DOE-EERE/NIST Joint Workshop on Combinatorial Materials Science for Applications in Energy

Working Dinner
November 6, 2008

A working dinner was held for the attendees of the DOE-EERE/NIST Joint Workshop on Combinatorial Materials Science for Applications in Energy on November 6, 2008. The results of breakout sessions held on the afternoon of November 6 were presented by Ned Stetson and Kate Beers. These presentations are summarized below.

Group 1 – Ned Stetson

The most important question discussed was how to build community between DOE and NIST. There was considerable discussion around how to match problems with solutions, other than by increasing funding. Mr. Stetson pointed out that DOE is soliciting proposals for funding for hydrogen storage solutions. Combinatorial methods can be used in proposals to DOE if they are focused on furthering hydrogen storage materials.

Combinatorial approaches and challenges and measurement techniques were also discussed. Specific topics included absorption/desorption, *in situ* desorption, Ramen/spectroscopic techniques, and ball milling (relating combinatorial methods to bulk samples). The group recommended reporting trends rather than absolute values, and it was noted that quantitative methods may not be needed if peaks can be qualitatively determined.

Group 1 recommended focusing on complex hydrides, most of which are at least tertiary. Complex hydrides are unstable; thus, approaches for these materials are challenging. This group also recommended using computational combinatorial methods to downselect materials approaches prior to experimentation, and to validate results.

Group 2 – Kate Beers

Group 2 focused on (1) the challenges with science and measurement needs, and (2) the barriers to meeting these needs.

Challenges with science and measurement needs

Challenges include handling/processing, probing synthetic pathways, preparing more diverse, well-characterized libraries, and scalability of measurements. XRD spectroscopy doesn't address all the problems of the entire range of materials. A direct measurement/screening technique would be a great first step. Reliability in the direct measures is still not where it should be for a HT technique. Pathways individualized for the various classes of materials are ok, too, and often necessary.

Group 2 concluded that a minor investment in a thought experiment would be of value. Combinatorial science can be used to develop ways to build a screen in the laboratory without a large investment. There may be lessons to learn from more mature combinatorial industries for building such screens.

Barriers to meeting needs

A common perception may be that the most significant barrier is cost. There are often alternate investments available that are not expensive and furthermore offer the opportunity to learn skills and techniques that are also applicable when using the more expensive equipment. It was noted that Combi and HT instrumentation skills have benefitted students in finding jobs. User centers such as the DOE Centers of Excellence may offer a way to gain new insights and ideas for methods.