program.
- This is a much needed activity for independent standardized testing particularly in view of the little unanimity of storage values reported so far in literature for carbon-based materials and contradictory storage claims.
- The goals of this effort are critical to the verification and validation of developmental claims of other components of the initiative. Hence this effort is critical to the realization of initiative goals.
- Key to accomplishing the hydrogen program goals.
- Focused on providing measurement/validation capability.
- This facility and its associated capabilities will be useful in the short term but will become progressively more critical to the HFCIT RD&D program in the longer term.
- Very relevant to the objectives of the DOE H<sub>2</sub> storage program. DOE requires an independent assessment of the storage capabilities of newly developed materials. Developers also need independent confirmation of their results.
- Provide independent validation of material performance.
- Important program in DOE portfolio. This program will not provide the breakthrough discovery, but will help to enable such a discovery.
- Establishing consistent measuring techniques is crucial to the variety of testing conditions that exist and chance for error in measurement.

**Question 2: Approach to performing the research and development**

This project was rated **3.0** on its approach.

- The approach is to develop facilities and protocols to characterize small quantities of solid state storage materials. SwRI visited the leading labs making measurements of hydrogen uptake and desorption when specifying and installing facilities. The lab is part of a round-robin testing program to verify its capabilities.
- Centralized location is probably necessary to ensure consistency.
- Largest impediment to project will be shipping restrictions on new materials imposed by DOT etc. Time to classify and approve these materials may hinder progress for individual PIs.
- Need to put more effort on characterizing smaller size samples (in the 5-50 mg range).
- The approach is not completely convincing.
- The main technical aspects related to the project objectives are not completely addressed or described.
- Good work developing and setting up lab.
- Good planning and methodology for a working solution.
- Extensive communication with researchers is important for moving forward.
- A well thought out facilities design was made and implemented. High quality components and testing and characterization equipment have been utilized in the preparation of the facility.
- The approach has been well reviewed and is appropriate.
- Good job has been done in the planning and implementation of this facility; application to samples, e.g., during the round robin stage, will undoubtedly bring some shortcomings to light, but this is to be expected--I'm sure they will be manageable.
- Multiple measurement capability.
- Development of sample handling protocols.
- Addresses pre-measurement sample conditioning.
- Gas purity levels in excess of typical laboratory.

**Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **3.0** based on accomplishments.

- PI has done a thorough job in setting up a safe and through facility and accommodating the needs of the users.
- Burst chamber for tanks will certainly be too small to test automotive scaled tanks.
- Hardware is in place but the PI did not show any meaningful results.
- After 75% of work completed, the facilities set up have not yet shown up experimental results, apart from the realization of the laboratory.
- The development of protocol is not clearly supported by a real progress: the same flow chart of last year without any comment supporting the progress.
- SWRI has assembled world class test facilities and personnel.
- Round robin testing of samples should provide confirmation of lab capabilities.
- Hard to evaluate this as not adequate information was given with respect to the standard operating procedures and the protocol development. Are these confidential data?
- There were delays in the round robin testing which will actually lead to the validation of the protocol development.
- Not enough information was supplied on the system testing.
- Reasonable progress has been made in the project thus far. A number of comments were made in the Q&A regarding the breadth of testing and certification procedures available. This is not meant as a criticism but to open the door to consideration as to whether the effort is broad enough to meet all the needs of the initiative.
- Not as much has been actually accomplished this last year, the vast bulk of this talk is also in last years talk; indeed many slides are entirely unchanged.
- Gas sampling system was installed.
- Full size system test pipe ready.
- Revising/upgrading SOPs.
- Completed and tested most subsystems. Started round robin testing. Have encountered some delays.

- Progress has been good. The facilities are installed and are being exercised as part of the round robin testing. Protocols and safety plans have been drafted and reviewed by experts in the field.
- Facility nearly operational.
- Progress in facility completion and validation seems to be slower than one might expect.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **2.7** for technology transfer and collaboration.

- PI could work with some more of the researchers to determine their individual requirements and develop the system to capture as many possibilities as possible.
- Could improve significantly as the project moves on to the next phase.
- The described collaborations appear insufficient and not adequate to the ongoing effort: collaborations with other projects testing components may assist the development of a "standardized" procedure.
- Good list considering scope of project.
- This is a very important project which is greatly benefiting from collaboration with the universities and government research laboratories.
- More interaction with industry is highly recommended for the transfer of procedures and protocols.
- Collaboration in the form of the round-robin testing scheme is to be complemented. Efforts of this type are critical to achieving and maintaining high credibility of results.
- Connectivity is low but this is not a big problem as DOE is doing the key connectivity item - the round robin.
- The presentation did not make clear what the partnering organizations are contributing.
- Collaboration with other organizations is good. It is particularly strong with developers of advanced storage materials.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- The future research is reasonable, but does not present clearly the activities on the system testing.
- PI should consider installing a larger burst tank should the industry find it necessary.
- Two issues: how to fully utilize the center in the future and how to maintain its independence.
- Effort should be focused on obtaining real systems accuracies.
- Expect round robin testing to confirm capabilities of lab and personnel to permit commencement of testing of samples for evaluation assessment.
- Good planning, moving step-by-step to a fully operational standardized testing facility.
- Future plans are reasonable. Have there been any efforts at international standards of testing and protocol development?
- Essentially the plan now is to measure samples and that is appropriate.
- Round robin is key to being trusted by DOE contractors.
- The future plans are sensible in the context of what the testing program is designed to do.
- Round-robin validation completion, final versions of testing protocols, and completion of construction is scheduled for the remainder of 2005. The facility should be ready to accept first samples in July 2005.

### **Strengths and weaknesses**

#### Strengths

- Through setup, excellent knowledge of lab setup and commissioning.
- Good hardware facilities.
- The establishment of an independent testing facility with a complete set of equipment and procedure is of paramount importance for the program.
- Excellent facilities appropriate for a verification/validation laboratory.
- Independent testing.

- At this point in time, it is difficult to recognize what strengths mean for this project because of its new/unique nature - in time, performance will reveal the strengths.
- The management of the project appears to be very good so far.
- SwRI is establishing its lab as a state-of-the-art facility that researchers can have confidence that the data generated will be correct.
- First rate equipment used in this facility.

#### Weaknesses

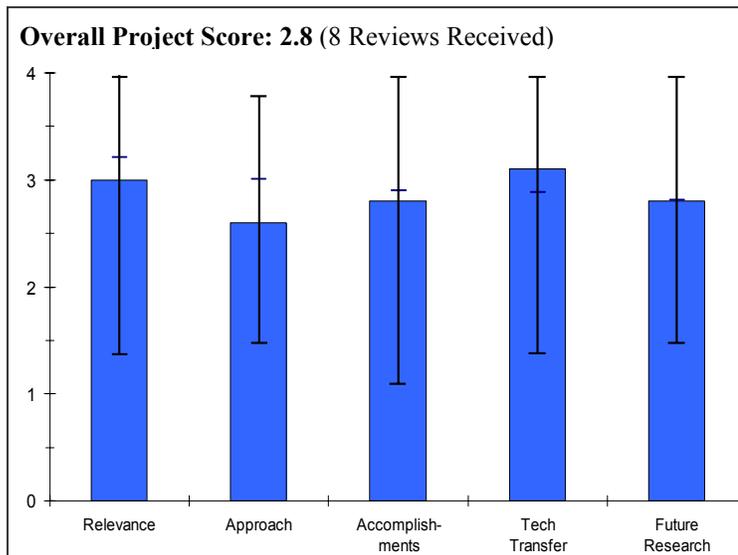
- PI could communicate more with researchers on requirements. Workshop at merit review is a good start.
- The use of commercial characterization equipment does not permit the kind of resolution needed to characterize small size samples.
- The lack of clear experimental validation data of the instrumentation raises doubt about the readiness and usability of the facility. The protocol is only limited to material characterization.
- Further development of technical expertise.
- Facility restricted to solid-state hydrogen storage.
- There is not enough evidence given on ability to obtain reproducible and accurate data.
- Hopefully, the test facility is ready to deal effectively with the wide variety of sample types it will be receiving
- What is going to happen when the test facility gets a significantly different (e.g., lower) value for the storage capacity of a sample than the provider claims? That's when the fun starts!
- Shipping samples to the facility may be an issue from a regulatory standpoint.
- It is not clear as to how well staffed this facility is or will be. What percentage of time do the PIs spend on the project at this time?

#### Specific recommendations and additions or deletions to the work scope

- The work on the protocols (material and testing) should integrate feedback from other projects (CoEs, UTRC and so on).
- Conduct thorough investigations to address reproducibility and accuracy of measurements. Publicize these results in order to gain full acceptance of the quality of the measurements by the research community. This will justify the role of an independent validation/verification testing facility.
- As new storage materials and concepts are emerging, added flexibility to evaluate those materials will be important (e.g., liquids).
- DOE team needs to enforce any improvements implied by the round robin results.
- In the early stages of the round robin testing, focus on samples that have straightforward sample handling/activation requirements, i.e., types that are like the ones used in sub-system testing.
- It won't go over well in future peer reviews to stand up and say that results for certain samples received from certain providers are proprietary; the results of measurements made in the context of this particular project should in all cases be available for review and comment.
- Try to determine if the facility/staff have the necessary equipment and skills to understand why measurements differ from those made by the researcher, as they most certainly will from time-to-time.
- In the future, the connections with the Centers of Excellence should be emphasized and perhaps even formalized.

**Project # STP-58: Development and Characterization of Novel Complex Hydrides***Zidan, Ragaiy and Motyka, Ted; Savannah River National Laboratory***Brief Summary of Project**

This particular project is a 3-year CRADA with United Technologies Research Center as part of their project, "Complex Hydride Compounds with Enhanced Hydrogen Storage Capacity," ST-6. Savannah River is employing its recently developed method to modify or form new complex hydride structures as potential high capacity hydrogen storage materials. The new method is based on fusing different known complex hydrides at elevated temperature and pressure at or near their molten state. This method, named the molten state process, is robust, efficient and can be scaled-up to produce large quantities of modified or new complex hydride materials.

**Question 1: Relevance to overall DOE objectives**

This project earned a score of **3.0** for its relevance to DOE objectives.

- The molten state process is a welcome alternative to the traditional methods of preparing metal hydrides such as ball milling and solvent ball milling methods. The molten state process will likely scale-up better than ball milling for volume production; however, the high pressures (3000-psi) may limit production to small batches at a time. The PI has created a process which allows hybrid forms of metal hydrides previously inaccessible to be explored. Still- these are alanate materials with poor conductivity and similar system integration issues. It would appear that much higher storage capacities will be required (>13wt.%) to create a practical storage tank.
- Will create more uniformity among the hydrides.
- This project holds significant promise toward meeting DOE's hydrogen storage goals. The outcome should facilitate an end-product that has a relatively low cost of manufacture and appears to be highly scalable.
- The project is relevant to the DOE's objectives.
- Clearly aims to develop new hydrides aimed at DOE 2010 targets. Materials chosen may have limits short of targets.
- This project supports the larger UTRC project [ST-06].

**Question 2: Approach to performing the research and development**

This project was rated **2.6** on its approach.

- New process has opened many opportunities and permutations. Covering these permutations may take a long time. PI should develop a rapid screening process similar to UOP or UTRC in order to cover as many possibilities as possible. Currently, PI requires one week to prepare and analyze each alloy- too long
- Addressed several hurdles need to overcome.
- The approach used builds on prior knowledge to be able to quickly explore new possibilities for promising compounds.
- Comparatively somewhat limited with other methods but meets the adequate. The minimum projected output from this project should be about 20 to 35 characterized alloys. However, it is not clear what internal vetting process will be used to down select alloys.

- The approach clearly stated specific technical challenges. The application of the molten salt process (MSP) may be of twofold use: further validation of the process and production of low-cost novel hybrid alanate compounds.
- CRADA with UTRC (Proj. ST6) a good approach. The MSP approach is innovative and offers a route to new materials. Not certain it can be extended beyond the low melting alanates and borohydrides. The project is oriented mostly toward alanates and related complexes. This area is overworked within the HFCIT program.
- Focused heavily on a specific material synthesis approach. Limited analysis of material hydrogen properties, e.g., only TPD measurements. Limited material analyses, e.g., mainly XRD.

### **Question 3: Technical accomplishments and progress toward project and DOE goals**

This project was rated **2.8** based on accomplishments.

- Reduction in dehydrating temperatures is very good progress. Demonstrating higher capacities is yet to be shown.
- Still very new project. [Project was funded in FY-04 and FY-05.]
- Progress this year has been significant given the funding level provided and results are exciting.
- Considering the amount of resources, the project has shown modest progress. The key is the potential usefulness of the project.
- The technical achievements are well in line with the planned activities and motivate an acceptable progress of the work. The results are promising and a focus on a few developed materials would be preferable.
- Good initial results with MSP. Will the MSP process (high pressure and temperature) be amenable to commercial scale-up?
- Some progress has been made in synthesizing a complex hydride phase. Modest progress may be due to limited funding of project.

### **Question 4: Technology transfer/collaborations with industry, universities and other laboratories**

This project was rated **3.1** for technology transfer and collaboration.

- PI has collaborated with presumably an industrial partner which will hinder transfer of knowledge to research community considering that this is still fundamental research. PI is otherwise fully capable of completing work themselves, not too much collaboration is required. If PI is collaborating with an OEM, then understanding of systems requirements should follow.
- Worked specifically with UTRC and Norway Institute Energy Technology.
- Collaboration with private industry and universities has been highly effective.
- The collaborations are adequate and well integrate with the planned work.
- Excellent national and international collaborations. Good opportunities for tech transfer.
- Partnerships limited to UTRC, which this project is a part of, and with analyses partners. Could use some materials development partners.

### **Question 5: Approach to and relevance of proposed future research**

This project was rated **2.8** for proposed future work.

- Seems to repeat some work that has already been shown to be unsuccessful as far as finding new complexes. Will help with uniformity of hydride production.
- Future plans are solid for becoming more focused on the investigation of new compounds.
- The future research is based on the previous results. The characterization must include some cycling test.
- Future work identified as continuation of current effort.

### Strengths and weaknesses

#### Strengths

- PI is a very capable and amenable researcher, to degree of legal limits, PI is willing to share knowledge. PI has very capable lab equipment and synergy with many other strong researchers in near proximity.
- Hits on several key issues needed to move forward with the hydride research. Molten state process.
- PI's prior experience and extensive work in the area. The basic technical approach is set. Can produce larger sample amount and potentially simpler route for large scale production.
- SRNL has an innovative preparation process (MSP) and facility to analyze the characteristics of the produced materials.
- Project is aimed at new materials discovery. Molten State Processing method of synthesis is novel, and may be utilized as one of the synthetic approaches for other classes of hydrogen sorbents.
- A new and innovative approach of making doped samples (MSP).

#### Weaknesses

- Material is still alanate based with all the drawbacks of alanates and poor system performance. PI will need to aim for greater than 7.5% density to achieve DOE goals. Achieving 7.5% at reduced temperatures and good cyclic qualities will still be impressive.
- Comparatively longer time is required for sample processing and characterization but larger sample amount is produced.
- The current IP arrangement could actually limit the PI's success and effectiveness in the long run.
- Main limitation of the project is focusing on alanate systems that have not shown any promise to meet gravimetric targets (system basis) nor produce novel phases. It has been also shown in the past (Jensen et al) that initial synthesis method is not important to the structures after cycling.
- Too much focus on the overworked alanates. They are covered in detail in other HFCIT and offshore projects. They also have some safety problems.

### Specific recommendations and additions or deletions to the work scope

- The alloy down select process should be aligned with the system analyses work.
- Continue on the current path. Develop rapid processing techniques to expedite research. Try to apply similar techniques to amineborane materials which have higher capacities and potentially similar molten states.
- Good plan to optimize the MSP process and determine its limits. Would help to have a go/no-go decision point on the alanates. When to move on?
- Still too new.
- The program should be supported but the progress and effectiveness of the technique must be periodically gauged against other competing methodology. When additional data are available within the next 12 months, the project scopes can be revisited.
- The addition of cycling test in the next research period may help in the material selection.
- Need to soon move to materials with higher gravimetric and volumetric hydrogen densities (e.g., borohydrides, amides and  $\text{AlH}_3$ ). The borohydrides may have some potential for MSP.