

WORLD CHANGING IDEAS

MATERIALS SCIENCE

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With supercomputers and the equations of quantum mechanics, scientists are designing new materials atom by atom, before ever running an experiment

*By Gerbrand Ceder
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In 1878 Thomas Edison set out to reinvent electric lighting. To develop small bulbs suitable for indoor use, he had to find a long-lasting, low-heat, low-power lighting element. Guided largely by intuition, he set about testing thousands of carbonaceous materials—boxwood, coconut shell, hairs cut from his laboratory assistant's beard. After 14 months, he patented a bulb using a filament made of carbonized cotton thread. The press heralded it as the "Great Inventor's Triumph in Electric Illumination." Yet there were better filament materials. At the turn of the century, another American inventor perfected the tungsten filament, which we still use in incandescent lightbulbs today. Edison's cotton thread became history.



Materials science, the process of engineering matter into new and useful forms, has come a long way since the days of Edison. Quantum mechanics has given scientists a deep understanding of the behavior of matter and, consequently, a greater ability to guide investigation with theory rather than guesswork. Materials development remains a painstakingly long and costly process, however. Companies invest billions designing novel materials, but successes are few and far between. Researchers think of new ideas based on intuition and experience; synthesizing and testing those ideas involve a tremendous amount of trial and error. It can take months to evaluate a single new material, and most often the outcome is negative. As our Massachusetts Institute of Technology colleague Thomas Eagar has found, it takes an average of 15 to 20 years for even a successful material to move from lab testing to commercial application. When Sony announced the commercialization of the lithium-ion battery in 1991, for example, it seemed like a sudden, huge advance—but in fact, it took hundreds or thousands of battery researchers nearly two decades of stumbling, halting progress to get to that point.

Yet materials science is on the verge of a revolution. We can now use a century of progress in physics and computing to move beyond the Edisonian process. The exponential growth of computer-processing power, combined with work done in the 1960s and 1970s by Walter Kohn and the late John Pople, who developed simplified but accurate solutions to the equations of quantum mechanics, has made it possible to design new materials from scratch using supercomputers and first-principle physics. The technique is called high-throughput computational materials design, and the idea is simple: use supercomputers to virtually study hundreds or thousands of chemical compounds at a time, quickly and efficiently looking for the best building blocks for a new material, be it a battery electrode, a metal alloy or a new type of semiconductor.

Most materials are made of many chemical compounds—battery electrodes, which are composites of several compounds, are good examples—but some are much simpler. Graphene, which has been widely hyped as the future of electronics, consists of a one-atom-thick sheet of carbon. Regardless of a material's complexity, one thing is always true: its properties—density, hardness, shininess, electronic conductivity—are determined by the quantum characteristics of the atoms of which it is made. The first step in high-throughput materials design, then, is to virtually “grow” new materials by crunching thousands of quantum-mechanical calculations. A supercomputer arranges virtual atoms into hundreds or thousands of virtual crystal structures. Next, we calculate the properties of those virtual compounds. What do the crystal structures look like? How stiff are they? How do they absorb light? What happens when you deform them? Are they insulators or metals? We command the computer to screen for compounds with specific desirable properties, and before long, promising compounds rise to the top. At the

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end of the process, data generated during that investigation go back into a database that researchers can mine in the future.

Since 2011 we have been leading a collaboration of researchers that aims to accelerate the computer-driven materials revolution. We call it the Materials Project. The goal is to build free, open-access databases containing the fundamental thermodynamic and electronic properties of all known inorganic compounds. To date, we have calculated the basic properties (the arrangement of the crystal structure, whether it is a conductor or an insulator, how it conducts light, and so on) of nearly all of the approximately 35,000 inorganic materials known to exist in nature. We have also calculated the properties of another few thousand that exist only in theory. So far some 5,000 scientists have registered for access to the database containing this information, and they have been using it to design new materials for solar cells, batteries, and other technologies.

We are not the only ones pursuing this approach. A consortium of researchers led by Stefano Cortarolo of Duke University has calculated tens of thousands of alloy systems; their research could yield lighter, stronger car frames, structural beams for skyscrapers, airplane skins, and so on. The Quantum Materials Informatics Project, which consists of researchers at Argonne National Laboratory, Stanford University and the Technical University of Denmark, has been using high-throughput computing to study catalytic processes on metal surfaces, which is particularly useful in energy research.

In the very near future, materials scientists will use high-throughput computing to design just about everything. We believe that this will lead to technologies that will reshape our world—breakthroughs that will transform computing, eliminate pollution, generate abundant clean energy and improve our lives in ways that are hard to imagine today.

THE MATERIALS GENOME

THE MODERN WORLD is built on the success of materials science. The advent of transparent, conductive glass led to the touch screens on our smartphones. The reason those phones can

IN BRIEF

Engineered materials such as chip-grade silicon and fiber-optic glass underpin the modern world. Yet designing new materials has historically involved a frustrating and inefficient amount of guesswork.

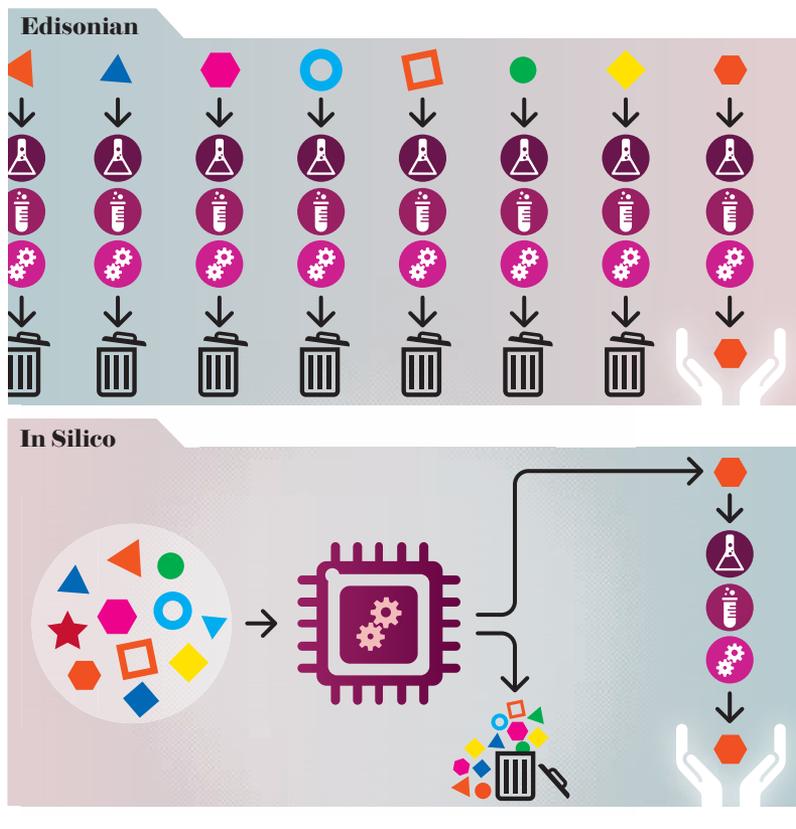
Streamlined versions of the equations of quantum mechanics—along with supercomputers that, using those equations, virtually test thousands of materials at a time—are eliminating much of that guesswork.

Researchers are now using this method, called high-throughput computational materials design, to develop new batteries, solar cells, fuel cells, computer chips, and other technologies.

BASICS

What a Difference a Supercomputer Makes

Roughly speaking, the Edisonian method of materials design consists of testing everything you can think of and throwing away what does not work. With high-throughput computational materials design, researchers can quickly screen candidates in silico—virtually, on giant supercomputing banks—saving time and money and preventing frustration. Once the computer has tested hundreds or thousands of materials and produced a list of the top 10 or so candidates, researchers begin synthesizing physical samples and testing them with conventional laboratory methods.



beam information around the world at the speed of light is that materials scientists found a way to make glass free of impurity ions, enabling fiber-optic communications. And the reason those phones last a full day on a charge is because in the 1970s and 1980s, materials scientists developed novel lithium-storing oxide materials—the basis for the lithium-ion battery.

It was our work on batteries that brought us to high-throughput materials design in the first place. We had spent our careers doing computational materials design, but until a 2005 conversation with executives from Proctor & Gamble (P&G), we did not think about what serious time on the world's most powerful supercomputers could make possible. These P&G executives wanted to find a better cathode material for the alkaline batteries made by their Duracell division. They asked us a surprising question: Would it be possible to computationally screen *all known compounds* to look for something better? On reflection, we realized that the only real obstacles were computing time

and money. They were happy to supply both. They committed \$1 million to the project and gave our small team free rein over their supercomputing center.

We called our effort the Alkaline Project. We screened 130,000 real and hypothetical compounds and gave P&G a list of 200 that met the criteria the company asked for, all of which had the potential to be significantly better than its current chemistry. By then, we were convinced that high-throughput materials design was the future of our field. We added staff, raised resources and, in 2011, launched a collaboration between M.I.T. and Lawrence Berkeley National Laboratory, which we initially called the Materials Genome Project. Teams at the University of California, Berkeley, Duke University, the University of Wisconsin-Madison, the University of Kentucky, the Catholic University of Leuven in Belgium and other institutions have since joined in the effort, all of them contributing the data they generate to our free, open-access central data repository at Lawrence Berkeley.

Before long, we dropped “Genome” from the project name to distinguish it from an initiative that the White House Office of Science and Technology Policy was launching. And to be fair, the properties of chemical compounds are not really “genes”—they are not hereditary bits of information that provide a unique sequence of data. Still, a direct relation exists between the function or property of a material and its fundamental descriptors. Just as blue eyes can be correlated to a certain gene, the electronic conductivity of a material, for example, can be traced back to the

properties and arrangements of the elements it is composed of.

These kinds of correlations are the basis of materials science. Here is a simple example: we know we can “tune” the color of minerals by introducing targeted defects into their crystal structure. Consider the ruby. Its red hue comes from an accidental 1 percent substitution of a chromium ion (Cr^{3+}) for aluminum in the common mineral corundum (Al_2O_3). When the Cr^{3+} is forced into this environment, its electronic states become altered, which changes the way the material absorbs and emits light. Once we know the origin—the fundamental descriptor—of a property (in this case, the redness of a ruby), we can target it with synthetic methods. By tweaking those chemical defects, we can design new synthetic rubies with perfectly tuned colors.

The equations of quantum mechanics can tell us how to do that tweaking—what elements to use and how to arrange them. Yet the equations are so complex that they can really only be solved by computer. Say you want to screen a group of

a few hundred compounds to see which ones have the properties you need. It takes an incredible amount of computing power to crunch those equations. Until recently, it simply was not possible, which is why so much of materials science has historically proceeded by trial and error. Now that we have the computing power, however, we can finally take advantage of the full predictive potential of quantum mechanics.

Suppose we are researching thermoelectric materials, which generate an electric current if they experience a large temperature gradient. (The reverse is also true: a thermoelectric material can sustain a temperature difference if you run a current through it; think instant cooling.) Society wastes an enormous amount of heat through combustion, industrial processing and refrigeration. If we had efficient, cheap and stable thermoelectric materials, we could capture this heat and reuse it as electricity. Thermoelectric devices could transform industrial waste heat into electricity to power factories. Heat from car exhaust pipes could power the electronics in the cockpit. Thermoelectrics could also provide on-demand solid-state cooling: little devices that we could weave into our clothing that, with a flip of a switch, would cool us down, no fans or compressors required.

One of the best thermoelectrics we know of today is lead telluride, which is far too toxic and expensive to use commercially. Suppose you are a researcher looking for a better thermoelectric material. Without high-throughput computing, this is how it would go: You would start by looking for known compounds that, like lead telluride, have a high Seebeck coefficient (a measure of the amount of electricity you get out for the temperature difference that goes in) but that, unlike lead telluride, are not made of rare, toxic or expensive elements. You would pore over tables and compare numbers. If you were lucky, you would come up with some candidate chemistries that, in theory, would seem like they could work. Then you would make those compounds in a lab. Physically synthesizing materials is an expensive, time-consuming and difficult job. Generally, you have no idea going in whether the new material will even be stable. If it is, you can measure its properties only after you have synthesized the compound and then repeated the process until you have a fairly pure sample. This can take months for each compound.

So far researchers have had no luck finding alternative thermoelectric materials. But they have not yet tried high-throughput computational materials design. That will soon change. Starting this year, we will begin working with researchers at the California Institute of Technology and five other institutions to perform high-throughput searches for new thermoelectric materials. We intend to keep at it until we find the chemical compounds that could make those energy-saving, miracle-cooling technologies a reality.

THE GOLDEN AGE OF MATERIALS DESIGN

OUR ABILITY TO ACCESS, search, screen and compare materials data in an automated way is in its infancy. As this field grows, what could it yield? We will venture a few guesses.

Many promising clean-energy technologies are just waiting for advanced materials to become viable. Photocatalytic compounds such as titanium dioxide can be used to turn sunlight and water into oxygen and hydrogen, which can then be processed into liquid fuels. Other photocatalysts can do the same thing with carbon

dioxide. The dream is an “artificial leaf” that can turn sunlight and air into methanol-like liquid fuels we could burn in cars and airplanes [see “Reinventing the Leaf,” by Antonio Regalado; *SCIENTIFIC AMERICAN*, October 2010]. Researchers at the Joint Center for Artificial Photosynthesis, a U.S. Department of Energy research center, are using high-throughput methods to look for materials that could make this technology feasible.

What about finding new metal alloys for use in those cars and airplanes? Reducing a vehicle’s weight by 10 percent can improve its fuel economy by 6 to 8 percent. U.S. industry already pours billions of dollars every year into research and development for metals and alloy manufacturing. Computer-guided materials design could multiply that investment. Significant advances in high-strength, lightweight and recyclable alloys would have a tremendous impact on the world economy through increased energy efficiency in transportation and construction.

Computing is another field in need of transformative materials. Recently we have seen many serious predictions that we are nearing the end of Moore’s law, which says that computing power doubles roughly every two years. We have long known that silicon is not the best semiconductor. It just happens to be abundant and well understood. What could work better? The key is to find materials that can quickly switch from conducting to insulating states. A team at U.C.L.A. has made extremely fast transistors from graphene. Meanwhile a group at Stanford has reported that it can flip the electrical on/off switch in magnetite in one trillionth of a second—thousands of times faster than transistors now in use. High-throughput materials design will enable us to sort through these possibilities.

This list is much longer. Researchers are using computational materials design to develop new superconductors, catalysts and scintillator materials. Those three things would transform information technology, carbon capture and sequestration, and the detection of nuclear materials.

Computer-driven materials design could also produce breakthroughs that are hard to imagine. Perhaps we could invent a new liquid fuel based on silicon instead of carbon, which would deliver more energy than gasoline while producing environmentally benign reaction products such as sand and water. People have talked about the idea for decades, but no one has figured out a workable formula. High-throughput materials design could at least tell us if such a thing is possible or if we should focus our efforts elsewhere.

All of this is why we believe we are entering a golden age of materials design. Massive computing power has given human beings greater power to turn raw matter into useful technologies than they have ever had. It is a good thing, too. To help us deal with the challenges of a warming, increasingly crowded planet, this golden age cannot start soon enough. ■

MORE TO EXPLORE

Opportunities and Challenges for First-Principles Materials Design and Applications to Li Battery Materials. Gerbrand Ceder in *MRS Bulletin*, Vol. 35, No. 1, pages 693-701; September 2010.

The Materials Project: A Materials Genome Approach to Accelerating Materials Innovation. Anubhav Jain et al. in *APL Materials*, Vol. 1, No. 1; July 2013.

SCIENTIFIC AMERICAN ONLINE

To see a slide show of materials and the atomic properties that make them behave the way they do, go to ScientificAmerican.com/dec2013/materials