Report on the Workshop on a

Drug Discovery Approach to Breakthroughs in Batteries

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Executive Summary

All that prevents conversion of our nation's automobile fleet from internal combustion with its need for liquid fuel derived from petroleum to electric drive powered by domestic sources of electricity is the availability of proper battery technology. In turn, the road to superior batteries is paved with advanced materials: better cathodes, better anodes and better electrolytes. However, 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 conclusion of a workshop held at MIT in September, 2008 under the sponsorship of the National Science Foundation is that by leveraging the advances in computational materials science and informatics with high-throughput experimentation, the rate of discovery of new materials can be greatly accelerated, enabling the development of superior battery technologies. Furthermore, based in part on lessons learned in the search for new drugs by the pharmaceutical industry, the workshop declared that:

1. High-throughput experimentation with informed test protocols is expected to reduce the time for assessment of candidate materials as well as to contribute fundamental property measurements to the materials database

2. The deployment of computational materials science and informatics is expected to enable rapid intelligent screening of materials resulting in the selection of the most promising candidates with targeted performance attributes.

3. Research on the anode, cathode, and electrolyte must be integrated, and mechanisms for data sharing are essential.

Accordingly, the workshop endorsed the injection of new funds by the federal government to support the search for advanced energy storage materials and further recommended that only research conducted by multidisciplinary teams comprising a strategically selected combination of theoreticians and experimentalists be eligible for sponsorship under the proposed new program.

Introduction: The Need for New Battery Technology

At a recent IEEE workshop for Congressional staff on plug-in hybrid cars[1], the questions were posed: "What is the probability that basic researchers in the US could come up with a new battery twice as good for cars as the newly emerging standard, the iron phosphate lithium ion battery? What could be done to maximize the probability that this goal is actually achieved, as soon as possible?" The workshop described here was conducted in order to attempt to answer the second question. Specifically, the question was viewed from the perspective of what could be done in the way of a new initiative by NSF in order to accelerate the rate of discovery and thereby compress the time line to implementation of new technology. Of particular interest in this regard was what can be done to take full advantage of approaches used in the pharmaceutical industry to create breakthroughs, where informatics enabaled high throughput experimentation, digital simulation and molecular modeling has made it possible to search a larger space of possibilities more quickly and more cheaply than would be the case using conventional approaches based upon a combination of chemical intuition and laboratory experimentation.

Energy is likely to be a major problem, perhaps *the* major problem, facing society over the next century. The development of domestic sources of energy is critical to the national interest. With an annual cost of $700B[2] associated with the importation of oil from unstable regions, national energy security and the economy are strong additional drivers for the development of new, domestic energy technology. Since transportation fuels account for approximately 30 % of the US energy demand (see Fig. 1), this energy sector must be addressed in any plausible sustainable energy scenario. Moreover, any forward leaning energy program must reduce the carbon footprint in order to address the growing criticality of global warming. Carbon-free transportation must necessarily rely upon electric power delivery which, in turn, cannot be viable in the absence of cost-effective energy storage technology - i.e. batteries.

> *Revolutionary breakthroughs in EES have been singled out as perhaps the most crucial need for this nation's secure energy future. The BES Workshop on Basic Research Needs for Electrical Energy Storage (EES) concluded that the breakthroughs required for tomorrow's energy storage needs will not be realized with incremental evolutionary improvements in existing technologies. Rather, they will be realized only with fundamental research to understand the underlying processes involved in EES, which will in turn enable the development of novel EES concepts that incorporate revolutionary new materials and chemical processes. Recent advances have provided the ability to synthesize novel nanoscale materials with architectures tailored for specific performance; to characterize materials and dynamic chemical processes at the atomic and molecular level; and to simulate and predict structural and functional relationships using modern computational tools. Together, these new capabilities provide unprecedented potential for addressing technology and performance gaps in EES devices.*
>
> DOE Basic Energy Sciences Workshop, April 2-4, 2007

Batteries provide a feasible alternative for transportation energy storage, provided that sufficient capacity (e.g. a 16kWh storage capacity supports a 40 mile range for a small car) can be achieved at reasonable weight, volume and cost. This approach also has the significant advantage that it can use the existing power grid structure as opposed to the need to develop a new distribution infrastructure, as would be the case for H_2. The battery technology required for this application does not lie beyond the realm of possibility. We see evidence of battery powered vehicles that are coming into production; however, cost is an issue if electric drive technology is to reach full market potential and displace internal combustion with its reliance on liquid hydrocarbon fuel. As of this writing, the cost premium for electric drive is estimated to be $3K for the Toyota Prius and $7K projected for the GM Chevrolet Volt. Even if costs come down with mass production, there is still a need for innovation in energy storage in order the enable the transition from hybrid electric vehicles (HEVs) to plug-in hybrid electric vehicles (PHEVs) and ultimately to all-electrics (EVs). Although an electric drive system has a number of components, the key bottleneck to higher performance is the absence of a superior battery boasting higher capacity, lower mass, and longer service lifetime (greater resistance to capacity fade).

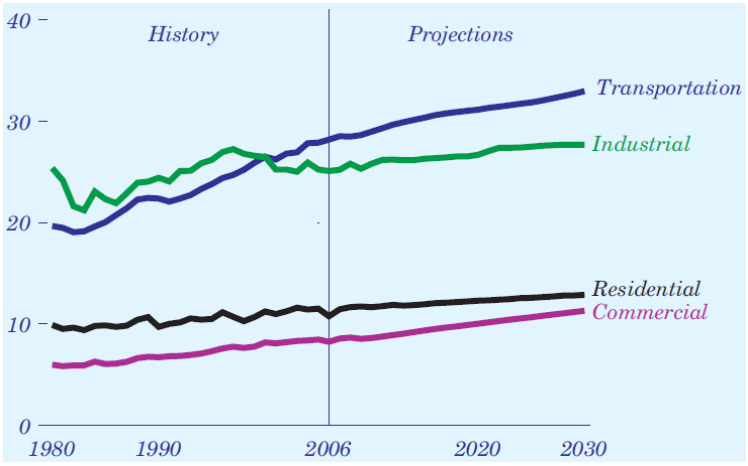


Figure 1: Delivered energy consumption by sector for 1980-2030 (quadrillion Btu). DOE Annual Energy Outlook 2008, p.6

Technologies to create, transfer, save, or store energy are critically dependent on materials innovation. The "hydrogen economy" is an excellent example of how materials properties can place limits on new energy concepts, i.e. at this point we lack not only the materials to store and release hydrogen at a reasonable gravimetric and volumetric density, but also the long-term stable catalysts to electrochemically produce and use it efficiently as an energy carrier. However, the need for rapid deployment of new battery technology is at odds with the typically slow rate of new material development.

Traditional materials development from "invention" to commercialization is an extremely long process, and one that is not commensurate with the current urgency of climate protection and energy security. It has been estimated that on average 18 to 20 years are required to bring an innovative materials idea to the market.[3] Several aspects contribute to this problem. Searching for novel materials has historically been typically a rather random and therefore somewhat unpredictable process. The initial focus on new materials is usually based on a single outstanding property (e.g. T_c for a superconductor, storage capacity for a battery material, dielectric constant for a new dielectric, etc.). Hence, attempts towards scale-up and commercialization often start without access to other key properties which can ultimately govern the economic viability of the new material, e.g., reliability, stability, processability, etc. Deficiencies of a material in any of these areas can throw a materials development program off track and lead to major iterations on materials selection and processing routes. Thus, an

accelerated materials development program for a new generation of batteries must include all material properties necessary for safe, cost-effective utilization and manufacture.

A novel and ambitious solution would be to deploy proven high-throughput experimental methods and computational methodologies to predict, screen, and optimize materials at an unparalleled scale. One needs to create a unique combined high-throughput experimental and computing platform for the full range of battery technologies; one that is well integrated and informed by a team of material and battery experts. This approach would provide a broad and comprehensive screen of materials for all relevant properties across a multitude of chemistries, in order to give application designers access to all the relevant properties before a materials development program is started. This approach, of providing maximal information on a material's behavior early on in the selection process, will lead to more informed and better choices, and as a consequence, a reduced time to commercialization.

The Vision

A new way of approaching energy storage research is needed in order to achieve the goal of widespread electrification of our transportation system on a foreshortened timescale. We call for an expanded use of computational materials science (i.e. applied quantum mechanics, molecular dynamics, etc.) working in tandem with interdisciplinary teams of experimentalists involved in high throughput synthesis, testing, and characterization of candidate materials discovered by digital screening, where all data is efficiently shared using informatics tools supported by modern cyber-infrastructure. The technical goal is to develop a new battery for automotive applications with the following metrics:

- storage capacity of 400 Wh/kg (or 800 Wh/L), which is twice the energy density of current best-in-class batteries
- composed of earth-abundant materials to help achieve the cost goals of the automotive market and avoid dependence on raw materials that have restricted access
- service lifetime of 10 years

Inverse and High-Throughput Materials Design.

Materials for EES [electrical energy storage] are likely to see the first benefits of large-scale computational materials science, which can be applied to calculating many of the required properties. One question is whether high-throughput search methods can be implemented with predictive modeling tools to scan large numbers of compositions, structures, particle sizes, etc., to find new electrode materials. New computational tools and analysis methods need to be developed to enable such large computational searches. In "inverse design," one tries to invert this problem and, rather than calculate properties for a well-defined composition or structure, to design materials or microstructures that have very specific properties. Mathematical techniques that enable such inverse design, starting either from key physical insights or from large amounts of data, are particularly needed.

Basic Research Needs for Electrical Energy Storage DOE Basic Energy Sciences Workshop, April 2-4, 2007

Computational modeling has become an indispensable tool in many scientific and engineering disciplines. Finite element modeling of deformation, fluid flow, heat flow, etc. have significantly reduced the amount of experimental prototyping required in manufacturing and design. Even large-scale systems such as the Boeing 777 have largely been designed with computer modeling before a single part was built. The opportunity to do the same predictive modeling of materials properties and integrate this capability into rapid materials design is now available. Using so-called *ab initio* computations, which start from the basic laws of physics at the atomic scale, it is possible to predict properties of materials without the need to synthesize them first, thereby creating the opportunity for a virtual design laboratory. This approach (shown schematically in Figure 2) has been demonstrated and verified for a large number of electronic, optical, magnetic, thermodynamic and kinetic properties of materials. Due to its potential for efficiency, computational modeling needs to play an important role in a program seeking advanced battery technologies which need accelerated materials design. There are several advantages to a computational approach to materials screening and design:

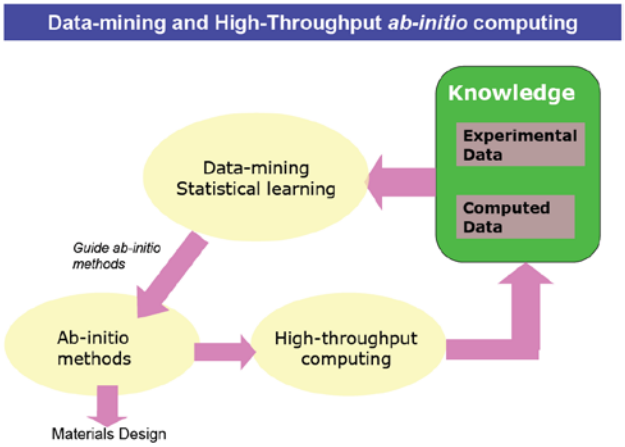


Figure 2: schematic of method combining computational with *ab initio* and data mining.

- Novel ideas for materials can rapidly be evaluated before one has to invest time and money in synthesis and processing routes.
- In a virtual laboratory "what-if experiments" can be performed to rapidly learn what the crucial chemical or structural attributes in a material are to determine a given property.
- Computational modeling gives full control (structural, chemical, morphological) over a system so that clear meaningful results can be established in a short time.
- Computing is perfectly scalable and with a reasonable amount of resources it is now possible to scan thousands of chemical systems in a matter of months. Computational modeling can reduce uncertainty in materials by providing broad coverage in its optimization.

Figure 3 is a schematic of the information flow that shows how model-building, coupled with experimentation, can accelerate both materials discovery and the creation of knowledge. At the beginning of this *Discovery Informatics*[4] process, an expert uses an inverse search based on his/her personal expertise to identify either descriptors or the materials he or she will generate in order to meet the performance objectives of the problem that has been defined. After a sufficient number of experimental tests, data on the performance achieved by specific materials is then used to begin the process of identifying material descriptors (i.e. physical, chemical, and

electrical quantities that are used by experts to communicate the essential phenomena that control a specific performance metric) and a model that quantitatively relates the descriptors to the performance. Typically the model will have two components. One is a dynamic response model that predicts the response of a given material or material system. The other is a model of the fundamental physics and chemistry that sets the parameters that drive that response. Several iteration loops will be needed to (i) identify improved descriptors, (ii) refine the descriptor-performance model, (iii) test the dynamic response model for specific materials with experimentally measured performance and (iv) relate material descriptors to material synthesis. The most difficult aspect of the forward model building is the development of fundamental relationship of how the parameters in the dynamic response model are quantitatively related to values of the molecular descriptors. Guidance in the development of this model can be obtained from detailed molecular simulations on model systems with tools such as density functional theory and molecular dynamics. Ideally, these computationally intense molecular simulations can be generalized through correlations that broaden the range and increase the speed of application of the model. As soon as an even crude forward model is in place, a guided stochastic inverse search of the descriptor space can be done by evolving the values of the descriptors sets so that the current forward model predicts the desired performance. The best predicted performers are then synthesized and tested. Comparison of the measured and predicted performance then provides opportunities to improve the model in cases where the predictions fail.

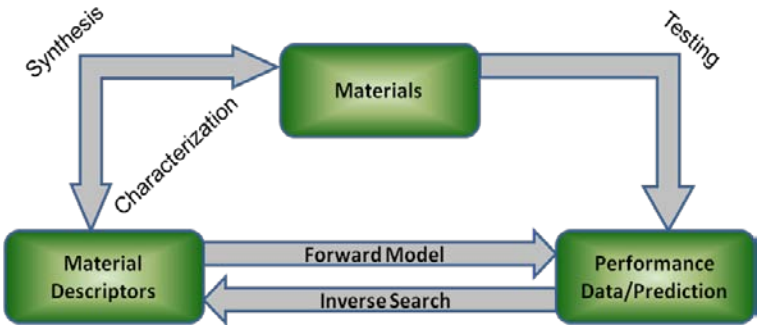


Figure 3: Data flow from descriptors to performance

These and other informatics-based strategies require large amounts of data to drive both model building and data mining. As described above, some of the needed input can come from high throughput computation, i.e. computation that is at least semi-automated to cover large parameter spaces. Ultimately, however, the models must be validated by direct experimental measurements. To support the speed of assessment needed for rapid discovery, these approaches need to be coupled with high throughput experimental (HTE) capabilities via either parallel or fast serial physical and/or chemical analysis. While there is almost always a tradeoff between data quality and speed, high speed screening can be followed sequentially by increasingly slower, but more informative, experimental tests on the most promising leads. The section below outlines successes of this informatics based approach in several different fields.

Demonstrated Success Stories

In the following subsections we will show how an information rich approach that combines high-throughput experiments, quantum chemical simulations, and model based engineering has transformed several fields. These examples provide a clear illustration of the types of technologies that will be needed to rapidly accelerate battery research in the 21st century.

Pharmaceuticals Transformed by HTE

High throughput screening (HTS) platforms have aided in the identification of countless compounds that have been forwarded to the chemist's bench for optimization, followed by early clinical trials, with an expected smaller number progressing to the late clinical phase. Documenting HTS-derived drugs can be difficult, as GSK's Robert Hertzberg explains, "Lots of compounds have 'mixed pedigrees' and there is little incentive for people to track the history." Nevertheless, number of notable drugs and late stage candidates have emerged from this pool:

- Bayer's renal cell carcinoma drug sorafenib (Nexavar), approved in December 2005.
- Merck's HIV integrase inhibitor raltegravir (Isentress), and sitagliptin (Januvia) the company's antihyperglycemic (dipeptidyl peptidase-4 (DPP-4) inhibitor), which originated from two screening hits that were combined;
- Boehringer Ingelheim's HIV protease inhibitor, tipranavier (Aptivus);
- Bayer's rivaroxaban (Xarelto; Factor Xa inhibitor) for thromboembolic disorders;
- Pfizer's HIV entry inhibitor, maraviroc (Selzentry; CCR5 antagonist);
- Novartis/Schering's antiangiogenic compound PTK787 (VEGFR tyrosine kinase inhibitor); GSK's atherosclerosis/cardiovascular risk Phase 3 candidate, Darapladib (lipoprotein-associated phospholipase A2 inhibitor);
- TPO mimetic eltrombopag (Promacta) from a GSK-Ligand Pharmaceuticals Inc. collaboration

Given the relatively long development time (10-15 years) involved in taking a drug through early discovery and clinical trials, one is only beginning to see the impact of HTS on approved drugs. Early HTS, which began in the late 1980s, was only a rudimentary version of what it has evolved to in the mid-1990s, where refinement is still taking place today and advanced versions of HTS are not even in place at every pharmaceutical company. Given this background, the measure of HTS as an accelerator of drug discovery is only now being fully realized. For example, the GSK-Ligand collaboration started in 1995 (when GSK was SmithKline Beecham), and in March 2008 eltrombopag received FDA review acceptance and was granted priority review for the treatment of short-term idiopathic thrombocytopenic purpura (ITP).

One only needs to visit Merck's external website to find the following endorsement of HTS in a statement about montelukast (Singulair), the company's current best-seller,

> *"As a starting point in their search for an effective antagonist for the target receptor, Merck Frosst scientists hand-screened tens of thousands of compounds from the Merck & Co. sample collection."*

The requirement to develop new and effective drugs in shorter time periods is only possible with the aid of advanced automated technologies. HTS and variations thereof are permeating all steps of drug discovery and development[5], and the more likely question in the next decade will be, "What newly approved drugs were not created with the aid of high throughput, informatics-based technologies?"

Computational Materials Science

An integrated approach employing computational materials science coupled with expert insight and focused experimentation was able to identify an unanticipated consequence of aluminum in a lithium ion battery[6]. The team involved four MIT faculty: Anne Mayes, Gerd Ceder, Yet-Ming Chiang and Donald Sadoway. Ceder explained what happens when the lithium ion intercalates into lithium cobalt oxide by using quantum mechanics applied to a many bodied ensemble large enough to give physically realistic and useful results. He found that when lithium ion enters the cobalt oxide crystal, the compensating electronic charge does not reside exclusively on the cobalt alone, but rather is divided between cobalt and oxygen which led to a new hypothesis of how to raise cell voltage by controlling the Fermi level. Ceder speculated that if one were to synthesize lithium aluminum oxide in the alpha-sodium ferrite crystal structure (same as that of lithium cobalt oxide) the open circuit voltage of the material would be 5 volts. Unfortunately, the electronic conductivity of lithium aluminum oxide is effectively zero. Chiang reminded the team that basic ceramics teaches that doping with an oxide of higher cationic valence could confer some degree of electronic conductivity. Ceder then calculated the cell voltage of the binary system lithium cobalt oxide – lithium aluminum oxide and found that there should be a monotonic increase in voltage corresponding to increasing aluminum concentration. Chiang's lab synthesized specimens containing 25%, 50%, and 75% (on a molar basis) aluminum in lithium cobalt oxide. Sadoway's lab constructed cathodes of these materials and tested them in a coin-cell battery configuration. The results were as predicted: aluminum raised the cell voltage. No one believed the results because aluminum is not a transition metal and so was thought to be inactive as a cathode constituent, i.e., its presence would simply serve as a diluent, which would reduce volumetric capacity and have no effect on cell voltage. This story is a good example of how conventional wisdom was overthrown thanks to the insight provided by computational materials science in collaboration with experiments and experts with complimentary areas of expertise.

HTE in Heterogeneous Catalysis

Heterogeneous catalysis is an area of materials research that has also embraced the idea of rapid materials testing to facilitate discovery and innovation. The European Commission sponsored several projects under the COMBICAT and TOPCOMBI initiatives[7]. One highlight of the resulting work was published by Grubert and coworkers[8] who employed evolutionary search algorithms within a high throughput experimental framework to discover copper-free Water Gas Shift catalyst leads. These leads are exciting because while it is known that copper makes an excellent catalyst, it is also known that the form of copper required for the catalysis is pyrophoric and therefore unsafe for widespread adoption in fuel cell systems.

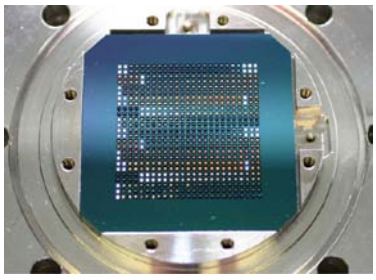


Figure 4: Image of the 625 well silicon wafer reactor or catalyst screening[9].

A second success was reported by Schüth and coworkers[9] who have developed synthetic protocols and reactors to perform syntheses and performance testing. Their synthesis techniques

create ternary or higher mixed oxides that are screened in reactors with 625 wells, as shown in Figure 4.

U.S. researchers Lauterbach and coworkers[10] have developed a 16 channel reactor with independent temperature control to properly randomize temperature programs in catalyst libraries for stage two testing. With this system they optimized the synthesis of an ethylene epoxidation catalyst leading to a threefold increase in conversion. This parallel reactor system has also been used to discover a new K-promoted Ru catalyst for ammonia decomposition.[11]

Another success has been reported by Bricker and coworkers at UOP[12] who combed through a library of 500 catalysts in 6 weeks where traditional methods would have required 3.5 years. They discovered non noble metal (i.e. much less costly) formulations for dehydrogenation catalysts for use in the petroleum industry.

Strasser and coworkers[13] have demonstrated that high throughput experiments can be supplemented with density functional theory calculations to facilitate understanding of observed trends. Such additional insights result in better library design decisions and speed up the cycle time for new catalyst development.

Model-Aided Catalyst Design

We note two examples of the successful implementation of the model building approach in catalyst design. In the first, DFT calculations have led to new understanding of aryloxide single site hexene polymerization catalysts.[14] The propagation rate constants for 18 catalysts were correlated to a wide variety of potential descriptors from the DFT results and two parameters were found to be sufficient to describe the results. One was the energy required to separate the anion from the catalytic cationic center and the other was the cone angle describing the space available for docking of the monomer at the metal center, prior to insertion into the growing polymer. The ability of the model to match the data is shown in Figure 5. The calculations also revealed that interactions of ortho substituents on the aryloxide ligand with the metal center contribute significantly to a lowering of the ion pair separation energy and ultimately led to synthesis of the 2-Br-phenoxide ligand to give one of the most active catalysts in this family[15]. This is an example of how the combination of computational chemistry with experimental studies on a library of catalysts, where informatics tools were employed to manage the large amount of data, has led to the first quantitative structure-activity model for this important class of polymerization catalysts – understanding that was exploited to develop a new catalyst with improved performance.

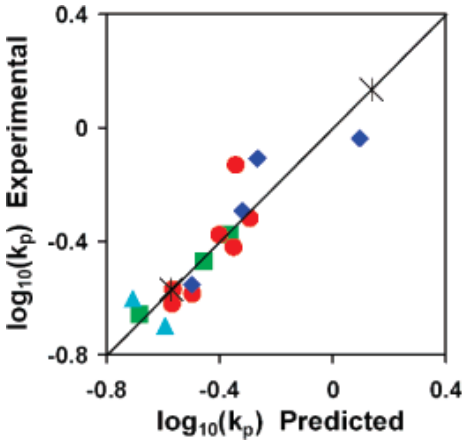


Figure 5: Parity plot of k_{pred} with points colored according to catalyst family.[14]

A second example draws even more heavily on computational materials science for screening potential catalysts. In a series of papers, Nørskov and coworkers have shown that adsorption energies can be correlated with the center of the d-band for their catalytic metal substrates[16]. Since many adsorbate fragments such as N, NH, NH_2, C, CH, CH_2, etc and appear to be linear in the d-band center energy, they are all linearly correlated with each other[17]. The use of Brønsted, Evans, Polanyi (BEP) relations for linear correlation of activation energies with adsorbate energies, then allows creation of a full energy diagram for a catalytic pathway and then optimization of the rate or selectivity by choosing the metal or alloy with the optimum energy of the d-band center. The so-called Sabatier volcano plot for steam reforming catalysts is shown in Figure 6[18]. While this approach will be best for systems where large changes in energies occur from one element to another and where subtleties of structure of the catalytic site do not dominate the activity, it has been shown to work for several important catalytic systems and represents a very effective approach for leveraging computational results for materials design.

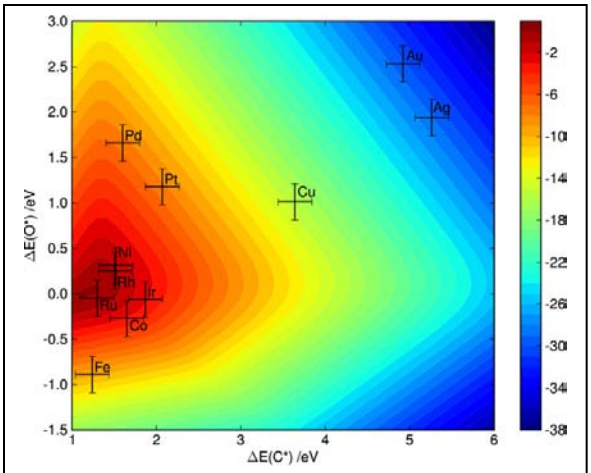


Figure 6: 2D volcano-curve of the turn over frequency (log^{10}) as a function of O and C adsorption energy. The error bars include an estimated 0.2 eV uncertainty in the adsorption energies.[18]

Computational Intelligence Helped Solve Antenna Design Challenge

Genetic algorithms (GAs) have been used to design complex antenna structures[19,20,21] to meet specific design requirements as shown in Figure 7. The key feature of GAs is that they can explore design variables that are both discrete and continuous, where the designer can impose additional constraints, e.g. each antenna is a single arm that is rotated 90° from its neighbors. In addition to the ability to automatically scan vast regions of design space, the GA approach can discover new, potentially interesting regions of design space that have been overlooked by expert designers who are often biased in their thinking. As an example, GAs were used to discover a number of known additive systems and a new oil additive systems that had been overlooked by expert formulators because the research team had engaged in 'group think' about exactly what molecular structure was needed for an effective oil additive.[22,23] As important as the development of new additive molecules, the GA approach was even more valuable in suggesting new directions for future research. GA and other automated design tools can potentially provide real value to the battery community that needs to develop these complex, integrated systems with multiple design requirements.

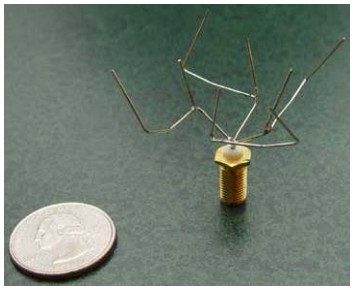


Figure 7: Photograph of prototype evolved antennas for design specification NASA's Space Technology 5 mission.[21]

Current State of the Art in Batteries

A number of battery systems have been developed. Figure 8 shows a some examples where the gravimetric energy density (Wh/kg) is plotted vs. volumetric energy density (Wh/liter). Included are primary (non-rechargeable) battery systems that have significantly higher energy densities than the current Li-ion systems; Some of these systems may be able to be adapted to serve as rechargeable systems, but in proven systems 200Wh/kg and 400Wh/L are the energy density limits for current technologies. These limitations will have to be addressed in any new material system for the next generation of batteries.

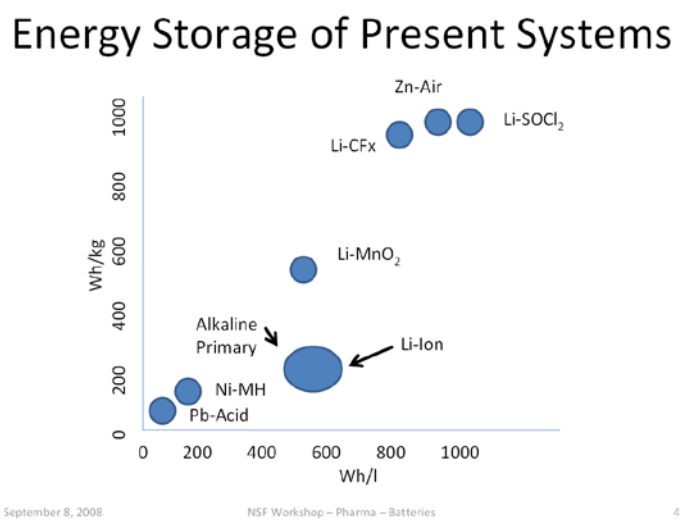


Figure 8: Energy storage capability of present systems, Broddarp, LLC 2008.

In addition to energy density, a major driver for any new battery system to be used in transportation will be the cost. The costs of the various components of a typical lithium-ion battery are summarized in Table 1. From this data it is evident that great gains in cost reduction can be achieved through innovation in electrolytes and separator technology since they interact with both parts of the cell and account for 30% or the total cost (compared to 23% for the electrode active materials). Efforts to improve energy density in present systems should help to meet the $/Wh goal, but expectation for significantly reduced cost over time may be unattainable. Moreover, batteries that employ lithium pose an additional challenge in that the world's supply of lithium is not unlimited, and the deployment of large numbers of electric vehicles will put pressures on the supply of lithium (see Figure 9). Thus, if lithium-based batteries are employed, instead of being able to ride the cost curve down as production of electric-based transportation vehicles ramps-up, the gains in manufacturing efficiency might be balanced or even undone by rising raw materials cost. Cost reductions can also accrue for material systems that

Material	% of cost per cell
Positive Active Material	22%
Negative Active Material	1%
Composite electrode construction materials	7%
Current collectors	7%
Separator	20%
Electrolyte	9%
Top parts & can	29%
Misc. tabs, etc.	4%

Table 1: Representative Bill of Materials (BOM) for the production costs of a lithium-ion 18650-type cell.

require less severe safety and containment measures.

Computational tools have the potential for dramatically accelerating the development of new batteries, where these tools will be needed for both the development of new materials as well as for the optimization of the individual components into a working system. The members of the workshop developed Tables 2 and 3 to describe the state-of-the-art in computational methods as they relate to battery technologies. For some of the properties, the predictive capabilities of the models are quite impressive as shown in Table 4, where the predicted and experimental voltage are given for several electrode materials that can be used in rechargeable lithium batteries. Such a predictive ability can be used to prescreen any new material for reasonable voltage and energy density. Although the predictive abilities of the models for other properties may not be as impressive, the current state-of-the-art is a good starting point for the development of improved models. However, there will need to be a significant extension of modeling capabilities in order to address the challenge of rapidly developing the next generation battery.

Resource limitations at work: Li-ion-battery light EVs

Scenario	'07	Likely '12	High '12
# HEVs, 2012	500,405	2,700,000	4,000,000
% Li-ion	0.1% (hobbyists)	25%	25%
kWh (average)	1.3	1.3	1.3
# PHEVs, 2012	2,300	250,000	700,600
% Li-ion	20% (conversions)	90%	90%
kWh (average)	3.9	3.9	3.9
# pure EVs, 2012	1,000	40,000	700,000
% Li-ion	0%	95%	95%
kWh (average)	19.5	19.5	19.5
EV% of vehicles	0.7%	3.6%	6.4%
Li need (tons)	1.2	3,747	25,089
Li need as % production	**0.002%**	**6.2%**	**42%**

Figure 9: Model from Lux Research on the demand on world lithium resources due to battery deployment in electric vehicles. Low percentages of electric vehicle deployment in the US market alone strains the world production capability.

	What's been Done	**What needs to be done**
Voltage	- First done 10 years ago - High throughput computations for electrode materials (+/-200mV)	- Non-intercalating electrodes - In the presence of phase change
Diffusion	- Can do one ion at a time - E_D in the dilute limit	- Many body problem - In the presence of phase changes - Concentration-dependent diffusivity - High throughput
Electron transport	- Has been done once.	- Some methodology exists, more needed
Phase Transformation	- Thermodynamics	- Kinetics
Thermal Effect	- Driving force	- Kinetics
Stability	- Limited aspects	- Dissolution - Phase transformations - Mechanical

Table 2: State-of-the-art of Computational Models for the Determining Material Properties

	What's been Done	What Needs to be Done
Composite Electrode	- 1D model (mean field)	-3D
Electrolyte Properties	- Easier to measure than calculate	-Basic science of relevant physical chemistry and electrochemistry
Thermal management	- Done for cells - Done for pack (by industry)	-Cell and pack dynamics under real-world use patterns
Impedance	- Heuristic - Equivalent circuit	-Materials dependence

Table 3: State-of-the-art of Models for Battery Systems

	Experimental	Calculated
$LiCoO_2$	4.2	4.25
$LiFePO_4$	3.5	3.45
$LiNiO_2$	3.75	3.71

Table 4: Experimental and calculated voltage for three lithium battery cathode materials.

High-throughput computing

While computing has demonstrated its usefulness in studying individual materials problems, its true game-changing potential lies in its scalability. Once the methodology to compute a property has been developed, the computation can be automated, and hundreds to thousands of compounds can be evaluated in a fully- or semi-automated way. Hence, it is possible to perform a broad search through composition and structure space. Such a search can be integrated with data mining methods which extract knowledge from compounds already calculated to improve the searching strategy and suggest other potentially interesting compounds.

Fully comprehensive screening of the compositional possibilities in nature is now within reach of high-throughput computing. A typical first-principles computation of a materials property such as energy or electronic structure may take about 1 CPU-day. More complicated properties may take up to 10-100 CPU-days per material. Assuming that of the order of five properties need to be known per material, a platform with 1000 CPUs can screen several thousand compounds each month, once the infrastructure is set up. To put this in perspective, there are currently about 35,000 known crystalline inorganic compounds in the International Crystallographic Structure Database (ICSD), the largest collection of inorganic compounds. Hence, the scale of computing power is now such that comprehensive searches through all possibilities in nature are possible. While one often thinks of the possible chemical combinations as infinite, they are quite within reach of a high throughput approach. Counting about 60 useful elements in the periodic table (not counting noble gasses, radioactive or toxic elements, or very rare and expensive elements)

only about 34,000 ternary and 488,000 quaternary combinations can be made. Obviously, one would not randomly search through these for a given application, but rather perform a directed search whereby acquired information is constantly used to direct the computations to interesting parts of composition space. We believe that such a comprehensive approach, whereby the entire chemical landscape is scouted, can radically change the way materials development is performed:

1) Multiple properties will be available for each interesting compound leading to a better justified choice of which materials should be further investigated in an experimental development program.
2) The wealth of available computed information about a prospective material – rather than the single piece of data that is often available with an experimental discovery – can be used to anticipate possible problems in experimental work and scale-up (e.g. a computed phase diagram information can be used to investigate the processability of the material and possible degradation).
3) The fact that a large compositional space has been searched – most of the possibilities in nature, one could argue – will remove some of the financial risk associated with investing in a novel material.

High-throughput computing is likely to become the new paradigm for materials design and development. A six to twelve month rapid screening of thousands of materials can result in a more focused and highly accelerated experimental research program, and ultimately lead to the more rapid introduction of materials into applications. Other fields, such as biology, have been transformed when detailed quantitative and comprehensive information became available. Large-scale and high throughput gene sequencing in biology is rapidly changing the nature of medical research and drug design in that field. We believe that high throughput ab initio computing will do the same for breakthrough battery research.

Finally, there must be a comment on the state of the infrastructure for battery research in the US. Battery research in the United States is fragmented. There are loose consortia such as USABC, BATT, etc. which do some integration, but for the most part the battery research community consists of disconnected specialists in the various disciplines needed to build a battery. The fragmentation of battery research poses some significant organizational challenges that must be addressed if the US is to credibly address the development of a new generation of batteries to meet the challenges of the 21st century.

Transformative Research Opportunities in Batteries

As part of the workshop, Dr. Ralph Brodd (a well know electrochemist in the battery arena) proposed the following list of nine key criteria for rechargeable battery chemistry:

1. Mechanical and Chemical Stability
2. Ability to Recharge and Deliver Power
3. Cycle Life
4. Temperature Range of Operation: -40 to +85°C
5. Low Self-Discharge

6. Shape of Discharge Curve
7. Cost
8. Charge Time
9. Overcharge/Overdischarge Protection

It is clear that any new battery or constituent material that significantly improves on these criteria without sacrificing anything in the others will result in an important advance for batteries. With these criteria in mind, the workshop participants discussed the options available for transformative breakthroughs in battery technology which can be achieved in an accelerated timeframe. The two areas identified as most promising (new battery chemistries and electrolytes) are covered in more depth below along with two important new approaches to collaborative battery research.

New Battery Chemistries

A schematic of the various components of a typically battery are shown in Figure 10.[24] In practice the various components are much more complex, e.g. the anode and cathode are complex composites that contain active material, polymeric binders and conductive diluents such as carbon black, where the composite has sufficient porosity to allow the liquid electrolyte to penetrate into the structure. The development of new materials for the 21st century battery will have to address the complexity of the various material systems as well as the interaction between the systems, e.g. the reactive sites on the anode or cathode can potentially degrade a polymeric electrolyte thus affecting long term performance.

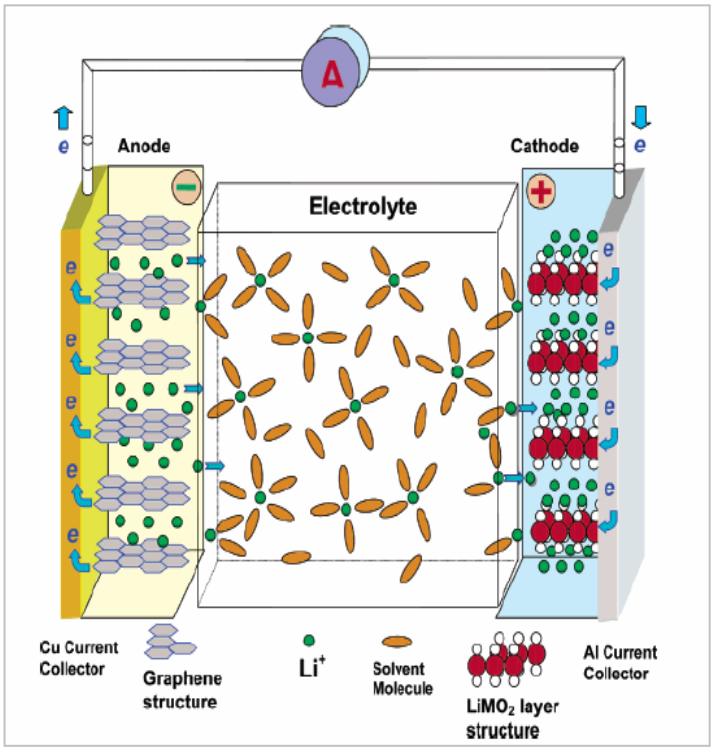


Figure 10: Components of a typical battery[24]

It is true that by the metric of energy per unit mass, lithium-ion seems very attractive. However, its viability in large format applications is still in doubt. For one, there is the high cost, but perhaps this can be combated by economic tools, e.g., subsidies, tax relief, etc. More of concern is the potential shortage of the necessary raw materials. Neither lithium nor cobalt is well distributed throughout the earth's surface. One of the design constraints on breakthrough battery materials should be that the candidate battery material must be derived from earth-abundant resources. Otherwise, the technical success is axiomatically resigned to remain in the laboratory. Cost considerations will condemn it as not commercially scalable.

The main opportunities for improving energy density (as well as reducing the costs due to safety considerations) lie in alternate cathode chemistries. The workshop participants identified the opportunity to use non-lithium charge carriers as a way to boost the energy density of the battery system. In an intercalation battery, the energy storage capability goes as the square of the charge on the mobile species and lithium is singly charged as compared to other earth-abundant systems that have higher valence states available. Additionally, it is even possible to imagine displacement batteries with higher valence mobile species which might be inherently safe, lower cost and sufficiently high energy. There is no single best battery, as there is no single best wine. Without context, it is impossible to recommend the appropriate battery technology. It has never been considered to develop an energy storage technology from scratch for automotive applications. Breakthroughs in this area will require that new chemistries be considered, old prejudices be put aside and all ideas be welcomed (up until the breaking of the laws of thermodynamics is proposed!). The path to better batteries is paved with advanced materials.

Electrolytes

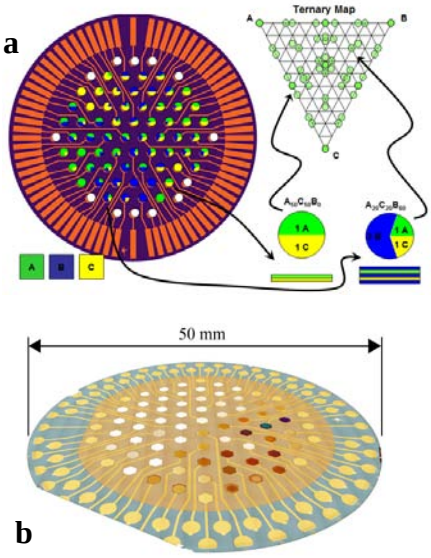
Electrolyte development is an area with tremendous opportunity for impact on the performance goals of the system. The electrolyte is the one component that touches all of the components in the battery, almost like the glue that holds it all together. That means that there are tremendous materials compatibility requirements on the selection of the electrolyte, but also that there are large opportunities for impact on performance. Simply widening the voltage window of the battery by, for example 25% by the use of an electrolyte with higher breakdown voltage, boosts energy density by 25%. Since the electrolyte portion of the battery cost is significant, so too are improvements in cost performance also significant. However, the question of electrolyte design has received a relatively small amount of attention from the research community. We recommend an improved dedication to funding research in this area.

The computational component related to electrolytes provides some interesting scientific challenges. Modeling of the liquid state is difficult, especially in multi-component systems with a plurality of solutes, mass and fluid transport, and coupled electric loads. This defines a fertile area for research. In parallel, there is the question of the solid/liquid interface which is represented by the boundary between the surface of the electrode and the electrolyte. There is ample evidence in the battery literature to indicate that failure to efficiently manage the electrode/electrolyte interface can lead to parasitic power losses in the form of voltage penalties associated with the activation energies required to facilitate electron transfer or ion transport or both. The nature of electron transfer is of sufficient intellectual value that Rudy Marcus received the Nobel Prize in Chemistry in 1992 for his pioneering work in this area.

Other areas for innovation in electrolyte research relate to the mobile charge carriers. By moving to non-lithium charge carriers (such as Na, Ma, Al, V, Ti, etc.) improvements in cost as well as energy density and safety become possible. Innovation in the solvent systems employed also hold promise for meeting performance goals. Liquid aprotic solvents, such as carbonates, have been the standard for advanced battery systems such as lithium-ion. Innovation in the nature of the solutes might enable lower cost, non-volatile alternatives with improved safety. Candidate solvents that might serve as supporting electrolyte include ionic liquids and solid polymer systems.

High Throughput Experimentation

In the drug industry the field of combinatorial chemistry was developed as a means to permit *high throughput experimentation* for efficient and systematic exploration of various chemical families for signs of biological or chemical activity. More recently this approach has been adapted to the field of solid state materials.[25] As typically practiced the HTE approach employs parallel (or automated serial) processing to create large "libraries" of material compositions, followed by parallel (or automated serial) testing to characterize the compositions for a specific property of interest. The information is then fed back into a database for mining through various informatics approaches, and subsequently used in modeling to suggest subsequent library designs. Much of the potential of the HTE approach depends on the development of tools for rapid screening of libraries for the properties of interest. Ideally, the intent is for only one variable to change (e.g. composition) while all others (grain size, surface area, etc) remain constant.



11 a) Schematic Layout of a sputter deposited thin film combinatorial library on a Si wafer. b) photo of actual thin film library

McGinn at Notre Dame has pioneered thin film combinatorial approaches for improved fuel cell electrode materials. [26,29,30,31] These studies have included thick film and fuel cell validation of thin film predictions,[27,28] and recently they have fabricated individual thin film solid state batteries. The preparation of combinatorial composition libraries and the subsequent electrochemical testing has been described in detail in several papers.[29,30] Combinations of high purity materials are sputter deposited through shadow masks to yield an array of discrete multilayer spots on 50 mm diameter silicon wafers as shown in Fig. 11. The samples are rapidly thermal annealed after deposition to transform the multilayer samples into homogenous alloys. Automated x-ray diffraction including an area detector for more rapid scans is used to determine the structure of the annealed library elements. For a given ternary system, specific regions (e.g. the A-rich corner) or the entire system can be surveyed based on the chosen mask sequence. If a region of interest is identified, a follow-up study can be performed focusing on that area. A commercial multielectrode potentiostat system (Scribner Multichannel Microelectrode Analyzer - MMA) is used for fuel cell catalyst testing by cyclic voltammetry (CV). A specially designed sample cell permits simultaneous collection of CV curves from all of the combinatorial library members. This is shown schematically in Figure 9,[31] where the ternary plot shows oxygen reduction onset potentials for candidate fuel cell electrocatalysts.

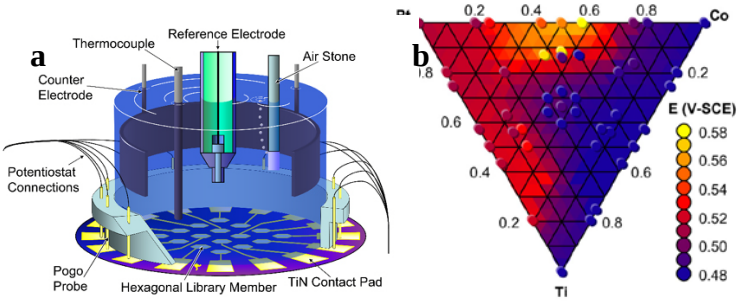


Fig. 12 Combinatorial test cell for fuel cell electrode electrochemical evaluation b) example of library activity map from analysis of cell test results

Computational Chemistry

As has already been discussed, high-throughput computing can provide a method for screening vast numbers of candidate materials, enabling the out-of-the-box thinking regarding new battery materials. These tools can (i) provide simple-to-compute properties for a range of materials, (ii) help develop descriptors that can be used in the construction of empirical and fundamental structure-property relationship models, and (iii) provide data that can be mined to determine statistical relationships between performance and the descriptors.

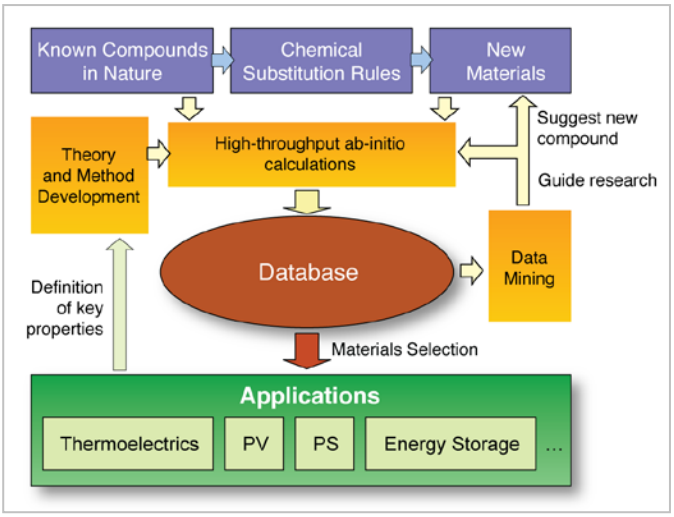


Figure 13: Data flow overview

To further illustrate how this approach would be used, a potential high throughput simulation environment is shown in Figure 13. The computing framework could operate around an internal database, which stores all aspects of a computational run including structural details, computational parameters, results, and even motivation for the particular computation. Compounds would be linked by chemical or structural prototype relations. Even more complex connections can be made such as topotactic relations (e.g. structure α is the same as β but with an ion removed, as is relevant for Li-battery electrodes). The chemical space that would be searched would start from all known compounds as found in databases such as the Inorganic Crystal Structure Database (ICSD), CrystMet, the Powder Diffraction File, etc., but augmented with new hypothetical compounds. The latter will be generated through chemical perturbation strategies from known compounds or by direct design based on the rules and information generated by the data mining methods. It is possible to develop seamless integration between structural databases, the computational environment, the data analysis and data mining. The objective would be to create an environment in which meta-questions can be asked about materials: e.g. "*How is the redox couple of Mn^{3+}/Mn^{4+} affected by structure and anion chemistry (for Li battery applications)?*", or "*How does the bandgap relate to structure and chemistry of materials?*" Such a fully automated high-throughput environment is not science in itself, but by providing a virtual rapid testing ground for materials, it will generate new materials, ideas, and intuition. Indeed, data mining materials design based on HTE has already been proven successful in the field of catalysts and polymers.

Ab initio Property Computation

In order to calculate the full suite of properties and structural aspects of materials for energy applications, several algorithms and methods need to be integrated with the HT environment. Currently, Ceder's group at MIT has begun some HT integration with basic DFT codes, such as the *Vienna Ab Initio Simulation Program (VASP).*[32] This enables the calculation of total energies for crystal structures and can, for example, be used to evaluate the electrode potential for possible electrode materials for rechargeable lithium batteries.[33] Figure 14 shows a scatter plot (with compound names removed) of the theoretical capacity versus the calculated electrode voltage for 3708 compounds.

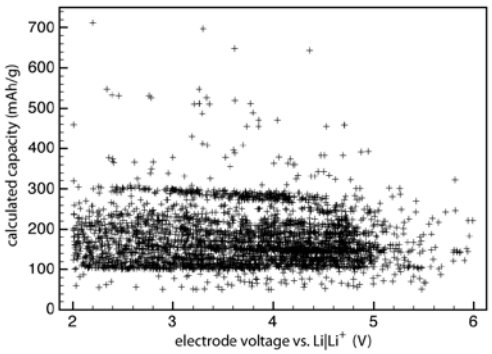


Figure 14: Calculated Theoretical Capacities vs Voltage for 3708 Compounds

Data Mining and Characterization of Structure/Chemistry Property Relations

Data mining and statistical learning form a key ingredient of this HT materials design environment. Once *ab initio* methods have generated a substantial amount of data, it is then possible to develop and apply extensive data mining and statistical learning methods to analyze the data in order to discover predictive relationships between descriptors and material properties.

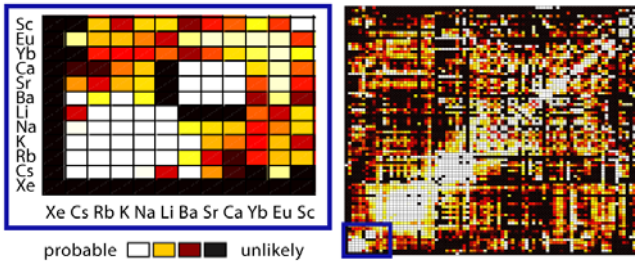


Figure 15: Probability to substitute atom 'A' (x axis) for 'B' (y axis) calculated over all compounds in the ICSD, where high probability is represented by the light colors (white is highest probability and black lowest).

A challenging problem within the materials design context is the generation of plausible new compounds, using existing data and the "hidden" rules of nature. To achieve computational efficiency, only hypothetical compounds with a reasonable chance for stability should be proposed. An intuitive way of doing this is to use the known compound space and propose new materials simply by replacing the atoms in known compounds with other chemical combinations. The success of such a method relies heavily on how intelligently the substitution is performed. Predictive rules can be obtained by data mining calculations of known compounds to find which atoms are likely to substitute for each other while retaining the same crystal structure. Using all the oxides structures in the ICSD the probability of any possible atomic interchange that would keep the structure stable was determined. Figure 15 shows the pair correlation in color code for this model and indicates how likely an element could directly substitute for one another (white represents a high probability of success). The inset shows a magnified part of the table where, for example, Li readily substitutes for most alkali ions (despite large differences in ionic sizes) but not for Ba, Sr, and Ca. The information captured in Figure 15 is particularly useful as it captures all of the known intuitive substitution rules based on ionic size, charge and chemical similarity, but does

so without bias and only by relying on actual ground state data. Employing this data when proposing new compounds, greatly increases the chance of finding stable compounds compared to random combinatorial guesses.

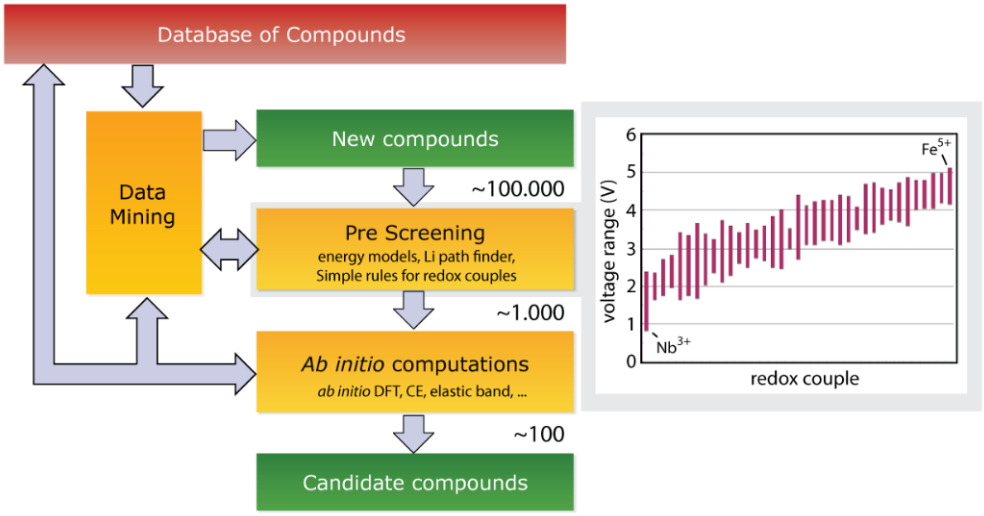


Figure 16: Overview of high-throughput screening process, specified for Li battery case and approximate number of compounds at each stage of the screening. The picture inset shows voltage ranges of cations, based on 3500 compound calculations, which can be used for pre-screening target voltages in new compounds.

Example of a HT design flowchart to Find Better Li Battery Materials

Figure 16 gives a general example of how high-throughput screening would be performed in order to find new electrode materials for rechargeable Li batteries. A HT design project for predicting any new material starts with defining the target element and structure space. As an example, the combined search space can consist of all non-toxic, non-radioactive elements and all structures contained in the ICSD. To find new Li-intercalation electrodes, step 1 would for example generate a set of hypothetical compounds by substituting redox-active cations into suitable structures, the latter which are chosen by approximately evaluating the Li diffusivity of the compound by empirical models. This initial set is large, usually on the scale of 100,000 compounds and needs to be pre-screened by efficient data mining algorithms.

There are a number of important Li battery materials properties, and they can be computed rigorously by ab initio methods as well as efficiently but less accurately by heuristic methods for pre-screening purposes. As an example, the capacity between some voltage limits of a hypothetical compound can be efficiently estimated using the capacity for simple binaries with same valence states. The stability can also be evaluated using data mining schemes for the electrostatic energy of mixing cations and coordination preferences trained on the data of existing compounds. Thus, using capacity and stability pre-screening tools, the set of new hypothetical compounds is reduced drastically, to the order of thousands of compounds. This set can be calculated by ab initio methods to yield accurate voltage, capacity, Li mobility, and stability evaluations by which the compounds are ranked. The most promising ones are then

further investigated using more sophisticated statistical mechanics methods to generate accurate phase diagrams, Li diffusivities and electronic conductivities.

Sustainability and Recyclability

New battery chemistries will likely involve mixtures of metals and metal oxides whose sustainability and recyclability are not well understood. Breakthrough battery materials composed of such materials will not be economically viable unless methods of recovering and separating the metals are developed. Recycling other parts of the battery will be important as well. Research into modular manufacturing of battery cells that can be replaced while keeping the underlying control circuitry intact will help drive down total cost of ownership. Finally, scale up of manufacturing techniques and assessment of material availability and strategic access will need to be addressed to ensure that successful lab scale experiments can be mass marketed.

Integration and System Modeling

It is clear from issues discussed above that batteries are complex systems. In fact, each component is already sufficiently complex on its own, that performance breakthroughs in those specific areas are highly challenging. Impact in the energy arena, however, will require a new and fully optimized operating battery *system.* Not only will communication between teams focusing on individual components be essential, full system optimization will further require integrated models that quantitatively capture the interplay between components. In addition to the basic storage function, battery systems will have to also address stability, reliability, safety and cost. While these issues can be addressed at a variety of levels, the highest level, which would aim for a global optimization, would draw on sufficiently large, coupled databases that it may raise interesting new challenges for the modeling of complex systems.

Enabling Technologies

HT Synthesis and Screening techniques

It is clear that the acceleration of breakthroughs needed to reach the research goals for enhanced battery performance outlined here cannot be done without a change in research approach. Based on successes in other fields, close coupling of high throughput modeling with high throughput experimentation can substantially increase the growth of knowledge and has the potential to support the proposed goals. While HT tools for new materials synthesis may be adapted from other materials fields like fuel cells, new tools will have to be developed for battery material applications. The technology in this area is relatively limited, especially with respect to high-throughput characterization of battery materials, so development of these tools will have to be a major component of any funding program targeting battery advancement.

In-situ characterization Tools with time and space resolution

In tertiary testing of the most promising new materials and components in situ characterization methods will give the most valuable information because they will reveal changes in the materials and their properties under the stress of operation. Time resolution will help define stability issues while special resolution will address material heterogeneity in operation.

Opportunities for this work might develop through collaboration with National Laboratories which house some of the most advanced spectroscopy and microscopy facilities.

Nano Technology

Since band structure, composition constraints, defect density, and other physical and chemical properties are strongly perturbed in nanosized materials, such materials may substantially broaden the search space for new components for battery application.[34] While the methodology for preparing nanoclusters of chosen size and structure is growing rapidly, guidance from computation of the pertinent properties of specific nanomaterials may be needed to restrict the search space. Stability of such systems will also be an issue that needs to be considered.

Multi-scale Material Modeling

A battery system spans length scales from the 0.1 nm atomic components to the roughly meter sized integrated system. Quantum level modeling of the atomic scale will guide materials discovery, as discussed above, but system optimization and issues of cost and stability will require integrated modeling over the whole 10 orders of magnitude change in length scale. Some aspects of this multiscale modeling are already in hand, but others will need to be developed in new research initiatives.

Domain Specific Modeling Tools

The value of HTE can only be realized if the model building and evaluation takes place at a rate commensurate with the data rate from HTE. A variety of domain specific modeling tools have been developed in other research areas to aid the researcher in rapidly constructing and/or modifying new models. In the area of chemical kinetics, domain specific compilers have been developed for a variety of reactions types including combustion,[35,36] propane aromatization,[37] vulcanization,[38] single site polymerization, [39] industrial chemistry,[40] electrochemistry,[41,42] and biology.[43,44,45,46,47,48,49] These systems assist the researcher in generating the appropriate differential equations that describe simple to more complex kinetics. There are also numerous domain specific modeling tools in MatLab[50] and Comsol[51] as well as a number of second party vendors that use the MatLab and Comsol platforms. As one example, a fairly general simulation module for a NOx after-treatment reactor has been developed that enabled the facile input of new candidate NOx adsorption/reduction kinetic models in either 1D or 2D models of the transport of reactant/products in the channel of the after-treatment system as well as the surface chemistry.[52,53] This simulation module enabled the rapid assessment of new kinetic mechanisms for NOx adsorption/reduction and the evaluation of new operating protocols for the after-treatment system. The development of such a domain specific modeling tools along with a well developed user interface can enable the more rapid development of new models of batteries as well as enable the more experimentally inclined researchers to make use of these predictive tools without the need for detailed understanding of the requisite numerical algorithms and implementing the associated software.

Need for Collaborative Infrastructure

The technical challenges described above span a variety of engineering and scientific domains. From a research perspective the various knowledge domains are currently disconnected. However, the development of breakthrough battery technology will require integration between various areas of expertise. For example, the development of a more efficient cathode material is

of little value if it does not also mitigate the long-term catalytic degradation of the electrolyte. This is just one example of the types of difficulties that occur because of the lack of research integration.

Consider what a potential integrated research team might look like. Team A: PI-Materials engineer researching new intercalation compounds with co-PIs that (i) provide high-throughput experimental capabilities, (ii) molecular modeling using DFT calculations to support the experiments and (iii) unique materials characterization and analysis at one of the national laboratories. And Team B: PI-Chemical engineer modeling the transport of ions in new electrolytes with co-PIs that include (i) a materials engineer looking a new anode or cathode systems, (ii) a electrochemist designing new electrolytic solutions and (iii) a computational intelligence expert using genetic algorithms to discover unique designs for the overall system. Such intra-team collaboration faces challenges because of the differences in technical expertise among members and these challenges only multiply with inter-team collaboration. Nevertheless, it is the formation of these cross-disciplinary teams for conducting research that offers the most significant potential for breakthrough battery technology.

The workshop participants concluded that performing research by means of integrated research teams is central to any funding initiative aimed at accelerating breakthrough battery technology. Individual research projects must work together to effectively leverage the limited resources to reach to goal of not just publishing papers, but rather developing the enabling technology for at least a 2-fold increase in battery performance/weight at reduced cost. Publishing data in scientific journals has been the traditional mode for community interaction; however, the timescale for this activity is much too long for the various research teams to effectively influence the work of other teams while the funded projects are still active. Annual or bi-annual working meetings between the participants of the program would provide a vehicle for faster communication, but even then the exchange is too slow and typically the amount of information that is shared is limited. Moreover, these working meetings are typically a presentation by each member of the team on what they are doing with little modification of the pre-ordained directions for research.

Success in development of breakthrough battery technology will require an open and transparent collaboration, where both inter and intra group members can access, review, model and make comments on all data as soon as it is collected. This approach allows researchers with different perspectives to review experiments and see if apparent failures in one context are not a potential opportunity in another. Moreover, modelers and informatics experts in different groups must be able to access all available data while the research is being conducted in order to maximize the knowledge content of their models and increase the probability of finding a new breakthrough.

Modern cyber-infrastructure can enable the needed collaboration. The key component of the cyber-infrastructure would be a relational database with a well defined but flexible architecture, where the physical location of the database could be central or federated. The database architecture needs to allow new experiments and types of data to be added as research progresses and leads from high throughput experiments are followed with more intense scrutiny. The database needs to be directly connected to an electronic lab notebook so that data does not have be entered a second time with additional effort and potential for error. Provenance and metadata

for each material tested and experiment performed must be maintained so that validation of data can be made by any user at any time. Additionally, an integrated software environment like SciAether^{TM} (sciaether.org) that includes an electronic lab notebook with IP protection, relational database, ontological based database queries, a linked analysis environment and domain specific visual analytics can greatly facilitate the use of such a database, especially by battery researchers that are not experts in database and/or cyber-technology.

Legacy data provides difficult, if not insurmountable, challenges for database development because it typically (i) is stored in conflicting formats and (ii) does not have sufficient meta-data so that anyone other than the individual researcher can make sense of the data. Because the US battery community is just beginning to organize (and hence there is not a large amount of legacy data), this would be an excellent opportunity for the NSF sponsored cyber-infrastructure research program to demonstrate how cyber-infrastructure can accelerate research productivity in an area of immense national importance.

Community Readiness

As mentioned earlier, the current battery research community is highly fragmented. This is due in part to the lack of sustained funding in this area over the last several decades. However, the various components in the larger research community are ready to take advantage of a new NSF sponsored large scale research intuitive in the battery area. Specifically,

- There are currently is a sufficient number of experts in electrochemistry to drive an initial research effort, although they have not recently been focused in the battery area.
- There are a significant number of researchers in allied areas in surface science, nanotechnology, computational materials science, informatics, control systems, etc. that are essential technologies needed to create a new paradigm for battery research in the 21st century.

The fact that there is not currently a firmly entrenched battery community affords some real advantages. First, there is the opportunity to bring in an array of new research groups with interesting technologies without the need to displace existing research groups, and second, the community can be structured to encourage data sharing rather than competitive hording of data. The research community is ready to take advantage of a major battery initiative once significant funding becomes available.

Workforce Development

Significant changes are under way with the ingress of materials scientists invigorating the field of battery research. To a great extent the acceleration of battery development will also depend on the development of human resources: electrochemical science & engineering need sustained support to attract and retain the best and brightest researchers. Only then can we create a vibrant and stimulating intellectual environment that will allow innovation to take root, much as is the case in the life sciences which have enjoyed huge investment over a long period of time. Now is the opportune time to benefit from the growing restlessness among students and young scientific researchers who want career paths that allow them to live their convictions in their professional lives, i.e., science in service of humanity, and sustainable use of energy and resources.. These are exciting times for applied science and engineering.

Conclusion

The conclusion of a workshop held at MIT in September, 2008 under the sponsorship of the National Science Foundation is that by leveraging the advances in computational materials science and informatics with high-throughput experimentation, the rate of discovery of new materials can be greatly accelerated, enabling the development of superior battery technologies. Furthermore, based in part on lessons learned in the search for new drugs by the pharmaceutical industry, the workshop declared that:

1. The deployment of computational materials science and informatics is expected to enable rapid intelligent screening of materials resulting in the selection of the most promising candidates with targeted performance attributes. A good start has already been made is some critical materials areas.

2. High-throughput experimentation with sophisticated test protocols is expected to reduce the time for assessment of candidate materials as well as to contribute fundamental property measurements to the materials database. The development of HT experimentation currently lags behind that of HT computation in this area.

3. Research on the anode, cathode, and electrolyte must be integrated, and mechanisms for data sharing are essential.

Accordingly, the workshop endorsed the injection of new funds by the federal government to support the search for advanced energy storage materials and further recommended that only research conducted by multidisciplinary teams comprising a strategically selected combination of theoreticians and experimentalists be eligible for sponsorship under the proposed new program.

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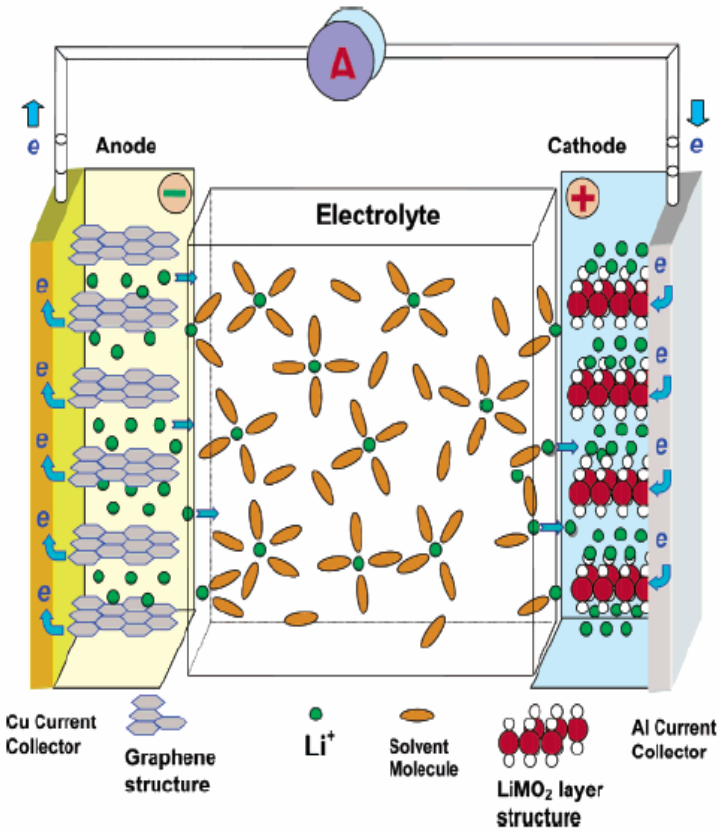
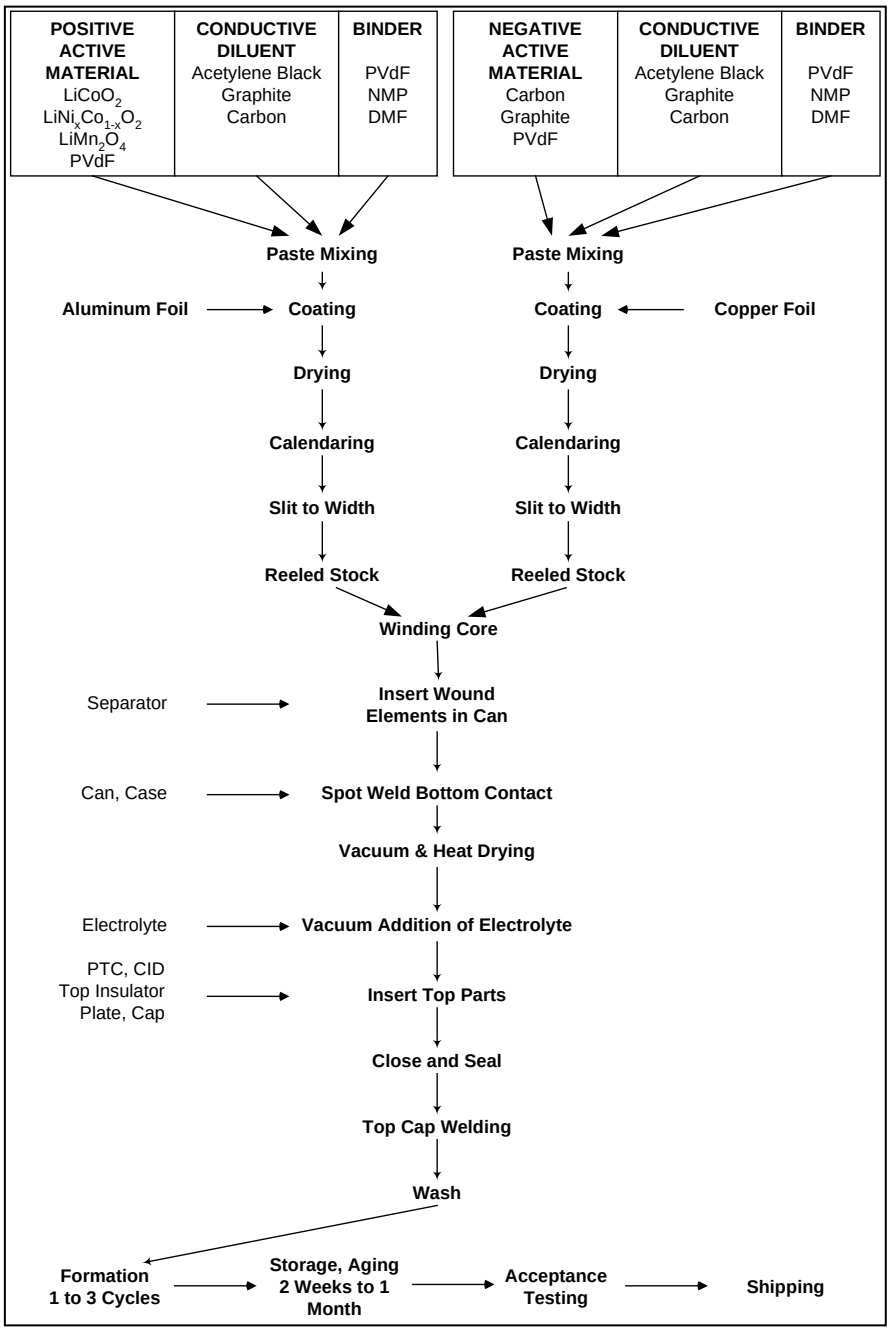
Appendix 1. Battery Tutorial[24]

What Is a Battery?

A battery contains one or more electrochemical cells; these may be connected in series or parallel to provide the desired voltage and power. The anode is the electropositive electrode from which electrons are generated to do external work. In a lithium cell, the anode contains lithium, commonly held within graphite in the well-known lithium-ion batteries. The cathode is the electronegative electrode to which positive ions migrate inside the cell and electrons migrate through the external electrical circuit. The electrolyte allows the flow of positive ions, for example lithium ions, from one electrode to another. It allows the flow only of ions and not of electrons. The electrolyte is commonly a liquid solution containing a salt dissolved in a solvent. The electrolyte must be stable in the presence of both electrodes. The current collectors allow the transport of electrons to and from the electrodes. They are typically metals and must not react with the electrode materials. Typically, copper is used for the anode and aluminum for the cathode (the lighterweight aluminum reacts with lithium and therefore cannot be used for lithium-based anodes). The cell voltage is determined by the energy of the chemical reaction occurring in the cell. The anode and cathode are, in practice, complex composites. They contain, besides the active material, polymeric binders to hold the powder structure together and conductive diluents such as carbon black to give the whole structure electronic conductivity so that electrons can be transported to the active material. In addition these components are combined so as to leave sufficient porosity to allow the liquid electrolyte to penetrate the powder structure and the ions to reach the reacting sites.



Appendix 2 – Battery Construction



Appendix 3 – Workshop Organization

The workshop was funded by NSF grant to Purdue University with W. N Delgass and James M. Caruthers as co-PIs.

The workshop organizers were:

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

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

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

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

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

The advice and perspective of Paul Werbos were and important contribution to defining the workshop objectives. Many details of the logistics, planning and execution of the workshop were ably handled by Luis A. Ortiz, Department of Materials Science and Engineering, Massachusetts Institute of Technology

Attendance was by invitation with the organizers attempting to represent a broad spectrum of experience and expertise in battery related science and technology.

Appendix 4 – Workshop Agenda

Massachusetts Institute of Technology
Cambridge, Massachusetts
September 8, 2008

Workshop Overview
1:30 - 1:50 pm
Paul Werbos
Program Director
National Science Foundation

Overview of High-throughput method
1:50 – 2:15 pm
W. Nicholas Delgass
School of Chemical Engineering
Purdue University

Informatics in Drug Discovery
2:15 – 2:55 pm
Ernst R. Dow, Ph.D.
Senior Information Consultant/Principal Research Scientist, Discovery Informatics
Eli Lilly and Company

Electrochemical energy storage and extended-range electric vehicles
2:55 – 3:25 pm
Mark Verbrugge
Director, Materials and Processes Laboratory
General Motors Research and Development Center

Break

Data handling and informatics tools for model-based discovery
3:40 – 4:20 pm
James Caruthers
School of Chemical Engineering
Purdue University

New High Energy/Power Devices
4:20-4:50 pm
Ralph J. Brodd
2161 Fountain Springs Dr .
Henderson , NV 89074

High-throughput ab-initio computing and data mining methods for the prediction of crystal structure

4:50 – 5:20 pm

Gerbrand Ceder
Department of Materials Science & Engineering
Massachusetts Institute of Technology

Materials Informatics: An "omics" approach to materials based design for battery technology

5:20 – 5:50 pm

Krishna Rajan
Department of Materials Science and Engineering
Iowa State University

September 9, 2008

8:30 – 8:40 am
Charge for Breakout Sessions

8:40 – 10:15 am
Breakout Session 1

10:30 – 10:50 am
Reports from Breakout Session 1

10:50 am – 12:20 pm
Breakout Session 2

1:30 – 2:00 pm
Reports from Breakout session 2

2:00 – 3:30 pm
Concluding Discussion

Appendix 5 - Participants

George Adamson, Vice President of Product Development, ZPower, Inc.

George Adamson was formerly the head of Virtic, LLC, a company providing contract engineering and scientific consulting. Prior to Virtic, Dr. Adamson was previously the vice president of research and development at Valence Technology Corporation, a firm developing and manufacturing lithium-ion polymer batteries, where he was responsible for setting the company's strategy for its intellectual property portfolio and launched the company's first three mass-produced product lines. Dr. Adamson was also the senior research scientist for Zinc Air Power Corporation, a start-up company developing a commercial electric vehicle battery. In this position, Dr. Adamson directed an electrochemical research and catalyst testing program to develop a commercial bi-function air cathode. Dr. Adamson is the holder of three U.S. Patents, with seven additional under application. He's been published extensively, in such journals as Journal Power Sources, Chemistry of Materials, Electrochemical and Solid-State Letters, Journal of Chemical Physics, and Journal of Molecular Spectroscopy. B.S. Chemistry, University of California, Riverside, 1988; Ph.D. Physical Chemistry, Massachusetts Institute of Technology, 1994.

George Blomgren, Chief Scientist, Lion Cells

Dr. George E. Blomgren evolved from a theoretical chemist into a battery expert, first by earning a B.S. in chemistry from Northwestern University in 1952 and a Ph.D. in physical chemistry from the University of Washington in 1956. After a post-doc at Columbia University, he began a 41 -year career with Union Carbide Corp. which evolved into the Eveready Battery Co. His early work with UCC involved statistical mechanical theories of liquids, electrolyte solutions, and molten salts. This led to a group leader position in the Battery Products Division in 1963 with a focus on the then-new lithium batteries. His work on electrolytes prepared the way in 1971 to filing the first patent on lithium liquid cathode batteries in which the liquid (e.g., thionyl chloride) serves as both the solvent for the electrolyte salt and the active cathode material. This dual role allows very high energy to be packed in the container, thus forming the highest energy primary battery in use today. His work also led to the lithium-ion disulfide battery, which the company developed into a commercial product, first as a button cell and then as an AA and AAA cell. His reward was the highest technical position at Eveready - Senior Technology Fellow.

After retirement he started a new career consulting with companies around the world on battery technology and applications. He also has presented invited papers at many meetings in the U.S., Europe, and Asia to the delight of his wife Gerry, who is always ready to pack up and go with him. George was Associate Editor of the Journal of the Electrochemical Society, Chair of the ECS Battery Division, and adjunct professor at Carnegie Mellon universities. He continues as adjunct professor at Case Western Reserve University in the Department of Chemical Engineering. With the formation of the new company "Lion Cells, Inc.", George became a founder and the Chief Scientist in 2006.

Ralph J. Brodd, President, Broddarp of Nevada, Inc.

Ralph J. Brodd is President of Broddarp of Nevada, Inc.,a consulting firm specializing in technology assessment, strategicplanning and battery technology, production, and marketing. He received a B.A. degree in chemistry from Augustana College, Rock Island, Illinois, and M.A. and Ph.D. degrees in physical chemistry from the University of Texas at Austin.

Dr. Brodd began his career at the National Bureau of Standards in Washington, D.C., studying electrode reactions and phenomena that occur in battery operation. He taught physical chemistry in the U.S. Department of Agriculture Graduate School and lectured in electrochemistry at Georgetown University and American University.

In the 1960s and 1970s, Dr. Brodd served in a variety of technical and management capacities with a number of battery companies. In 1961, Dr. Brodd joined the L.T.V. research Center of Ling Temco Vought, Inc., in Dallas, Texas, where he established a group in fuel cells and batteries. In 1963, he moved to the Battery Products Technology Center of Union Carbide Corporation, with technical management responsibilities for nickel-cadmium and lead acid rechargeable batteries, alkaline and carbon-zinc product lines, and exploratory R&D. He joined ESB (INCO Electroenergy, Inc.) in 1978, establishing a technology surveillance group, and moving to the position of Director of Technology with oversight and policy responsibility for R&D laboratories serving product areas ranging from primary and secondary batteries to uninterruptible power supplies and small electric motors. He was a member of the INCO Long Range Technology Committee and the technical advisory panel for North America Capital Venture Fund.

In 1982, Dr. Brodd established Broddarp, Inc., a consulting firm specializing in battery technology, strategic planning, and technology planning. A consultancy with Amoco led to his moving to Amoco Research Center as project manager of a rechargeable lithium sulfur dioxide battery project. He subsequently moved to Gould, Inc., to establish their Lithium Powerdex Battery Venture and then to Valence Technology, a venture group developing a solid polymer electrolyte battery system for rechargeable batteries for portable consumer devices. He served as staff consultant/marketing director and then Vice President, Marketing.

Dr. Brodd was elected President of The Electrochemical Society in 1981 and Honorary Member in 1987. He was elected National Secretary of the International Society of Electrochemistry, 1977-1982, and Vice President, 1981-1983. He is past chairman of the Board of Directors of the International Battery Materials Association. Dr. Brodd has over 100 publications and patents.

Valerie Browning, ValTech Solutions, LLC

Valerie Browning is an independent consultant and subject matter expert for ValTech Solutions, LLC. She serves as a subject matter expert for a number of DoD and other government activities in the areas of advanced materials and alternative energy.

Prior to forming ValTech Solutions, LLC in December 2007, Dr. Browning served as a Program Manager in the Defense Sciences Office at the Defense Advanced Research Program Agency. During her tenure at DARPA, she assumed full responsibility for the strategic planning, operating management, leadership and development of multiple R&D programs providing innovative technologies in power and energy, radar, telecommunications, and biotechnology for diagnostics, therapeutics and chem./bio warfare defense. She also served as the DARPA liaison to the DoD IPT on Energy Security and served as Acting DSO Office Director prior to her departure from government service. In addition to her time at DARPA, Dr. Browning spent 16 of her 24 years of government service as a research physicist at the Naval Research Laboratory. Her primary areas of research were thermoelectric materials, high temperature superconductors and magnetic oxide materials. She has published over 40 peer review manuscripts including three book chapters.

Born in South Ruislip, England, Valerie is a 1987 graduate of Virginia Tech where she received her B.S. in physics. She also holds a M.S. in physics from the University of Maryland and a Ph.D. in physics from the Catholic University of America.

James Caruthers, Professor of Chemical Engineering, Purdue University

Director, Center of Integrated Materials and Product Design (CIMProD)
S.B.(Chem) Massachusettes Institute of Technology, 1975
S.M. Massachusettes Institute of Technology, 1976
Ph.D Massachusettes Institute of Technology, 1977

Professor Caruthers' aim is to develop models to describe the behavior of a variety of chemical, polymeric and biological systems. His research interests include the design of formulated rubbers, the nonlinear mechanical behavior of glassy polymers, the rational design methods for catalysts, and the origins of the glass transition.

The modeling of complex systems requires the analysis of large amounts of data, which includes high throughput experimentation (HTE) and high throughput computations (HTC) as well as high throughput modeling tools to keep pace with data flow. In order to keep pace with this data flow, we are developing a cyber-infrastructure for chemical and materials discovery, which we call SciAetherTM. A team of professionals and students are developing an integrated platform that includes data ingress, data storage and retrieval using domain specific ontologies, data analysis and modeling, and rich visualization that using domain specific images. The system is scaleable, using computation capacity that ranges from a desktop PC to workstations to supercomputers and visual output that can be a PC's dual screen monitor to a multi-head display to a large tiled wall.

Gerbrand Ceder, R. P. Simmons Professor of Materials Science & Engineering, MIT

Gerbrand Ceder received an engineering degree in Metallurgy and Applied Materials Science from the University of Leuven, Belgium, in 1988, and a Ph.D. in Materials Science from the University of California at Berkeley in 1991 at which time he joined the MIT faculty. Dr. Ceder's research interests lie in computational modeling of material properties and the design of novel materials. Currently, much of the focus of his work is on materials for energy generation and storage, including battery materials, hydrogen storage, thermoelectrics, and electrodes and electrolytes for fuel cells. He has published over 210 scientific papers in the fields of alloy theory, oxide phase stability, high-temperature superconductors, and Li-battery materials, and holds 5 current or pending U.S. patents. He has received the Battery Research Award from the Electrochemical Society, the Career Award from the National Science Foundation, and the Robert Lansing Hardy Award from The Metals, Minerals and Materials Society for "exceptional promise for a successful career." He has also received three awards from the graduate students at MIT for best teaching. As a faculty member at MIT he has been involved with distance education offering a course on Atomistic Modeling life over the internet. He is currently a group leader for the

Research Program on High Performance Power Sources in the Center for Materials Science and Engineering. At MIT he has served on the Committee on Intellectual Property and on MIT's Presidential Council on Energy. He is the founder of Computational Modeling Consultants.

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

B.S. University of Michigan, 1964
M.S. Stanford University, 1966
Ph.D Stanford University, 1969

The goal of Professor Delgass' research in heterogeneous catalysis is to understand the surface chemical origins of catalytic activity and to use that fundamental knowledge in a process called Discovery Informatics for the design of catalysts. Steady state reaction and transient isotopic tracing provide quantitative chemical kinetic evaluation of catalytic performance, while spectroscopic measurements yield details of the chemistry of catalytic surfaces. X-Ray photoelectron spectroscopy gives a quantitative chemical analysis of catalyst surfaces prepared in situ. Solid state NMR and infrared spectroscopy reveal further details of the chemical state of the surface and the bonding of adsorbed species. Discovery Informatics is a framework that enables management of complexity, accumulation of knowledge, systematic testing of hypotheses by interaction with experiments, and the efficient search for new materials with desired performance characteristics. Six chemical engineering professors at Purdue have teamed together to apply this methodology to catalyst design. The approach uses high throughput experiments and quantum level theory to gain information on catalyst performance and chemistry and then uses a variety of systems tools to guide and execute building models that capture catalytic knowledge and discover new catalysts. Current areas of research interest include the water gas shift reaction, NOx traps, olefin polymerization, and biomass conversion.

Ernst Dow, Group Leader, Discovery Informatics, Eli Lilly and Company

After receiving his B.S. in Chemistry with a Computer Science option from the University of Pittsburgh in 1988, Dr. Dow joined Eli Lilly and Company focusing on computational chemistry. Following an AI Fellowship with Digital Equipment Corporation in neural networks he worked on QSAR and then took an educational leave, obtaining his Ph.D. from the University of Illinois at Urbana-Champaign in Biophysics and Computational Biology under Dr. Thomas Anastasio in 1999. He has been in Bioinformatics leading the effort to gain insight into biology from microarray and other high information content studies. His current focus is integrating information from many sources to allow a scientific question driven approach to access the proper data.

L. Louis Hegedus, Ret. Sr. VP R&D, Arkema

L. Louis Hegedus, Ph.D., was most recently senior vice president of research and development, for Arkema Inc. (formerly Atofina Chemicals, Inc.). He was responsible for all research and development (R&D) in North America and R&D coordination between the U.S. and France. Arkema research supports the company's businesses in Thiochemicals, Organic Peroxides, Fluorochemicals and Hydrogen Peroxide, Additives, Technical Polymers, and polymethyl methacrylate.

Prior to joining the Company in 1996, Dr. Hegedus was vice president of the corporate technical group at the Washington Research Center of W.R. Grace. His 16 years of experience with that company included different positions as director of inorganic research and vice president of research for the company's specialty chemicals businesses.

Prior to joining W.R. Grace, Dr. Hegedus was affiliated with the General Motors Research Laboratories, where he managed research on the development of the catalytic converter for automobile emissions control. His previous employment with Daimler Benz AG in Mannheim, Germany, as group leader of the materials testing department was followed by attendance at the University of California, Berkeley, from which he received his Ph.D. in chemical engineering. His earlier education was completed at the Technical University of Budapest, where he obtained his M.S. in chemical engineering.

Dr. Hegedus has produced 75 publications and patents, mainly in chemical reaction engineering and industrial catalysis. His honors include the Catalysis and Reaction Engineering Practice Award and the Management Division Award by the American Institute of Chemical Engineers (AIChE), an honorary Doctor of Engineering from the Technical University of Budapest, and the Professional Progress and R.H. Wilhelm Awards from the American Institute of Chemical Engineers. He is a fellow of the AIChE, a member of the National Academy of

Engineering(NAE), a past chairman of the NAE's Chemical Engineering Section, and a past chairman of the Council for Chemical Research. As a member of the Board on Chemical Sciences and Technology, he chaired the National Research Council's Report on Critical Chemical Technologies. Dr. Hegedus is a member of the Advisory Board of Chemical and Engineering News (ACS).

Lonnie Johnson, Founder and President, Excellatron

Lonnie Johnson is President and Founder of Johnson Research & Development Co., Inc., a technology development company, and its spin-off companies, Excellatron Solid State, LLC, and Johnson Electro Mechanical Systems, LLC.

Johnson holds a B.S. degree in Mechanical Engineering, an M.S. degree in Nuclear Engineering, and an honorary Ph.D. in Science from Tuskegee University. Upon graduation, he joined the Air Force and served as an Advanced Space Systems Requirements Officer at Strategic Air Command headquarters. He was twice awarded the Air Force Achievement Medal and the Air Force Commendation Medal. After leaving the military, he joined the Jet Propulsion Laboratory (JPL) in California. During his nine year career with JPL, he received multiple achievement awards from NASA for his work in spacecraft system design for the Galileo Mission to Jupiter and the Mars Observer projects, and was instrumental in the Cassini Mission to Saturn.

In 1989, he formed his own engineering firm and licensed his most famous invention, the SuperSoaker® water gun, to Larami Corporation. Two years later, the SuperSoaker, which has generated over $1 billion in retail sales, became the number one selling toy in America. Currently, Lonnie Johnson holds over 100 patents, with over 20 more pending, and is the author of several publications on spacecraft power systems. Johnson's companies, Excellatron Solid State and Johnson Electro Mechanical Systems (JEMS), are developing revolutionary energy technology.

A. Refik Kortan, Program Manager for Physical Behavior of Materials, Materials Sciences and Engineering Division, Office of Basic Energy Sciences, Department of Energy

M.S. in Physics, University of Maryland, 1976
Ph.D. in Physics, University of Maryland, 1979

Dr. Refik Kortan earned his Ph.D. degree in surface physics from University of Maryland in 1979. He was a post-doctoral fellow at the Physics Department in MIT before he joined then AT&T Bell Laboratories in 1984. Dr. Kortan utilized high-resolution x-ray scattering to study novel phase transitions in reduced dimensions, liquid crystals, and graphite intercalation compounds while he was at MIT. During his 20 years stay at Bell Labs, Dr. Kortan has received numerous AT&T Exceptional Contribution Awards. He has published over 200 papers, presented 182 invited and contributed talks, and held 13 patents. He has been recognized as one of the most cited physicists due to his pioneering research, receiving 4497 and 6947 citations during the span of 1981-1997 and 1991-2003, respectively. He was elected Fellow of the American Physical Society in 1996 for his experimental studies of phase transitions on surfaces, liquid crystals, and intercalated systems; and his work on new materials such as quasicrystals and fullerenes.

Paul McGinn, Professor of Chemical Engineering, University of Notre Dame

B.S. Metallurgical Engr. & Materials Science, University of Notre Dame (1980)
M.S. Metallurgical Engr. & Materials Science, University of Notre Dame (1983)
Ph.D. Metallurgical Engr. & Materials Science, University of Notre Dame (1984)

Professor McGinn's primary research interests are in the areas of the processing and properties of advanced materials. Current research programs are aimed at developing the processing tools and screening instrumentation for combinatorial materials development and discovery. The combinatorial approach to materials research employs parallel (or automated serial) processing to create large "libraries" of material compositions, followed by parallel (or automated serial) testing to characterize the compositions for a specific property of interest. Much of the potential of the combinatorial approach rests on the development of rapid means to screen libraries for a property of interest. Over the past several years his group has developed and put in place a wide range of automated processing and characterization tools for combinatorial research.

Dagmar Niebur, Program Director, National Science Foundation & Associate Professor of Electrical & Computer Engineering, Drexel University

Dr. Dagmar Niebur joined the National Science Foundation in March 2007 as a Program Director for the Power, Controls and Adaptive Networks (PCAN) Program of the Electrical, Communications and Cyber Systems (ECCS) Division in the Directorate for Engineering (ENG). Her responsibilities within the PCAN program

include Power and Energy Systems and Networks, Renewable and Alternate Energy Sources: Generation and Integration into the National Grid, and Interdependencies of Critical Infrastructures in Power.

Dr. Niebur is on an IPA assignment from Drexel University, where she is an Associate Professor and the Assistant Department Head of Planning and Development in the Department of Electrical and Computer Engineering. Before joining the faculty at Drexel, she held research positions at the Jet Propulsion Laboratory, Pasadena, CA; the Swiss Federal Institute of Technology, Lausanne, Switzerland; the University of Lausanne; and was a summer Visiting Professor at CEPEL, Rio de Janeiro, Brazil. Dagmar Niebur holds a Diploma in Mathematics and Physics from the University of Dortmund, Germany (1984), and her Diploma in Computer Science (1987) and Ph.D. in Electrical Engineering (1994) from the Swiss Federal Institute of Technology, Lausanne, (EPFL) Switzerland. Dr. Niebur is a member the Institute of Electrical and Electronics Engineers (IEEE), where she serves as member of the IEEE-PES Technical Council Advisory Board and chair of the IEEE-PES Subcommittees on Intelligent Systems and Research in Power Engineering Education. She is also a member of the American Society for Engineering Education, the Editorial Advisory Board of the International Journal of Engineering Intelligent Systems for Electrical Engineering and Communications, and the Board of Directors of the International Conference on Intelligent Systems for Power Systems.

Luis Ortiz, Visiting Scientist, MIT

Luis is a Visiting Scientist focused on advanced battery technologies. An accomplished technologist, Luis has six years of experience in the battery industry serving as both an independent consultant and Program Manager for technology transfer while with Valence Technology. Prior to entering the energy sector, Luis was a Six Sigma Blackbelt in Honeywell's Electronic Materials Division. Luis holds an SB and ScD from MIT's Department of Materials Science & Engineering. Always keen to social side of learning, Luis developed a number of organizations and programs while a student which served to bring technologists and members of the business community together.

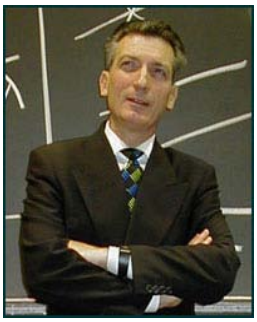
Kristin Persson, Chemist Research Scientist, Lawrence Berkeley National Laboratory

Dr Kristin Persson as been working on predicting new battery materials from ab initio computations, together with Professor Gerbrand Ceder, since 2005. She received her graduate degree in Theoretical Physics from the Royal Institute of Technology, Sweden in 2001 after which she came to MIT and held two postdoctoral associate appointments between 2001-2002 and 2004-2007. In 2008 she joined the Battery for Advanced Transportation Technologies effort at the Lawrence Berkeley Livermore Laboratory. She has co-authored 15 peer-reviewed publications.

Krishna Rajan, Stanley Chair in Interdisciplinary Engineering, Iowa State Univ.

B.A.Sc. – University of Toronto, 1974; Sc.D. – Massachusetts Institute of Technology , 1978

Krishna Rajan received his BASc in Metallurgy and Materials Science from the University of Toronto and the ScD in Materials Science.. He was also a postdoctoral fellow at MIT and Cambridge University. He served as a research scientist with the National Research Council of Canada in the 1980s after which he joined the faculty at Rensselaer Polytechnic Institute before coming to Iowa State University in 2005. He holds appointments in the Department of Materials Science & Engineering and the Bioinformatics and Computational Biology Graduate Program. He is director of the National Science Foundation's International Materials Institute for the Combinatorial Sciences and Materials Informatics Collaboratory. Prof. Rajan. has held numerous visiting appointments, including the Max Planck Institüt für Metallförschung, Stuttgart, the NRC Eastern Europe Fellowship at the Slovak Academy of Sciences, and the CNRS visiting professorship at the University of Rennes in France . He serves on many national and international committees including the US National Committee on Data Science and Technology (CODATA) of the US National Academies, co-chair of the National Science Foundation Panel on Cyber Infrastructure for Materials Science, the CODATA International Task Group of Materials Data Exchange and Operability and most recently appointed delegate to the US-China Bilateral Roundtable on Scientific Data Cooperation.



Donald R. Sadoway, John F. Elliott Professor of Materials Chemistry , MIT

B.A.Sc., Engineering Science, University of Toronto, 1972
M.A.Sc., Chemical Metallurgy, University of Toronto, 1973
Ph.D., Chemical Metallurgy, University of Toronto, 1977

Professor Sadoway's research seeks to establish the scientific underpinnings for technologies that make efficient use of energy and natural resources in an environmentally sound manner. This spans engineering applications and the supportive fundamental science. The overarching theme of his work is electrochemistry in nonaqueous media.

Specific topics in applied research are the following: environmentally sound electrochemical extraction and recycling of metals, lithium solid-polymer-electrolyte batteries for portable power, high-amperage energy storage devices for stationary applications, advanced materials for use as electrodes in fused-salt electrolysis cells and batteries, electrochemical synthesis of compound semiconductors, and electrochemical synthesis of diamond coatings.

The related fundamental research is the physical chemistry and electrochemistry of molten salts (including molten oxides), cryogenic electro-lytes, and solid polymer electrolytes. As the owner of 13 US patents and more than 100 technical publications, Professor Sadoway provides expertise in battery materials and key experience and track record with United States Military research contracting.

Susan B. Sinnott, Professor of Materials Science & Engineering, Univ. of Florida

Susan Sinnott is Professor of Materials Science and Engineering at the University of Florida. She received a B.S. in Chemistry from the University of Texas at Austin and a Ph.D. in Physical Chemistry from Iowa State University. After working as a National Research Council Postdoctoral Fellow in the Surface Chemistry Branch of the Naval Research Laboratory, she became an Assistant Professor in the Department of Chemical and Materials Engineering at the University of Kentucky before moving to the University of Florida in 2000. Her research uses theoretical and computational tools to study the design, processing, and properties of materials. Problems of current interest include examining polymerization, thin film growth, and the targeted chemical modification of surfaces through particle-surface deposition, calculating the electronic structure of metal oxide defect structures, and predicting the properties of heterogeneous interfaces. Prof. Sinnott has published over 100 articles in peer-reviewed technical journals and has given over 100 invited presentations at technical conferences and institutions. She has also assisted in the organization of several symposia and conferences in her field. Recent awards include Fellow of the American Vacuum Society in 2005, NSF Creativity Award in 2005, and the University of Florida Materials Science and Engineering Faculty Excellence Award in 2002, 2003, 2004, 2005, 2006, and 2008.

Patrick Trapa, Principal Scientist, Pfizer, Inc.

Patrick Trapa received his S.B. and Ph.D. from MIT with research specializing in nanoscaled self-assembling polymer electrolytes. He synthesized and characterized the systems, modeled ion transport through the electrolytes, and validated his findings with electrochemical experiments. Upon graduation, Patrick cofounded a battery company and later served as a director of electrochemistry at Electrovaya, a publicly traded battery company located in Canada. In 2006, he joined Pfizer as a principal scientist in Research Formulations (RF), and is an active member of project teams spanning from very early discovery through Phase II clinical trials. In 2007, he led a team tasked to improve, integrate, and assess various ADME models. The team also investigated the supporting in vitro assays which provide necessary input parameters to the programs.

G. Kumar Venayagamoorthy, Associate Professor of Electrical and Computer Engineering, Missouri University of Science and Technology

Dr. Ganesh Kumar Venayagamoorthy (S'91–M'97–SM'02) received the B.Eng. degree (Hons.) in electrical and electronics engineering from Abubakar Tafawa Balewa University, Bauchi, Nigeria, in 1994, and the M.Sc.Eng. and Ph.D. degrees in electrical engineering from the University of Natal, Durban, South Africa, in 1999 and 2002, respectively. He was a Senior Lecturer with the Durban Institute of Technology, Durban, prior to joining the Missouri University of Science and Technology (Missouri S&T), Rolla, USA in 2002. Currently, he is an Associate Professor of Electrical and Computer Engineering and Director of the Real-Time Power and Intelligent Systems Laboratory at Missouri S&T. He was a Visiting Researcher with ABB Corporate Research, Sweden, in 2007. His research interests are the development and applications of computational intelligence for real-world applications, including power systems stability and control, FACTS devices, power electronics, alternative sources of energy, sensor networks, collective robotic search, signal processing, and evolvable hardware. He has published 2 edited books, 5 book chapters, 60 refereed journals papers, and over 220 refereed international conference proceeding papers. He has attracted in excess US $6.5 Million in competitive research funding from external funding agencies.

Mark Verbrugge, Director, Materials and Processes Laboratory, General Motors Research and Development Center

Mark Verbrugge started his GM career in 1986 with the GM Research Labs after receiving his doctorate in Chemical Engineering from the College of Chemistry at the University of California (Berkeley). Mark has published and patented in topic areas associated with electroanalytical methods, polymer electrolytes, advanced batteries and supercapacitors, fuel cells, high-temperature air-to-fuel-ratio sensors, surface coatings, compound semiconductors, and various manufacturing processes related to automotive applications of structural materials.

Mark's research efforts resulted in his receiving the Norman Hackerman Young Author Award (1990) and the Energy Technology Award (1993) from the Electrochemical Society as well as GM internal awards including the John M. Campbell Award (1992), the Charles L. McCuen Award (2003), and the Boss Kettering Award (2007). In 2006, Mark received the Lifetime Achievement Award from the United States Council for Automotive Research.

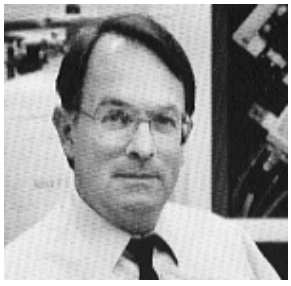
In 1996, Mark was awarded a Sloan Fellowship to the Massachusetts Institute of Technology, where he received an MBA. Mark returned from MIT in 1997 to join GM's Advanced Technology Vehicles (ATV) as Chief Engineer for Energy Management Systems. In 2002, Mark rejoined the GM Research Labs as Director of the Materials and Processes Lab, which maintains global research programs ranging from chemistry, physics, and materials science to the development of structural subsystems and energy storage devices. Mark is a Board Member of the United States Automotive Materials Partnership and the United States Advanced Battery Consortium, an adjunct professor for the Department of Physics, University of Windsor, Ontario, Canada, and he serves as the GM Technical Director for HRL Laboratories, LLC, jointly owned by GM and Boeing.

Paul Werbos, Program Director, National Science Foundation

Dr. Paul Werbos has core responsibility for the Adaptive and Intelligent Systems (AIS) Area within the Power, Control and Adaptive Networks (PCAN) Program of ECCS, and for the new area of Quantum, Molecular and High-Performance Modeling and Simulation for Devices and Systems (QMHP). He is the ECCS representative for Collaborative Research in Computational NeuroScience and for the Engineering working group in Adaptive Systems Technology. He initiated and has led the EFRI-2008 topic in Cognitive Optimization and Prediction. He has special interest in efforts to exploit higher levels of true computational intelligence in these areas, and in efforts which can seriously increase the probability that we achieve global sustainability. In 1994, he initiated an SBIR topic on fuel cell and electric cars which he coordinated for several years. He was part of the group which proposed and led NSF's earlier initiative in Learning and Intelligent Systems, and assisted the follow-on in Information Technology Research. He has at times handled the ECCS areas in electric power and wireless communications when there were gaps in those areas.

Dr. Werbos is an elected member of the Governing Board of the International Neural Network Society (INNS), for which he was one of the original three two-year Presidents. He has also served as an elected member of the Administrative Committee (AdCom) of the IEEE Computational Intelligence Society (CIS), which he continues to represent on the IEEE-USA Energy Policy Committee. For IEEE-USA and as chair of the CIS Task Force on Alternative Energy, he has given a number of major talks to Congressional staff on energy policy, and helped to organize the IEEE-USA workshop on plug-in hybrid cars. He also serves on the AdCom of the IEEE Industrial Electronics Society. He is a Fellow of the IEEE, and has won its Neural Network Pioneer Award, for the discovery of the "backpropagation algorithm" and other basic neural network learning designs such as Adaptive Dynamic Programming. He also serves on the Planning Committee of the ACUNU Millennium Project (see www.stateofthefuture.org), whose annual report on the future tends to lead global lists of respected reports on the long-term future. In 2002, he and John Mankins of NASA initiated and ran the NASA-NSF-EPRI initiative on enabling technologies for space solar power (search on "JIETSSP" at www.nsf.gov). In 2003, he participated on the interagency working group for the Climate Change Technology Program. He has a paper in press at Futures on a rational strategy for the economic development of space, and has been nominated for the Governing Board of the National Space Society.

He holds four degrees from Harvard and the London School of Economics in: (1) economics; (2) international political systems, emphasizing European economic institutions; (3) applied mathematics, with a major in quantum physics and a minor in decision and control; (4) applied mathematics for an interdisciplinary PhD. Prior to that, during high school, he obtained an FCC First Class Commercial Radiotelephone license, and took undergraduate and graduate mathematics courses at Princeton and the University of Pennsylvania.



M. Stanley Whittingham, Professor of Chemistry and Materials Science, SUNY at Binghamton

M. Stanley Whittingham read Chemistry at the University of Oxford, where he took his BA (1964), MA (1967), and DPhil (1968). After completing his graduate studies, Dr. Whittingham was a postdoctoral fellow at Stanford University until 1972. He then worked for Exxon Research & Engineering Company from 1972 until 1984. He then spent four years working for Schlumberger prior to becoming a professor at Binghamton University. For five years, he served as the University's vice provost for research and outreach. He also served as Vice-Chair of the Research Foundation of the State University of New York for six years.

Dr. Whittingham is a key figure in the history of the development of rechargeable batteries discovering the concept of intercalation electrodes. He is the holder of 16 US patents and has over 220 journal publications in his name. Exxon commercialized the first rechargeable lithium-ion battery, which was based on a titanium disulfide cathode and a lithium-aluminum anode. He developed the hydrothermal synthesis technique for making cathode materials, which is now being used commercially for the manufacture of lithium iron phosphate by Phostech/Sud-Chimie in Montreal, Canada.

He received the Young Author Award from the Electrochemical Society in 1971, the Battery Research Award in 2004, and was elected a Fellow in 2006 for his contributions to lithium battery science and technology.