

Project Description

In the search for superior batteries, the road to success is paved with advanced materials: better cathodes, better anodes, better electrolytes. The universe of candidates is so vast and the cost of selection and testing them is so great that conventional approaches to materials discovery are not likely to yield breakthrough results on a short enough time scale. The thesis of this proposal is that by leveraging the advances in informatics and high-throughput experimental and computational materials science we can greatly accelerate the rate of discovery of new materials and, in turn, the development of superior battery technologies. As a first step we propose a workshop at which will bring together leaders in battery research and those who have been successful in areas of materials and molecule discovery. Each of the roughly 20 participants will be strategically chosen for what they can contribute by way of synergy to this enterprise. Included are the following:

- Energy Storage: the knowledge of the central problem and the performance metrics of next generation batteries
- Materials Informatics, Computational Materials Science, High Throughput Experimentation for Materials Discovery: the knowledge of new tools for high throughput screening of candidate materials and of models and computation to guide an intelligent search for materials with targeted performance
- Discovery of Pharmaceuticals: the knowledge of how best to exploit high throughput approaches to the discovery of new compounds, including lessons learned along the way from previous success and disappointments

The interactions between researchers from different fields will be structured with a view to stimulating the battery community towards thinking about the problem of materials selection, testing, and utilization from new perspectives. In addition, by making battery researchers aware of new tools of inquiry we hope to increase productivity and interaction and, thereby, increase the likelihood of breakthrough thinking and true discovery.

The workshop will be held at the Massachusetts Institute of Technology over a day and a half, tentatively starting at 1 pm on September 8, 2008 and following for a full day on September 9, 2008. All participants will be invited and their expenses paid from this grant. The program will be organized and participants invited by a committee made up of

Donald Sadoway, John F. Elliott Professor of Materials Chemistry, Department of Materials Science and Engineering, Massachusetts Institute of Technology

Gerbrand Ceder, Richard P. Simmons Professor of Computational Materials Science, Department of Materials Science and Engineering, Massachusetts Institute of Technology

Krishna Rajan, Stanley Chair in Interdisciplinary Engineering, Department of Materials Science and Engineering, Iowa State University

James Caruthers, Professor of Chemical Engineering, School of Chemical Engineering, Purdue University

Nicholas Delgass, Maxine Spencer Nichols Professor of Chemical Engineering, School of Chemical Engineering, Purdue University

The starting structure of the Workshop (to be augmented and refined by the organizing committee) will be a series of lectures on day 1 to establish the current frontiers and visions for advancement in battery technology and to present new tools and approaches for materials and molecule discovery as practiced in pharmaceuticals, catalysis, and specific areas of materials science. This will be followed by breakout groups aimed at examining opportunities to use the new discovery tools to address breakthroughs in specific aspects of battery research. The groups will then report their findings to the whole group, which will try to turn the best ideas into a suggested structure of research targets and funding aimed at accelerating progress and increasing the likelihood of breakthroughs. Finally, breakout groups will be convened to capture the findings in written reports.

The deliverable from the workshop will be a report that prescribes a forward looking research program of research sponsorship.