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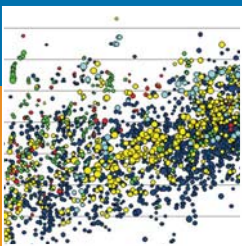
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Opportunities and challenges for first-principles materials design and applications to Li battery materials

Gerbrand Ceder

This article is based on the MRS Medal presentation given by Gerbrand Ceder (Massachusetts Institute of Technology) on December 1, 2009, at the Materials Research Society Fall Meeting in Boston. Ceder was awarded the Medal “for pioneering the high-impact field of first-principles thermodynamics of batteries materials and for the development of high-power density Li battery compounds.”

The idea of first-principles methods is to determine the properties of materials by solving the basic equations of quantum mechanics and statistical mechanics. With such an approach, one can, in principle, predict the behavior of novel materials without the need to synthesize them and create a virtual design laboratory. By showing several examples of new electrode materials that have been computationally designed, synthesized, and tested, the impact of first-principles methods in the field of Li battery electrode materials will be demonstrated. A significant advantage of computational property prediction is its scalability, which is currently being implemented into the Materials Genome Project at the Massachusetts Institute of Technology. Using a high-throughput computational environment, coupled to a database of all known inorganic materials, basic information on all known inorganic materials and a large number of novel “designed” materials is being computed. Scalability of high-throughput computing can easily be extended to reach across the complete universe of inorganic compounds, although challenges need to be overcome to further enable the impact of first-principles methods.

Introduction

The design of novel materials is critical for many potential new and clean energy technologies. Whether it is hydrogen or solar, thermoelectrics, or energy storage, the effectiveness of these technologies is severely limited by the available materials. Thermoelectricity is a good example: the material essentially *is* the device, converting heat to electricity through temperature-driven changes in its electron chemical potential. Similarly, materials for permanent magnets play an increasingly important role in the drivetrain of electric vehicles. But even older materials (e.g., cement, steel, and aluminum) are major contributors to CO₂ emissions in their production.

The importance of materials for developing a clean energy economy is both good and bad news for a materials scientist.

Some time ago, Eagar¹ at MIT showed that the average time required for new materials to be commercialized is 18 years, which is very bad news for material-based technological improvements. This is worse than the development of medical drugs. The lithium-ion battery is not very different. In 1976, Whittingham, working for Exxon Mobil (Exxon at the time), published the first paper demonstrating a functioning rechargeable lithium battery.² Sony started commercializing Li-ion batteries 15 years later, in 1991, and this technology is now about to be used in automobiles, some 20 years after Sony’s market introduction. There are other technologies with a similar delay; for example, high-temperature superconductors, which were discovered in 1986, are only now seeing nascent commercialization. The question is: how much time do we have to develop materials for clean energy

technologies? Depending on which model of climate change due to CO₂ emissions we consider, we have between minus 10 years and plus 40 years to solve the problem. Hence, if it takes 20 or 25 years just to commercialize and scale-up new materials technology, we need to act immediately and with approaches that are far more efficient and faster compared to the ones that we have used to develop materials in the past. It is unlikely that we will be successful with materials development as usual.

The Schrödinger equation in materials science

Can we design materials through computing? Computing would be an ideal research tool, since it can be easily scaled, is relatively inexpensive and versatile, and, in principle, the equations that describe atoms and electrons in matter are known. Solving the Schrödinger equation to predict the properties of materials is the idea behind *ab initio* computing. In most approaches to solve the Schrödinger equation, the many-body electron-electron interaction is replaced with an effective potential operating on one electron at a time, reducing the problem to a one-body problem. Starting with the key work of people such as Hartree, Fock, Slater, Hohenberg, and Kohn, considerable progress has been made on these one-electron methods, and today, a popular approach is to use density functional theory (DFT), either in the local density approximation (LDA) or the generalized gradient approximation (GGA). A review of the basic ingredients of these theories and how they can predict materials properties is given elsewhere.³

Using a computer, quantum mechanics, and codes downloaded from the Internet, we can achieve a great deal. We can compute basic quantities such as wave functions, charge density, band structure, and energy. Because these quantities are derived from approximate solutions to the Schrödinger equation, we should always be concerned about accuracy. But by far the biggest concern, from my 20 years of experience in attempting computational materials science, is *relevance*. No company or government agency has ever offered me a contract to compute band structures or charge densities. Instead, I tend to get approached with materials engineering problems: solve a corrosion problem; increase the strength of a metal; or develop a higher efficiency solar cell, a higher energy density battery material, or a better car.

The question is, can quantum mechanics help—can we make a better car using quantum mechanics? Unfortunately, there is no quantum operator for a better car (**Figure 1**). To turn the basic information obtained from solving the Schrödinger equation into relevant engineering information, one needs to, first, understand quantitatively the microscopic phenomena that control a macroscopic engineering property so that the problem (e.g., a “better battery”) can be translated into computable quantities, and, second, understand the technology to ensure that the right problem is solved. While this transfer of information from quantum mechanics

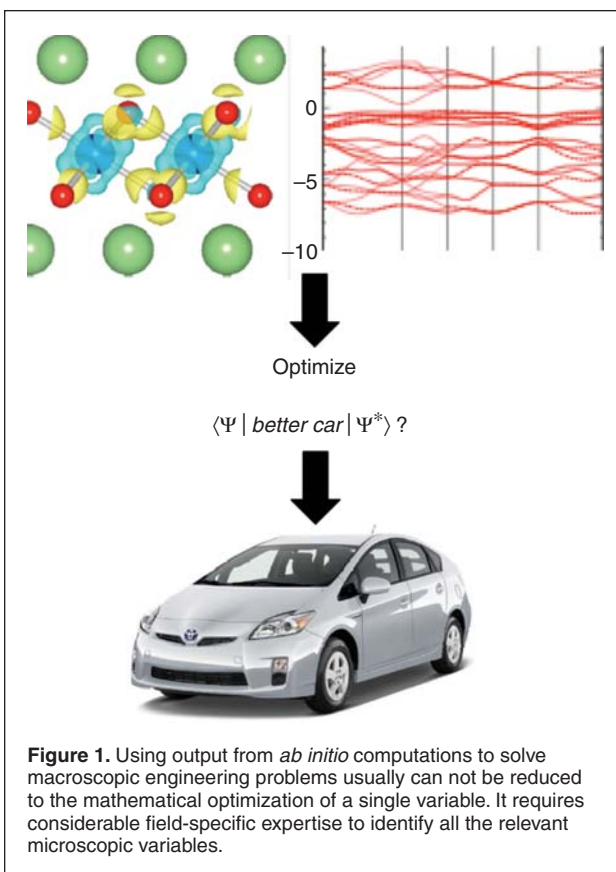


Figure 1. Using output from *ab initio* computations to solve macroscopic engineering problems usually can not be reduced to the mathematical optimization of a single variable. It requires considerable field-specific expertise to identify all the relevant microscopic variables.

to relevant engineering information is often called the length-scale problem, it is really a knowledge problem. Sadly, this field-specific knowledge is often neglected in computational materials science.

Lithium-ion batteries

This article illustrates these principles of computational materials design for the design and optimization of lithium-ion battery cathodes (**Figure 2**), in which lithium ions shuttle back and forth between two electrodes. The difference between the high chemical potential of lithium at the anode and the low chemical potential of lithium in the cathode drives Li⁺ ions through the electrolyte (an organic solvent) and the separator and electrons through the external circuit. This is the discharge of the battery. Upon charge, this process is reversed by applying a potential difference across the electrodes. I will focus on the cathode, where Li ions are stored by “intercalation” in the crystal structure of a material. There are a number of materials problems to be solved in designing an intercalation cathode. Its chemical potential for lithium sets the *voltage*: the lower the chemical potential of lithium, the higher the battery voltage. The *capacity* is determined by how much lithium can reversibly enter the crystal structures and re-emerge. The amount of lithium stored per unit weight and per unit volume is a key issue, as is keeping the cathode material stable for the hundreds or thousands of *cycles*

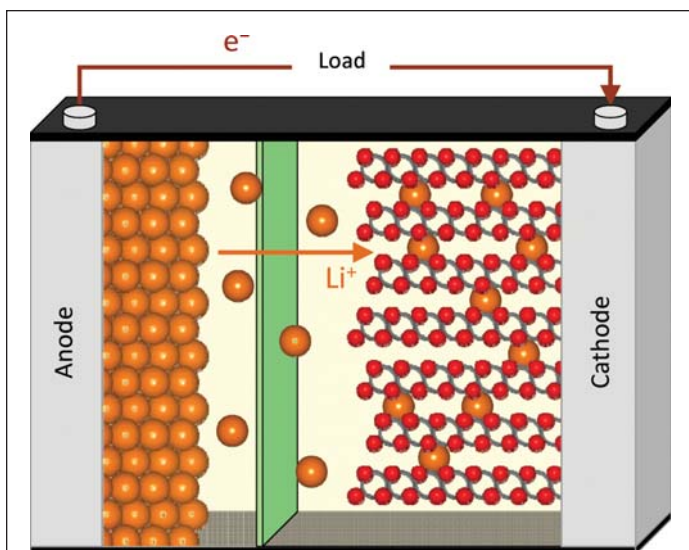


Figure 2. Schematic of a rechargeable lithium battery. Upon discharge, Li^+ ions flow from the anode to the cathode, where they are stored inside the crystal structure of a cathode material.

required from the battery. The faster we can move the lithium and the electrons in the cathode, the higher the *power density* out of the battery. Finally, safety and cost are a factor; in the long term, cathode material must cost less than \$15–\$20 per kg in order to meet automotive targets.

Voltage calculations

Voltage is one of the easiest properties to calculate from first principles for a potential electrode material, since it relates to the reaction energy of the cathode material with lithium through the Nernst equation.⁴ The reddish-brown circles in **Figure 3** show the error in

the voltage calculated using standard GGA for a few typical compounds. The errors are very large; for LiFePO_4 , the real voltage is about 3.4 volts, and the calculation underestimates this by 0.6–0.7 volts. For lithium nickel phosphate, the error is 1 volt.

Part of the problem is that standard DFT is very inaccurate in calculating the absolute energy of a solid or molecule. However, most physical properties are determined by energy differences, and as long as the two systems being compared are similar, the errors in their energies cancel. This is not the case for the reaction describing Li transfer from the anode to the cathode. In this process, an electron transfers from a metallic state, such as in lithium metal, to a transition metal state in an oxide. This electron transfer between very different orbitals lacks error cancellation and leads to an enormous error in voltage prediction by DFT.⁵ This problem also occurs in other redox reactions such as oxidation.^{6,7} Some of this error can be corrected with a method called GGA+U (green triangles in **Figure 3**),⁸ in which a Hubbard-type Hamiltonian is applied to the transition metal orbitals, which cancels much of the self-interaction. Unfortunately, the on-site repulsive energy in this method, U , is an adjustable parameter, which has to be fitted or determined from separate calculations. Even more advanced methods, such as Heyd-Scuseria-Ernzerhof hybrid functional (HSE) functionals (blue squares on **Figure 3**), which are essentially a mixing of Hartree-Fock methods with DFT, can calculate accurate voltages without adjustable parameters, but at a cost of 50 to 100 times more computing time than a regular DFT calculation.

Computation of rates

Materials kinetics, such as electron and ion mobility, or phase transformation rates in the electrodes, is important, as kinetics may control the power rate of the battery and its charge time. The lithium diffusion constant can be calculated in great detail by using kinetic Monte Carlo techniques,⁹ though very often simply obtaining the activation barrier for Li motion through the crystal can yield powerful insight.

One example where computation showed what might be possible—against conventional wisdom—is lithium iron phosphate.¹⁰ This is a very attractive cathode material for transportation, since it is potentially cheap because it contains iron and phosphate groups, and it is very thermally stable. The small green and grey spheres in **Figure 4a** show the diffusion paths for lithium. The low energy sites for lithium are in green, whereas the activated state is shown as a grey sphere. Morgan et al.¹¹ calculated that the barrier to Li^+ motion along that path is extremely low, giving Li diffusivities of the order of 10^{-7} to 10^{-8} cm^2/s , potentially enabling very fast charging and discharging of the cathode material. This prediction of extremely fast charging and discharging was recently confirmed by experiments¹² that were guided by computed phase diagrams.¹³ These phase diagrams showed that when LiFePO_4 is synthesized with the appropriate Fe and P deficiency, an amorphous fast Li^+ conducting surface and interface coating¹⁴ can be created on the material, enhancing Li transfer in

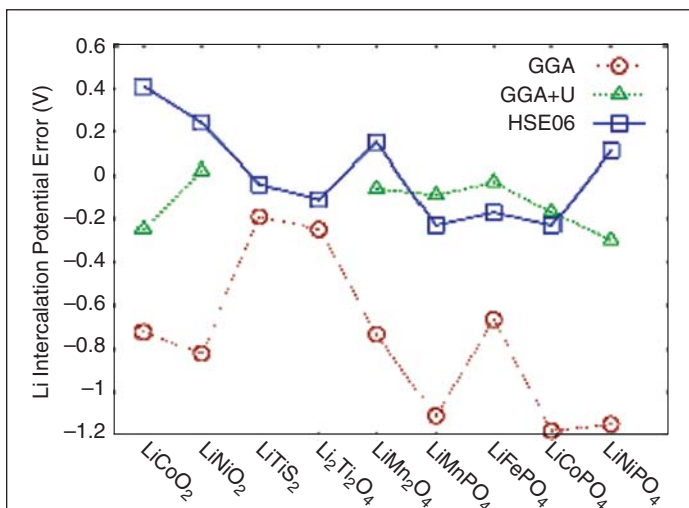
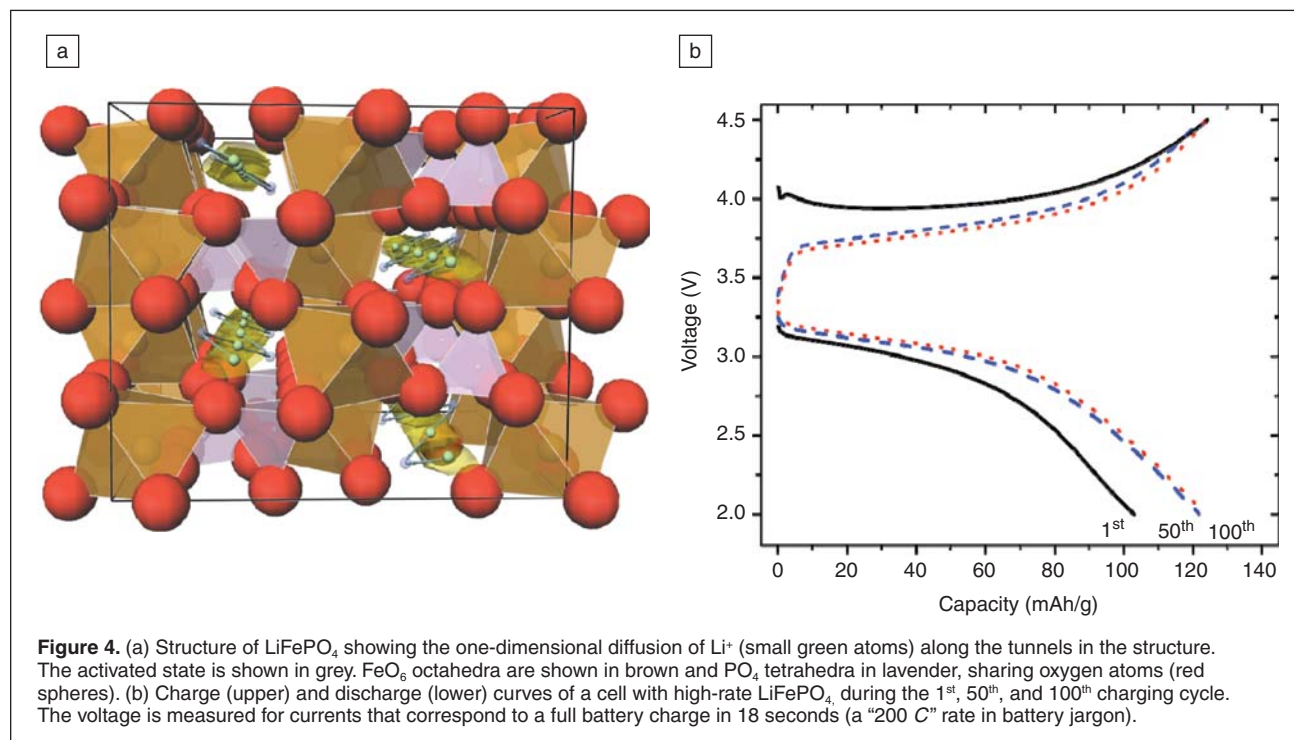


Figure 3. Error on calculated Li-insertion voltages for a series of cathode materials in standard GGA, GGA+U, and HSE approximation. GGA, generalized gradient approximation; GGA+U includes Hubbard “U”; HSE, Heyd-Scuseria-Ernzerhof screened exchange functional.



and out of the material. Figure 4b shows the voltage during charge and discharge of small batteries made with this material, under currents that correspond to a full battery charge in 18 seconds (a “200 C” rate in battery jargon, where 1 C current corresponds to complete charge or discharge in one hour). Even under these very fast conditions, the cathode material can store up to two-thirds of its maximal theoretical charge. Rates up to 1000 C, which are equivalent to 3 seconds to charge or discharge, have now been obtained in small lab-scale half cells. Though significant challenges exist to engineer all components of commercial cells and charging systems to sustain such a high rate, this material has clearly fulfilled the promise that computation gave it.

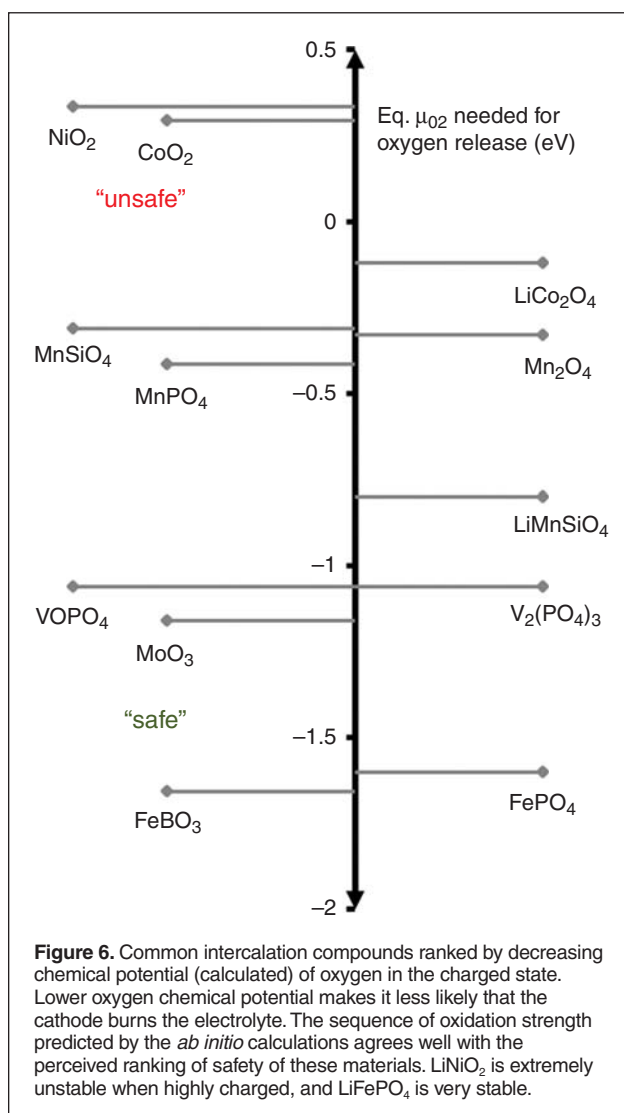
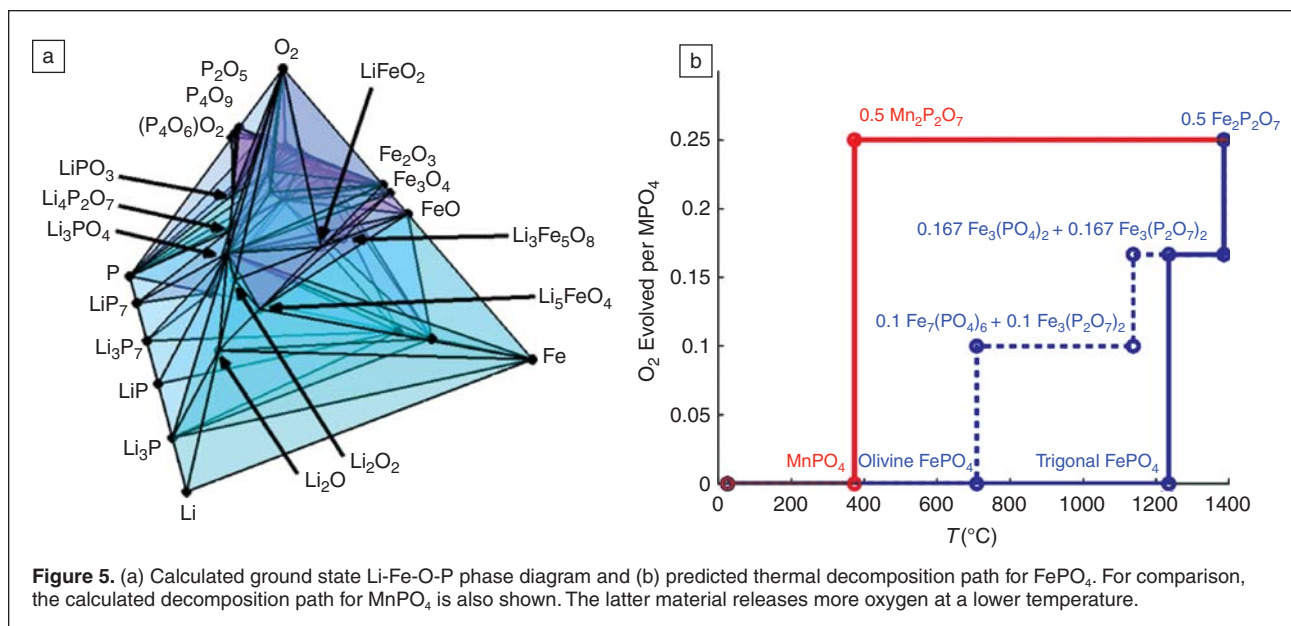
Safety

Safety of batteries is an engineering property that is much harder to translate into quantities that can be derived from *ab initio* computations, as it depends on a number of components and their interplay in a battery. Very often, the safety problem arises from the interaction of the highly charged cathode with the electrolyte. In their charged state, most cathode compounds are highly oxidizing. For example, in a lithium cobalt cell, which is used in cell phones and laptops, a large amount of Co^{4+} is present. This is not a particularly stable oxidation state, and Co^{4+} tries to reduce by liberating oxygen. While this reduction reaction is kinetically hindered at room temperature, any incident that heats the cell (such as an internal short) can activate the release of oxygen, which then reacts with the organic electrolyte. Essentially, the cathode burns the electrolyte. This insight makes it possible to relate

the computed oxidation strength of a material and correlate it with safety.⁷ The oxidation strength can be found practically by calculating the multi-component phase diagram of the system and projecting it under an increasingly reducing environment, simulating the heating of the charged cathodes. The oxygen chemical potential at which the material undergoes a reaction that releases oxygen and the amount of oxygen released are the critical measures of safety.

As an example, **Figure 5a** and **5b** respectively show the *ab initio* computed quaternary Li-Fe-O-P phase diagram and the reduction path of FePO_4 (the charged state of LiFePO_4) with temperature. For comparison, the calculated reduction path of MnPO_4 is also shown.¹⁵ The computed data show that, in agreement with observations, $(\text{Li})\text{FePO}_4$ is quite safe, as it only decomposes with oxygen release at a fairly high temperature. In contrast, LiMnPO_4 , often heralded as a potential improvement in energy density over LiFePO_4 due to its higher theoretical energy content, may not be nearly as safe, which is in agreement with two recently published experimental measurements.^{16,17}

Figure 6 shows the computed oxygen chemical potential at which many known cathode materials reduce in their charged state. Almost perfect correlation exists with the known safety of materials: Lithium nickel oxide is one of the worst materials in terms of safety. Lithium cobalt oxide is also poor, but it is used in cell phones and laptops. Lithium iron phosphate is probably one of the safest materials we can create; it is on the extreme end of the chemical potential scale. The computed results in **Figure 6** clearly show the benefits of polyanion groups such as PO_4 and BO_3 in achieving safe cathode materials.

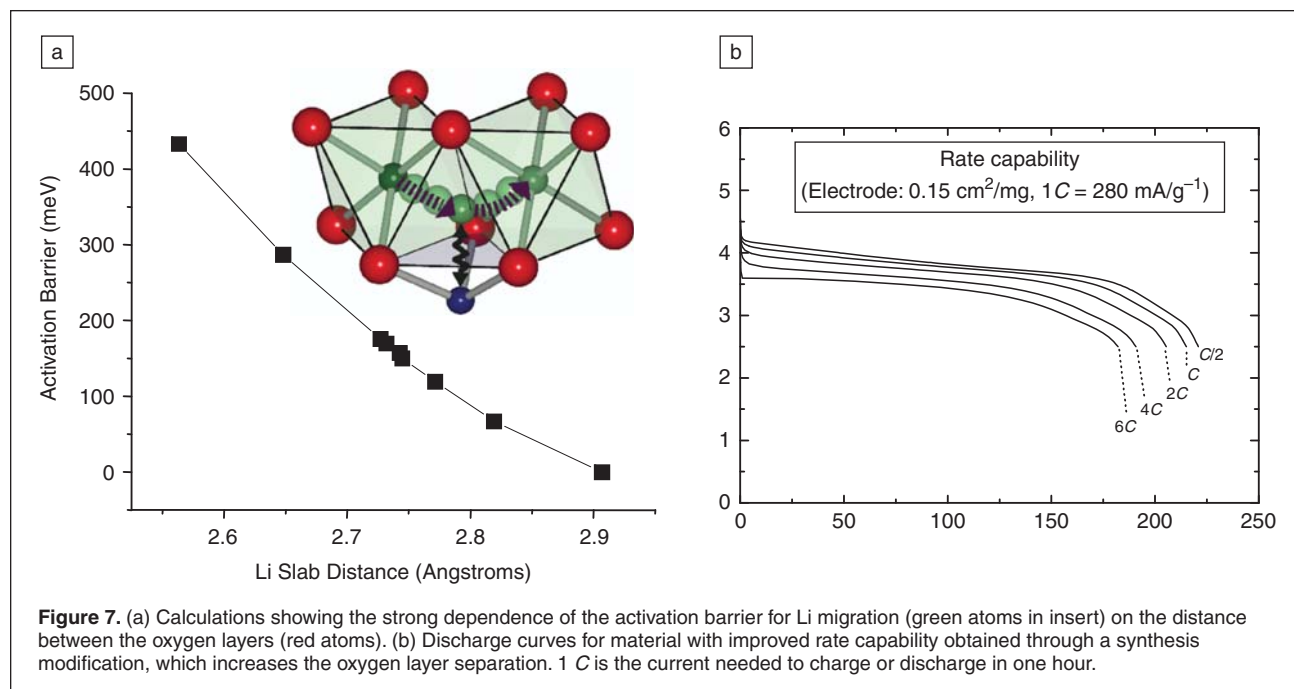


Computer-aided design

Before I go into large-scale computational searching for new materials, I will show an example of how materials can be improved on the basis of *ab initio* modeling.¹⁸ $\text{Li}(\text{Ni}_{0.5}\text{Mn}_{0.5})\text{O}_2$ is, in theory, an almost perfect cathode material. Mn is present as Mn^{4+} , which is one of the most stable transition-metal cations in close-packed oxygen frameworks¹⁹ due to its filling of only the lower manifold of *d*-states, which for ions in octahedral environments are split off from the higher energy *d*-states. The nickel ion, present as Ni^{2+} , can be fully oxidized to Ni^{4+} , providing two electrons per cation.²⁰ While this material works as a Li-intercalation compound at low rate, it loses most of its capacity at the charge/discharge rates that are needed for commercial operation.

Since rate limitations often relate to the mobility of ions, computation can be used as a virtual laboratory to find what limits lithium mobility in these materials. In layered oxides, such as $\text{Li}(\text{Ni}_{0.5}\text{Mn}_{0.5})\text{O}_2$, Li^+ migrates from one octahedral site to another through a tetrahedral site, which can be taken as the activated transition state for this migration process. In computations, one can virtually test what controls the migration energy through that tetrahedral site. **Figure 7a** shows the strong dependence of the calculated activation energy on the distance between the oxygen layers (red atoms) that define the tetrahedral site. As this spacing is squeezed down, the activated states are also squeezed down, and even with a small change of layer spacing, the barrier can change by 50 mV up or down. At room temperature, a change of 56 meV in the activation barrier of an exponentially activated process such as diffusion changes the rate by a factor of 10. The computations therefore clearly show that minor variations in structure and lattice spacings can produce very large effects on the diffusivity.

In $\text{Li}(\text{Ni}_{0.5}\text{Mn}_{0.5})\text{O}_2$, the oxygen layer spacing is controlled by the nature of the cations between the layers. When the material is synthesized through classic solid-state synthesis at high temperature, a certain amount of Ni^{2+} is present in the lithium layer,



and the presence of these higher valent ions contracts the oxygen layers. Calculations showed that a hypothetical material with no nickel in the lithium layer would have a larger distance between the oxygen layers, and, as a result, a lower activation barrier for lithium motion. Fortunately, such a perfectly ordered material can be made by first synthesizing $\text{Na}(\text{Ni}_{0.5}\text{Mn}_{0.5})\text{O}_2$, which is perfectly ordered due to the much larger size of Na^+ , and then ion-exchanging Na^+ for Li^+ . Tests on this perfectly ordered material showed that it has very high discharge rate capability (Figure 7b) even up to a 6 C (10 minutes to full discharge) rate.

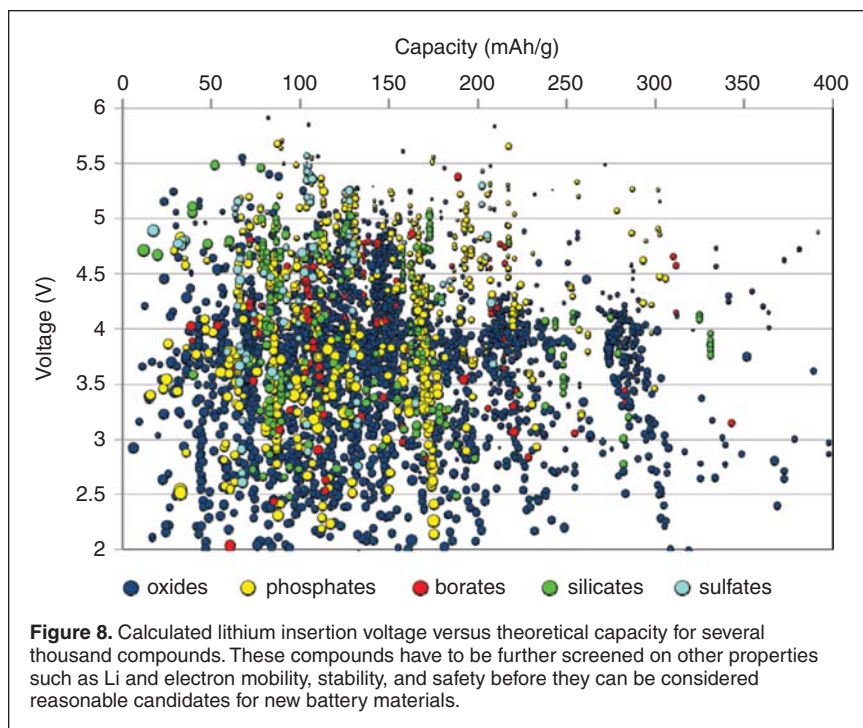
The future

In the last part of my presentation, I will discuss what I believe will happen in the future, but as Yogi Berra said, it is tough to make predictions, especially about the future. One of the major advantages of a computational research approach is the fact that it is scalable. If one can compute something once, in principle, it can be computed thousands of times, assuming enough computing power. Can we calculate the properties of all known—and many unknown—inorganic compounds? Today, there are about 60,000 inorganic compounds for which the crystal structure is known and tabulated in databases such as the Inorganic Crystal Structure Database. Of these compounds, only about half are stoichiometric, so it is possible that the number of distinct compounds is less. Even including less complete evidence of a distinct compound, such as the diffraction patterns reported in the Powder Diffraction Database without crystal structure assignment, the number of “discovered” compounds is no larger than 200,000. This scale is very computable. With

about 400 computing cores in our own laboratory, we have already performed *ab initio* calculations on about 60,000 real and hypothetical compounds. This comprehensive searching through all of nature is the idea of the Materials Genome Project at MIT.²¹ Still in its infancy, the Materials Genome Project aims to perform large-scale property computation on all known inorganic compounds and make that basic information available for materials research and materials discovery.

The Materials Genome Project has four major components: we created a *chemical space* from data on all known compounds and created substitution strategies to generate new compounds based on data-mined chemical rules. The *computing environment* is a complex series of job control scripts, which manage thousands of computations at a given time, detect errors, convergence problems, and automatically resubmit jobs when they fail. A sophisticated *database* stores all the data, and *analysis tools* allow us to operate on it and search through it. This environment makes it possible to engage in “meta questions.” For example, with a few commands, we can call up all the known molybdenum compounds that contain oxygen, look for possible sites in the structure that can hold lithium, and run voltage predictions on them. I believe that such a Google-like approach to chemistry and materials science is the way of the future.

As of February 2010, we have investigated about 25,000 real and hypothetical compounds for their relevant properties as lithium battery cathodes and performed some level of computation on about 60,000 compounds. **Figure 8** shows the calculated voltage versus the theoretical capacity of thousands of oxides, phosphates, borates, silicates, and sulfates. These data



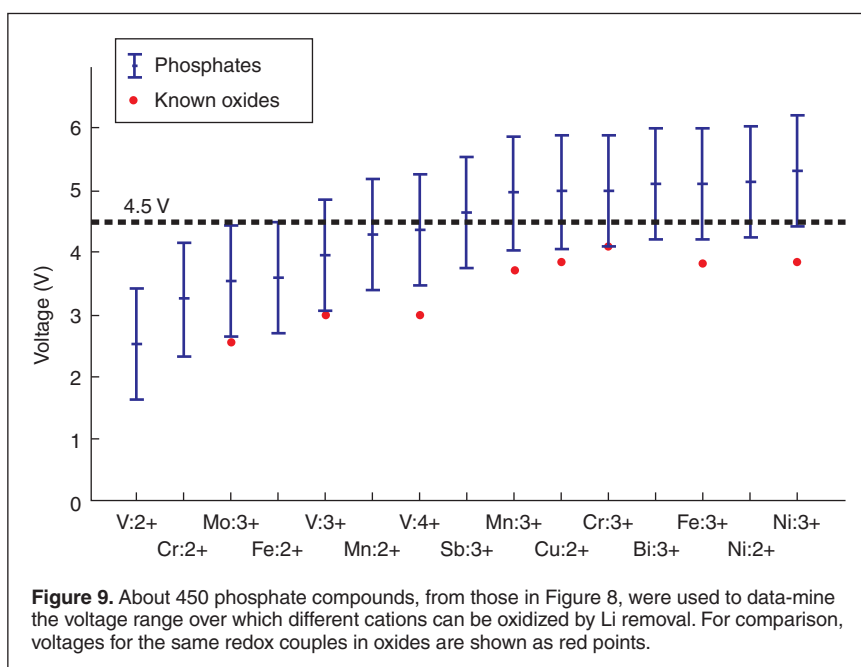
can be used for a first screening of materials to see if they can achieve a reasonable energy density. But other properties also need to be good for a material to function as a lithium storage cathode. As previously mentioned, high voltage often destroys the electrolyte and may result in high oxidation strength in the charged state, thereby reducing safety. High capacity, achieved by removing a large amount of lithium from the structure, often leads to structural instabilities and capacity-fade of the battery. In addition, lithium and electron mobility have to be good to enable reasonable charge and discharge rates. Hence, a tiered screening approach is followed, whereby materials that pass the basic energy density criteria are further investigated with more complicated property calculations.

A lot can be learned by systematically analyzing the large amount of computed data. We have mined the data in Figure 8 to find the voltage range over which each transition-metal redox couple can exchange an electron when paired with a phosphate (PO_4)³⁻ anion group. **Figure 9** shows a sample result of that analysis indicating that phosphates clearly operate at higher voltages than oxides for the same redox couple, as has been speculated before using theoretical bonding arguments.²² The information in Figure 9 can be used as a design tool to create materials operating in a particular voltage range.

For each compound calculated, we have approximate solid-state phase diagrams

available, created from the energies in the database. This information allows us to track, for every compound, its stability and oxidation strength as a function of temperature. As explained previously, this can be used as an indicator of safety of the cathode material. A thermodynamic analysis by Huggins and Godshall²³ indicated that high voltage of a cathode (important to obtain high energy density) also causes high oxidation strength of the charged cathode (bad for safety). While these authors analyzed this correlation on nine systems, we can now use computed information on several thousand compounds to investigate to what extent high voltage reduces safety. **Figure 10** shows the calculated voltage versus the oxygen chemical potential under which the charged state decomposes for oxides and phosphates. Overall, the data confirms the trend that Huggins and Godshall predicted: On average, high voltage leads to a more oxidizing state of the charged cathode. But more important may be the fact that there is considerable deviation from the trend, imply-

ing an opportunity for materials design. Even for the same operating voltage, the oxidation strength of different cathode materials varies by several electron volts, implying that safe high-voltage materials are possible. It also can be observed that for the same voltage, the phosphates are actually slightly less oxidizing, which is why they have better thermal stability. But, on average, borates and silicates are clearly even better. Such information can again be used in designing better materials.



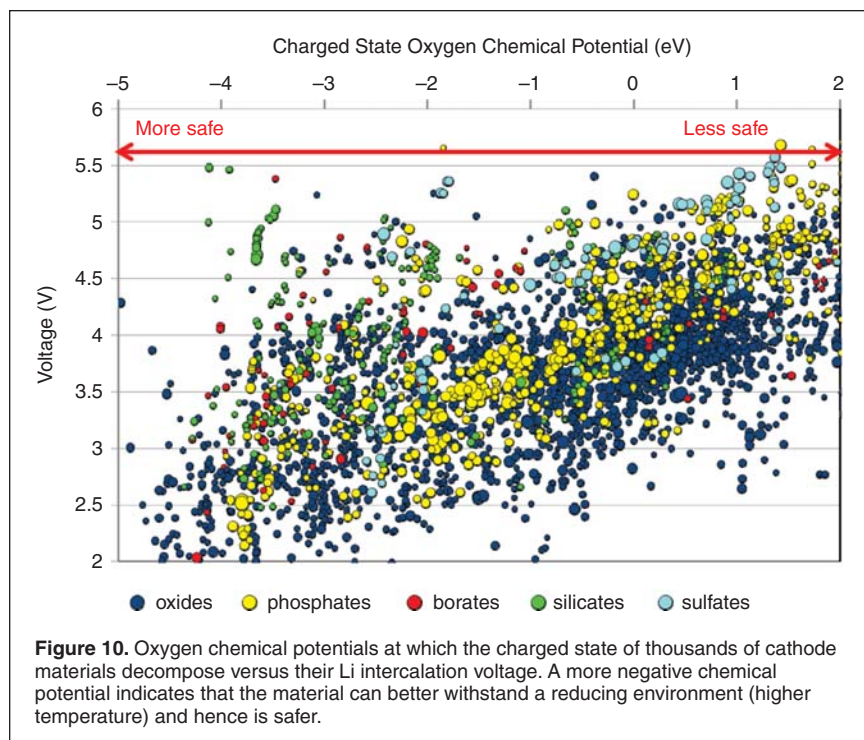


Figure 10. Oxygen chemical potentials at which the charged state of thousands of cathode materials decompose versus their Li intercalation voltage. A more negative chemical potential indicates that the material can better withstand a reducing environment (higher temperature) and hence is safer.

In the lab

While our computationally driven search is ongoing, several materials have already made it through all of the computational screening criteria, and attempts to synthesize and test them in batteries are under way. Finding a synthesis route for a new material has become the slow step in the materials design process, and it relies on significant know-how, intuition, and persistence. Clearly, the next challenge for computational materials science will lie in gaining a better understanding and predictive capability in how materials form and react.

Conclusions

I have not said much about the accuracy of *ab initio* predictions. The chemical breadth of high-throughput computations exposes a lot of problems of modern *ab initio* methods, and my research group and my students spend a considerable amount of time worrying how errors propagate through the data. The shortcomings of the classic approximations to density functional theory (DFT), such as the generalized gradient approximation (GGA) and the local density approximation (LDA), are particularly troubling when combining data from compounds with very different electronic structure (e.g., when creating a phase diagram between a metal and its oxides or when dealing with the different degrees of electron localization created by different anion chemistries). In studying such complex systems and equilibria in them, it is very easy to be misled by systematic errors in GGA/LDA-DFT. However, for many important technological applications, the most limiting factor today is still that it is very hard to find properties at the

microscopic scale that directly relate to these engineering properties. Batteries, the example that I have highlighted, are a good field for *ab initio* predictions, because the voltage, lithium mobility, and electron mobility can be well defined on the microscopic scale. There are also other areas where the Materials Genome ideas also can be applied to solve pressing materials development needs. For example, algorithms for many of the relevant properties of thermoelectric materials (thermal and electrical conductivity, Seebeck coefficient) are well established and could be integrated with our structure and stability predictions to look for efficient materials for heat to electricity conversion. But it is important to realize that for many materials problems, considerably more work needs to be done to understand and define the correlation between microscopic and macroscopic engineering properties.

My vision for the future is that, once we develop the insight and algorithms to tackle more complex properties, rapid progress can be made by making new capabilities available on tens of thousands of materials. Automation

of computation and appropriate data handling and dissemination will play key roles in this materials revolution. We should learn from the impact and growth of the Internet. The Internet did not become important because everybody had it. The Internet became important when Web crawlers and page-rank algorithms were invented to automate the process of information gathering. Materials science will evolve to a similar situation. In my opinion, it will take no more than 10–15 years before the properties of all known compounds can be computed, so as scientists, we can focus on doing interesting things with them.

Acknowledgments

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Data courtesy of Dr. Masashi Watanabe,
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