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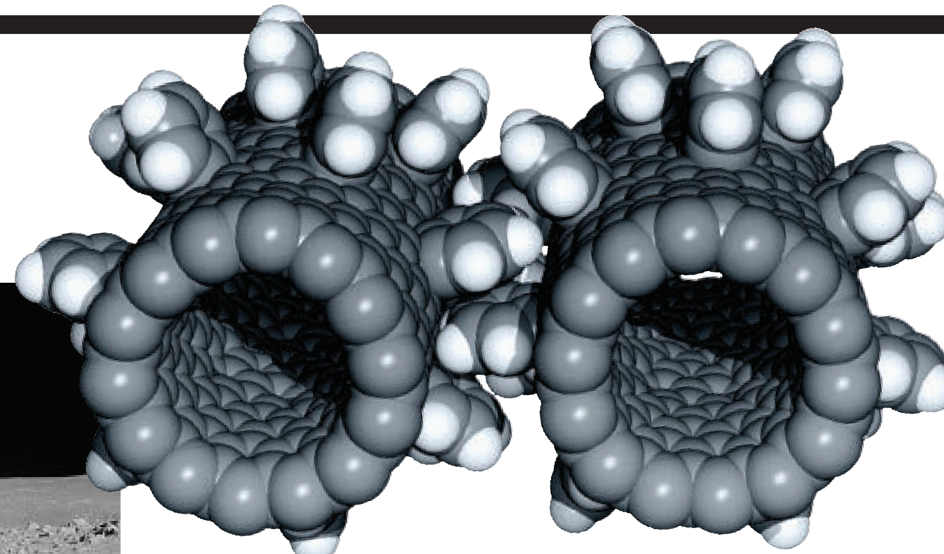

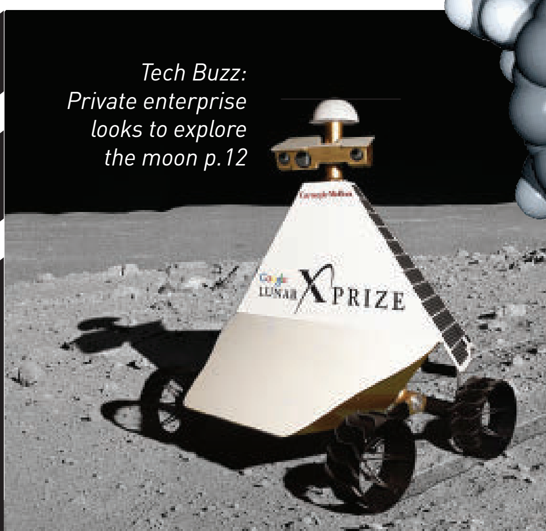

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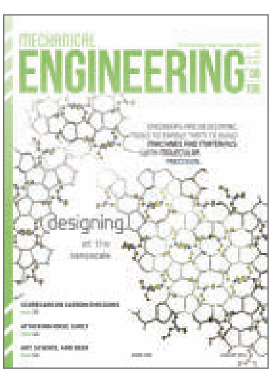
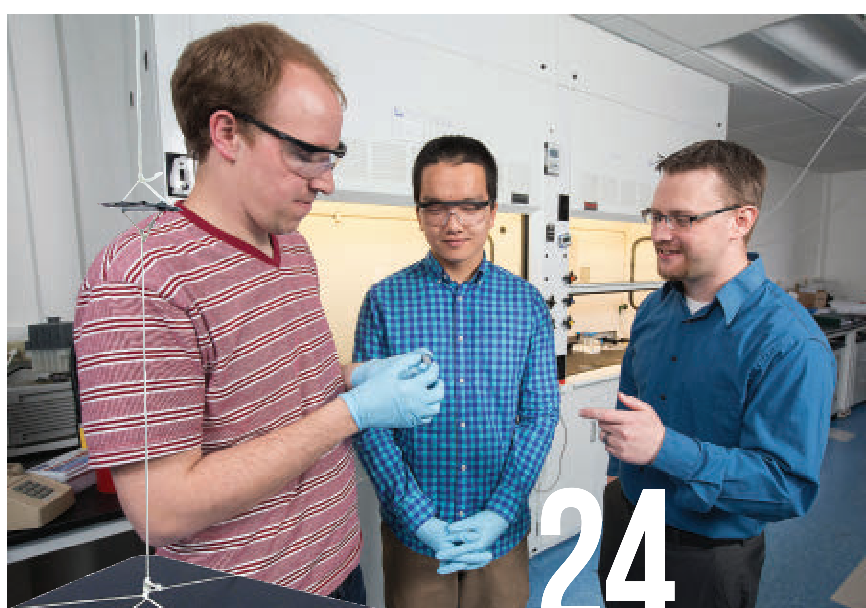




ASME
SETTING THE STANDARD

John G. Falcioni
Editor-in-Chief

ADVANCED MATERIALS FOR GAMES OF ALL SIZES

Not too distant from the collection of smiley, sad, angry, and other round-faced emoticons on your smartphone or IM dashboard is an image of the iconic black-and-white-patched soccer ball. But even if you're one to use these hackneyed little critters in e-mails and texts, chances are you probably never even realized the soccer ball was there, let alone think to use it.

I admit to inserting the ball into text messages a few times in the past weeks as my team, the Albiceleste, kept me on the edge of my seat during the quadrennial FIFA World Cup that ended last month. As it turns out, the real black-and-white soccer ball, with its 32 panels comprising 12 black pentagons and 20 white hexagons stitched together, isn't as ubiquitous as one might think, at least not in international competition.

The German company Adidas, maker of the official ball of Fédération Internationale de Football Association (FIFA) sanctioned tournaments, has designed five different soccer balls for international play—none of them had black pentagons and white hexagons. Remarkably, the traditional soccer ball has not been used in the World Cup since the tournament was played in West Germany in 1974. The search for the optimal soccer ball for use in the highly fêted World Cup has included the Tango, the Azteca, the Questra, and the much maligned Jabulani, which was used four years ago in South Africa. This year, for the World Cup in Brazil, Adidas created Brazuca.

Each new ball is engineered with material advances to make the sphere more aerodynamic, more waterproof, and easier to control. If the goal (no pun intended) of ball technology is to make play more competitive, then the Brazuca can lay claim to being a huge success. Pundits (yours truly included) say this year's World Cup was one of the best in recent history.

The Brazuca, along with many other soccer balls, it turns out, is made in Sialkot, a town in the northeast region of Pakistan recognized as the soccer ball capital of the world. Before China got involved a few years ago, seven out of 10 soccer balls in the world were made in Sialkot and factories there produced more than 60 million soccer balls a year. Now it's down to about 40 million. The Brazuca is produced at an Adidas factory where 40 percent of the workforce is comprised of women—no small feat in Pakistan. The ball has six patches that are glued together, not stitched. This makes these soccer balls, according to Adidas, the most aerodynamic ever made.

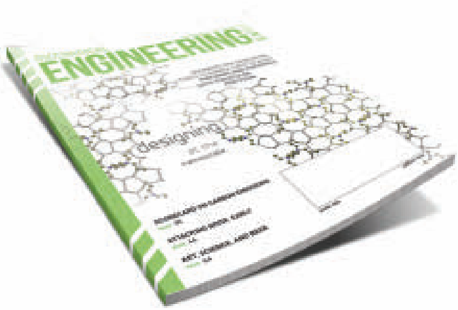
Testing included smashing it against a wall at 45 mph, dredging it in water to ensure it wouldn't absorb moisture, and baking it at 130 °F for seven days so that it stood up to the heat of the Amazon, where some of the games were played this year. Wind tunnel tests showed that unlike the Jabulani, which was made in China and tended to change directions in flight when it was kicked, the Brazuca remained stable.

Our cover story this month focuses on advances in material design for different types of applications—nano, meso, micro, and macro scale manufacturing processes. The work is being conducted by the Georgia Institute of Technology's Multiscale Systems Engineering Research Group.

I'm wondering whether the researchers from Georgia Tech will manufacture a high-end soccer ball for those exciting nano foosball games I like to watch. ☺ **ME**

FEEDBACK

What has been the most critical technological improvement in sports? Email me.
falcionij@asme.org



CAD AT THE NANO SCALE

RESEARCH AT GEORGIA TECH SEEKS TO GIVE ENGINEERS THE ABILITY TO CUSTOMIZE MATERIALS AS THEY DESIGN.

BY YAN WANG

THE TIME HAS COME FOR ENGINEERS TO BE ABLE TO **CUSTOMIZE THEIR MATERIAL EXACTLY TO THE PIECE THEY'RE DESIGNING.**

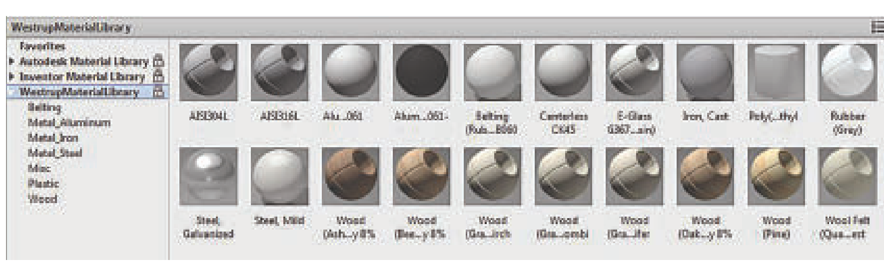
As the advent of flexible electronics attests, the materials with which things are made are at the root of today's product innovations.

The Georgia Institute of Technology's Multiscale Systems Engineering Research Group, where I'm a faculty member, is working to integrate the modeling and simulation features of today's CAD with materials design capability. These integrated features would be available at the nano, meso, micro, and macro scales, which we call multiscale CAD.

Integration would allow engineers to create customized materials (that is, materials that contain pores or voids, or super alloys that have coexisting phases) to meet their needs while performing structural and shape design at the macro scale.

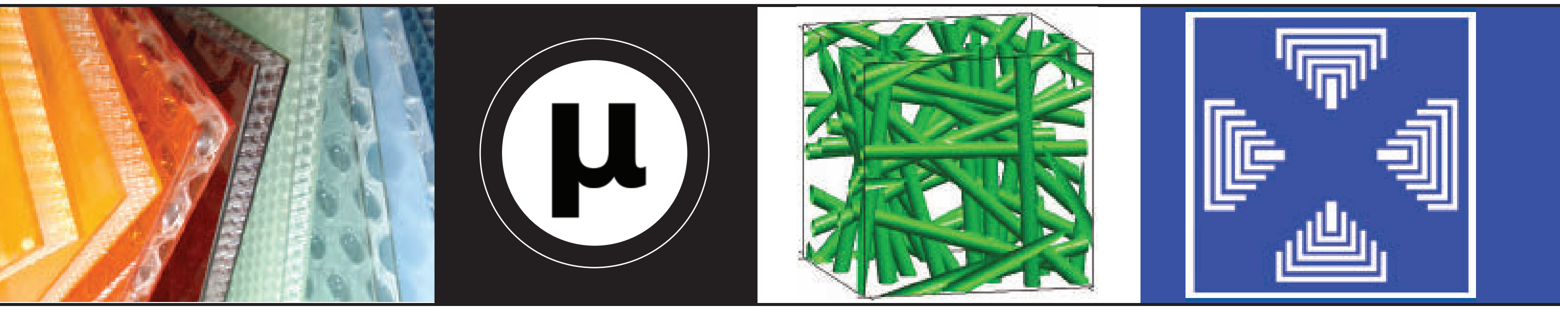
Similar to the conventional CAD as the first tool for virtual prototyping, the primary function of multiscale CAD is to allow the efficient construction and interactive modification of geometric models for microstructures. Existing boundary-representation-based parametric modeling approaches have become inefficient in model construction at

CUSTOMIZING MATERIALS: CAD systems of the future may be able to model synthetic materials on the order of ultra-porous zeolite. At right, part of the current materials browser in Autodesk Inventor.



nano and meso scales where geometry and topology are highly complex. New modeling and representation techniques are thus needed and this is the goal of our research.

In future CAD systems, engineers will be able to zoom in to specify material morphology and distributions. They'll be able to combine material design at the nano or micro scales, with geometrical and topological design at the macro scale to optimize the product's performance.



MODELING SUBJECTS: Engineers would be able to design and model materials including, fom left, polymers, fibrous porous media, silicon, graphene, or textiles.
At far right, a schematic of ionized physical vapor deposition, a nanoscale manufacturing process.

In this way, design engineers will be able to customize materials to their design in much the same way they select and change part geometries today. They'll be able to simulate the product with the selected geometries and materials in place. These would be available in an all-in-one package so engineers could create specific materials while they are designing a new product.

What we're envisioning is to allow engineers to define their own materials rather than use those already discovered.

NEW MATERIALS' FUTURE

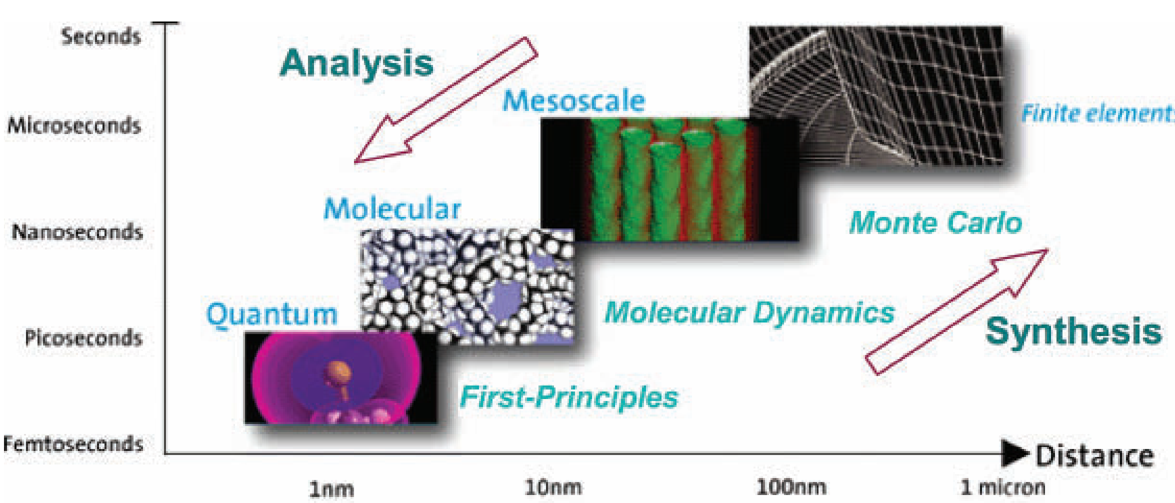
As it stands now, there's a divide between materials creation and product design. Bringing them together within the same system will allow for all kinds of new material properties and structures that currently haven't been used in the engineered world.

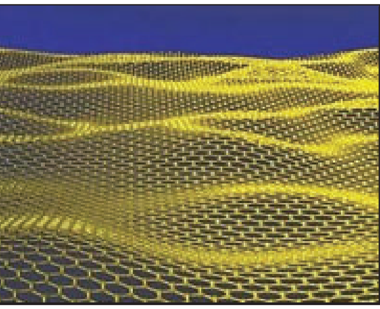
Integrating those two functions would allow engineers to customize and design material properties on any portion of their CAD design by simply zooming into the specific region, specifying material compositions, designing atomic or crystalline configurations, and simulating material performance within the product to ensure it will work as needed. If it doesn't, engineers can redesign the material, the part, or both, and test again.

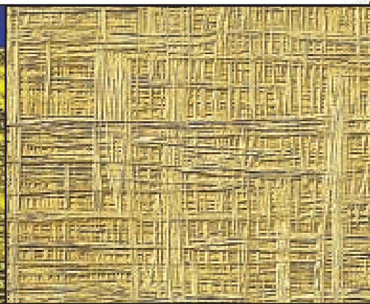
This is of interest because design decisions made at the microscopic level determine a material's properties, which, in turn, determine product behavior.

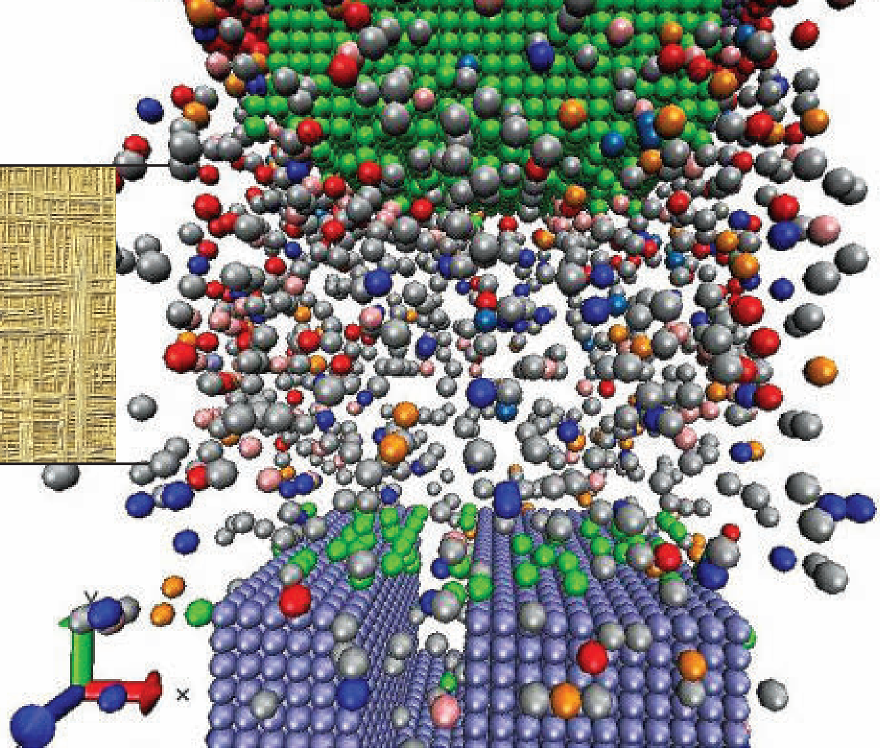
In today's CAD-enabled design processes, design engineers select available materials from databases. They select the materials they deem best suited to their products' specifications and their designs.

The conventional material selection approach that design engineers usually take is based on the isolated databases that were built without the input of problem-specific needs. Such a one-directional approach to discover, devise, and deploy new materials has a long development cycle and is not cost-effective. Even the materials science and engineer-









ing community has realized that this "lack of design" approach limits the rapid advancement of engineering materials.

To discover new materials, scientists run many experiments. In a process that is analogous to baking a cake, various ingredients are mixed and processing conditions are tried based on scientists' own experiences. If a cake is too hard or if it falls, a baker will tinker with the recipe, and materials scientists have had a similar practice.

It's only after materials scientists discover a new material through these experiment-driven approaches that product engineers consider how it can be best used within an engineered product. They also enter the new material into the materials database used by CAD designers today.

So from an engineering design perspective, discovery is not design. Design starts with asking the question: "What are the problems I have and what are the materials I need to solve it?"

The existing product development process doesn't integrate material design for the product into CAD. Say a mechanical engineer wants to design a vehicle from design specifications that call for the car to be light but strong. Currently, the engineer can only play around with different geometric shapes and topologies within the CAD design.

Materials are given. They can only be selected from the existing materials database.

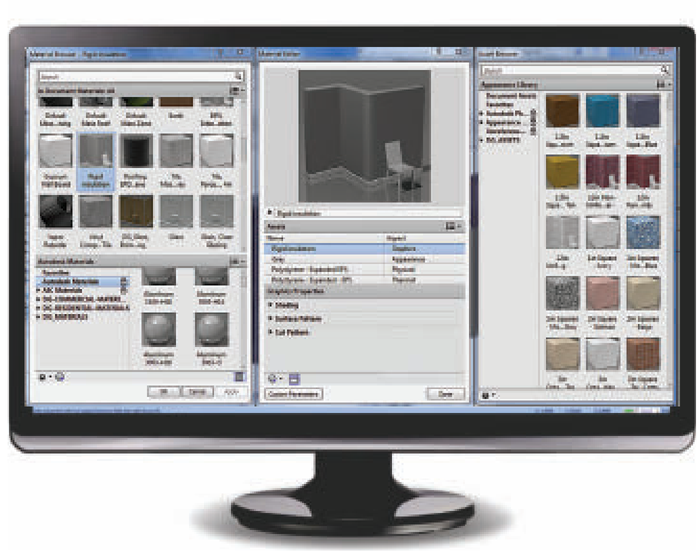
Therefore, the available "degrees of freedom" that design engineers control to optimize the performance of products are restricted to the geometry and topology offered within CAD systems. The addition of material properties in the design space would offer design engineers more degrees of freedom. Customizable materials would provide extra flexibility to realize increasingly intricate product functionality.

In other words, materials selection should be replaced by materials design to better meet customers' requirements in realizing modern products.

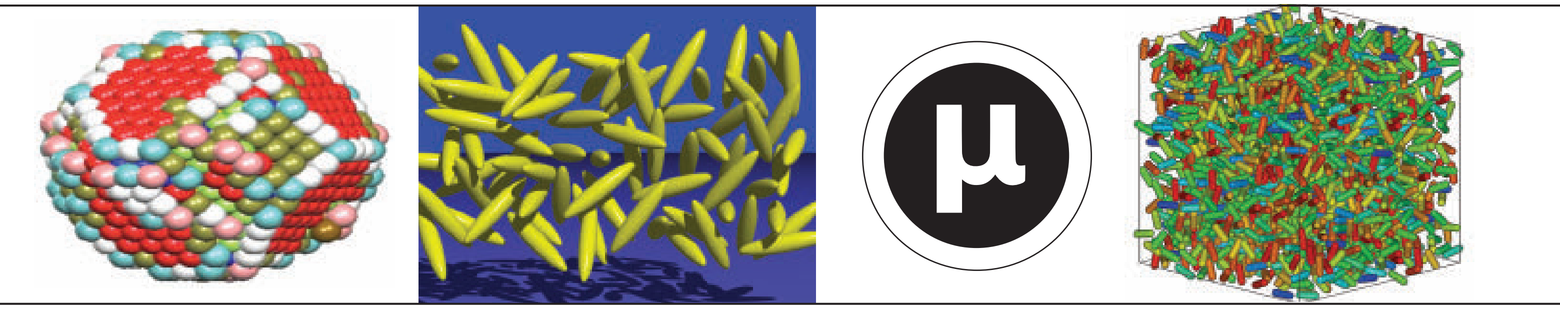
AS IT STANDS NOW, THERE'S A DIVIDE BETWEEN MATERIALS CREATION AND PRODUCT DESIGN.

BRINGING THEM TOGETHER WITHIN THE SAME SYSTEM WILL ALLOW FOR ALL KINDS OF NEW MATERIAL PROPERTIES AND STRUCTURES THAT CURRENTLY HAVEN'T BEEN USED IN THE ENGINEERED WORLD.

MATERIALS ARE GIVEN. THEY CAN ONLY BE SELECTED FROM THE EXISTING MATERIALS DATABASE.



MATERIALS IN THE LIBRARY: Contemporary CAD systems let engineers specify materials from a range of choices, but do not zoom in for the design of materials with special features on the nano or mesoscale.



CLOSE-UP VIEWS: From left, a gold nanoparticle, a liquid crystal, a Monte Carlo simulation of particles in an isotropic stage, a synthetic zeolite crystal, and transis-

COMPUTE INSTEAD OF EXPERIMENT

Simulation software tools would also be used to analyze the material at multiple scales. The engineer could use them to compute the physical properties instead of experiment. The tools can quickly answer questions to verify the design; for example, what is the modulus of elasticity of the newly designed material? This mechanical property can be directly calculated and predicted from material configurations done at the atomic scale.

Nano scale materials simulation can predict mechanical, thermal, optical, and electrical properties for some particular atomistic structure. The calculated properties from nano scale simulations can be plugged into traditional FEA for overall structure analysis. So it's kind of a chain reaction of calculations. Computation allows engineers to predict material properties and use those numbers to run FEA at the macro scale.

The value of a multiscale CAD environment lies in knowledge shared and used across disciplines. Do mechanical engineers have to learn more about materials in order to use multiscale CAD in the future? No. In fact, today's engineers don't have to know all details of how to formulate and solve differential equations behind FEA and CFD software in order to run simulations.

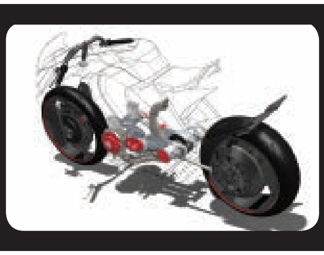
Similarly, our goal is to develop integrated software tools that will allow engineers to design materials in the same way they run FEA analyses, without the need of knowing all chemistry and physics behind them. We aim for software tools that simulate materials and predict their properties by simple mouse clicks.

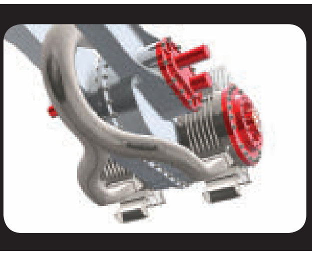
We began working on this concept a few years ago. One challenge has been how to allow computers to represent shapes and structures at the nano or meso scales, which are much more complex than the structures at the macro level, as currently done in CAD. We are also working on a new area called computer-aided nanomanufacturing that can predict whether or not the design of nanostructures and nanomaterials are manufacturable.

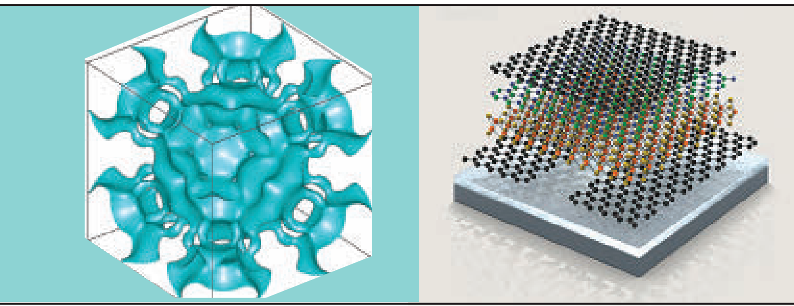
RADICALLY DIFFERENT SHAPES

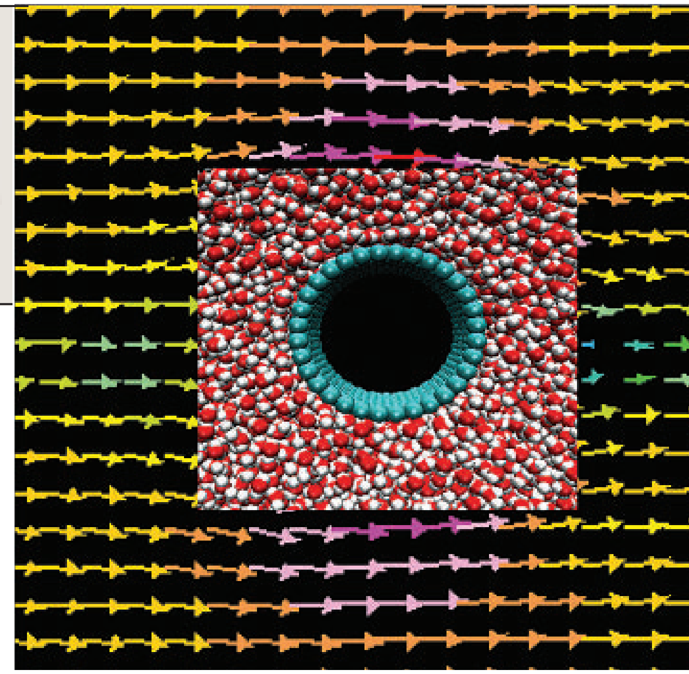
Offering the capability of designing materials in CAD requires the representation of many different kinds of shapes. Compared to the geometries at the nano scale or in nature, traditionally used geometries in engineering design are very simple and mostly flat, such as buildings, chairs, and computers, because that's what the current CAD can do today.

Natural shapes, like sea urchin, and kale, and geometries at nano scales, like zeolite, and polymer, are very complex. Part of our effort is to see how we can present these atomic configurations and porous structures by computer.









tors made of 2-D materials. At far right, a bio nanosensor.

WE AIM FOR SOFTWARE TOOLS THAT SIMULATE MATERIALS AND PREDICT THEIR PROPERTIES BY SIMPLE MOUSE CLICKS.

The engineer using the nano CAD software would first design the complex shapes interactively, simulate properties of the design, and optimize toward the need. The engineer could then apply the designed material in the macro scale simulation using FEA software.

The multiscale CAD would also allow engineers to design better functional materials, such as state-change materials. Examples of these materials, used for their state transformation properties every day, include batteries for energy storage, DVDs for information storage, and shape-memory alloys for orthopedic surgery. Charged and discharged batteries are two states of the material, as are burned and erased DVDs, and deformations of shape-memory alloys.

For instance, erasable DVDs depend on special materials with certain optical properties. When a laser pulse burns them, the materials change between transparent and non-transparent. This optical property change is used to store the binary information of zero or one.

The designer of DVD materials needs to decide the speed of burning and the amount of energy required to finish the state transformation. Atomistic simulation can be used to predict the required energy for the transformation. The designer can determine the material compositions and atomic configurations best suited to meet target performance.

The geometric modeling of microstructures that make up material is still in its infancy. The efficiency and controllability of complex and porous shapes are the most important research topics for the interactive modeling and design of microstructures. ME

YAN WANG is an assistant professor of the Woodruff School of Mechanical Engineering at the Georgia Institute of Technology in Atlanta, and a faculty member at the institution's Multiscale Systems Engineering Research Group.

DESIGN ON A NEW SCALE: Just as current CAD software models parts and assemblies, future systems may be able to zoom in and model materials on the molecular level to give them novel properties specifically suited to a given product.

MORE THAN 30 YEARS AGO, ENGINEER **K. ERIC DREXLER** STARTED WORKING ON THE CONCEPT OF **NANOSCALE MACHINERY** AND **MANUFACTURING**.

He recently spoke with *Mechanical Engineering* associate editor Jean Thilmany about the present state and future prospects of this most advanced form of manufacturing.

AT ITS HEART, atomically precise nanomechanical engineering—the building of machines and factories on the scale of large molecules—is mechanical engineering writ small.

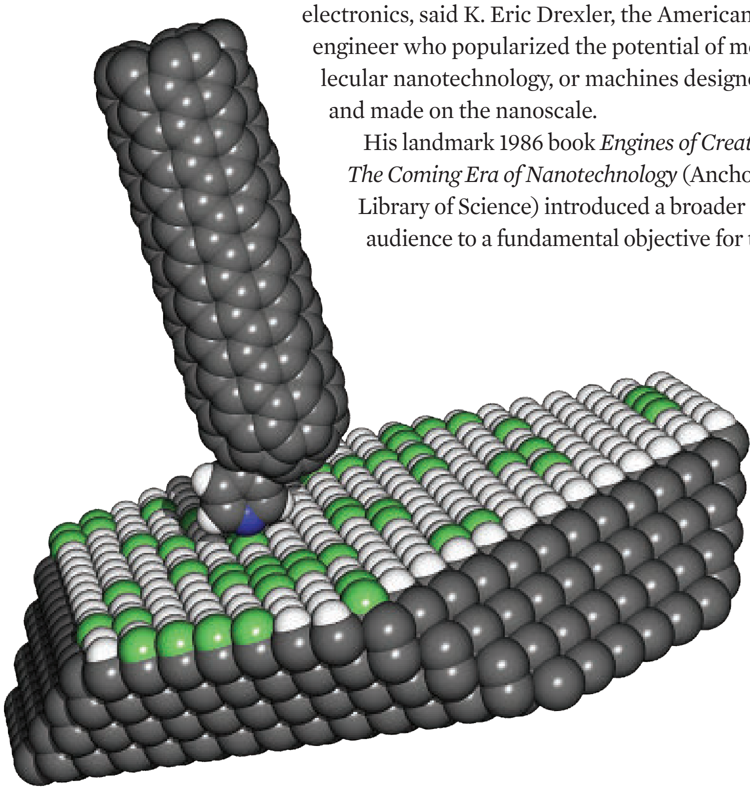
With a theoretical factor of one million advantage in throughput of both energy and materials, nanomechanical technology promises to revolutionize everything from automobiles to medical devices, just as the ability to fit billions of transistors on an integrated circuit transformed electronics, said K. Eric Drexler, the American engineer who popularized the potential of molecular nanotechnology, or machines designed and made on the nanoscale.

His landmark 1986 book *Engines of Creation: The Coming Era of Nanotechnology* (Anchor Library of Science) introduced a broader audience to a fundamental objective for the technology: using machines that work at the molecular scale to structure matter from the bottom up.

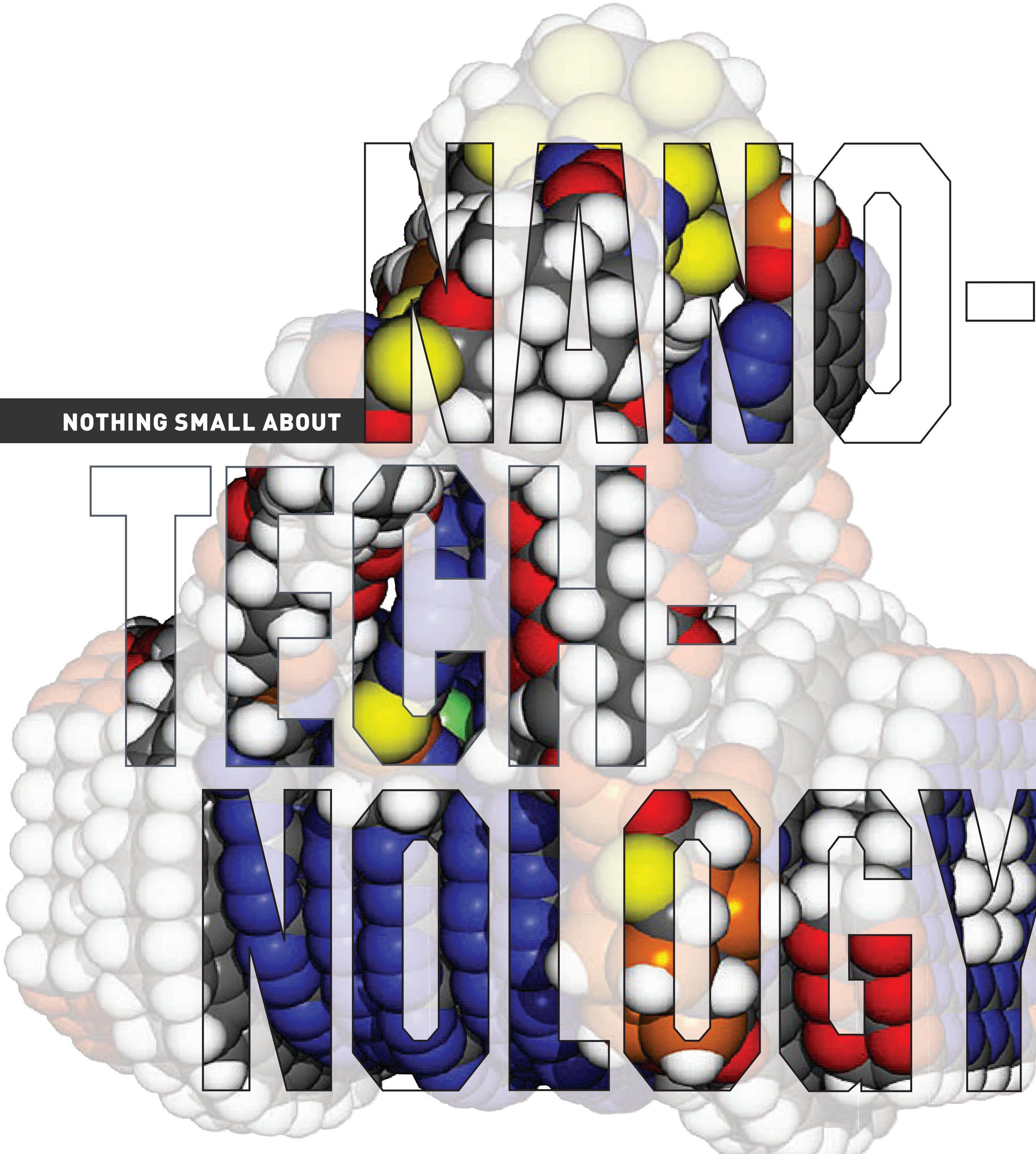
Drexler's 1991 doctoral thesis in molecular nanotechnology from the Massachusetts Institute of Technology was expanded and published as the book, *Nanosystems: Molecular Machinery Manufacturing and Computation* (Wiley, 1992). More recently, he authored *Radical Abundance: How a Revolution in Nanotechnology Will Change Civilization* (PublicAffairs Books, 2013).

The nanomechanical revolution Drexler predicts would open up new jobs to mechanical engineers. For right now, however, the key to progress is at the intersection between mechanical engineering and the molecular sciences, where atomically precise fabrication has reached the scale of designing and building structures with millions of precisely arranged atoms.

Drexler spoke to *Mechanical Engineering* from his home in England, where he works with the Programme on the Impacts of Future Technology at Oxford University.



We have a **nanotechnology revolution** in progress today.



NOTHING SMALL ABOUT NANO-TECH-NOLOGY

Complex functions can be accomplished through machines built at the molecular scale. At left, a design for a computer memory system uses a nanotube probe. Above, this motion controller was developed by Drexler.

INTERVIEW By JEAN THILMANY

J.T: Can you tell us a bit about what you mean by "nanomachinery"?

K.E.D: What I mean by this term is a particular kind of nanomachine-based technology on the horizon today, one that has enormous potential. The best way to understand the potential is by comparing this machine technology to the leading nanoscale technology in the world today.

Today we have a nanotechnology revolution in process, nanoelectronics, the ubiquitous chip technology that has already transformed many industries. It's not commonly called "nanoelectronics" or "nanotechnology," but that's what it is. We still use the prefix "micro," though the technology has gone beyond this.

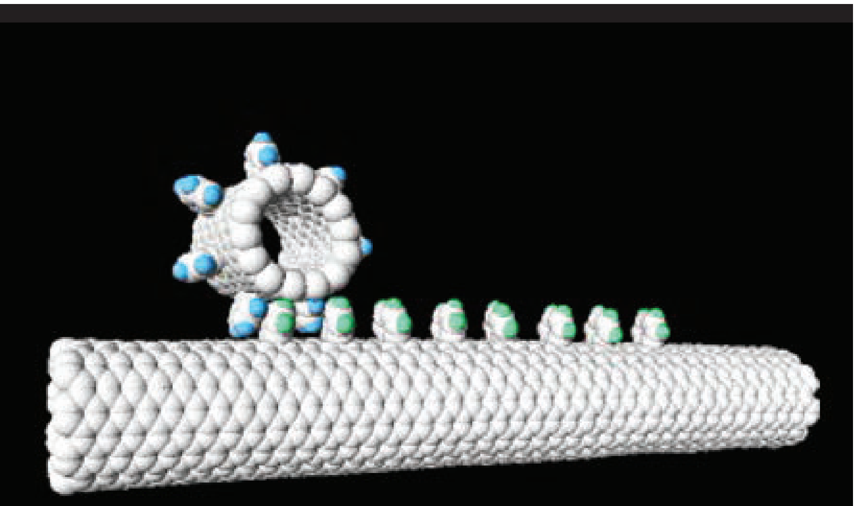
Nanoelectronics today is based on intricate systems with features as small as 20 nanometers. Like future nanoscale machines, these nanoscale electronic systems operate at high speeds and perform useful functions. "Nanoscale" refers to the component level, since chips with billions of devices are built on a centimeter scale, and future nanomachine-based systems with trillions of devices can be much larger.

The impact of electronic nanotechnology has been enormous. Today's digital electronics—cell phones, computers, and so on—are based on nanoelectronic technologies.

These electronic systems are based on arrays of nanoscale components that work together at high frequencies and process little discrete things. In the case of electronics it's bits of information.

Nanomechanical production technology will likewise be based on arrays of nanoscale components that work together at high frequencies and handle small, discrete things. But in the nanomachine world the things aren't bits packaged in bytes, they're atoms packaged in molecules.

This kind of technology is already surprisingly well understood, even though making the actual physical devices is still beyond reach of today's fabrication technologies. What we do have is the modeling tools needed to do detailed computational simulations and explore the design space, and these tools can be used by mechanical engineers to design nanomachines.



Engineered molecules, such as these nanotubes with attached nodules, can act as simple machines. Many working together could make a factory.

J.T: What will nanomachines look like?

K.E.D: In a literal sense, nothing, because the smallest components will be invisible, just a few nanometers in diameter, and only barely resolved by an electron microscope. Useful systems of machines, of course, will often be large.

In terms of their structures, when atomically precise fabrication capabilities become more advanced, it will be possible to build a class of nanoscale machines that is quite extraordinary, with every atom in a position chosen by designers, and densely bonded to form strong, stiff materials. This class of nanoscale machines will have components with shapes and functions very similar to devices designed by mechanical engineers today.

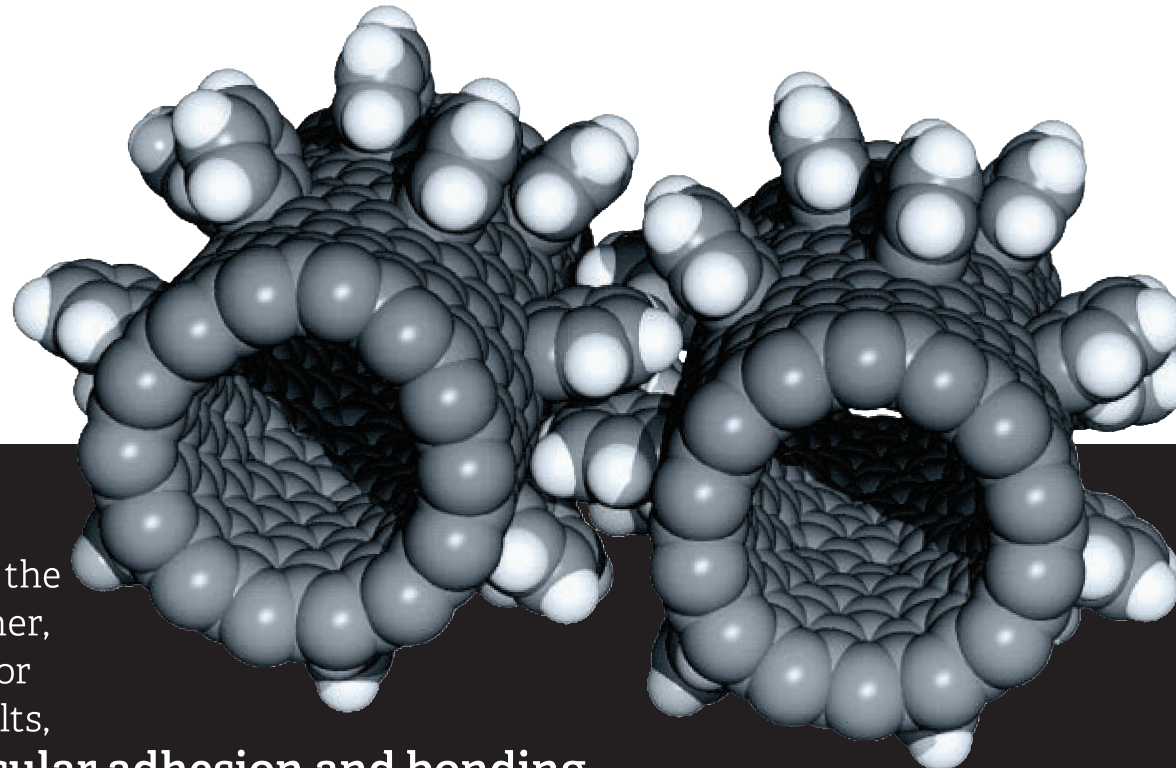
The prospect for this kind of technology includes ultrastrong materials and high-performance mechanical systems of all kinds. The machines will be built on a range of scales, but they'll demonstrate their most extraordinary properties at the nanoscale.

Because of basic mechanical scaling laws, nanoscale machines can operate at high frequencies, and nanoscale production systems will be able to process many times their own mass in a short time. For both energy and materials, there's a factor of one million advantage in throughput per unit mass between nanomachines and similar machinery at the macro level. The consequence is that you don't need a whole lot of machinery to get a large result. A thin-film configuration would be typical.

At this scale, you can get enormously higher power densities in motors and gear boxes—for example, a power density on the order of 100 GW per kilogram is natural, just because of scaling laws. Of course, you couldn't use a kilogram of machines like that all in one in place, because cooling will only be possible with much smaller amounts of hardware or lower power densities.

J.T: Where does the development of nanomachines stand today?

K.E.D: Both the physics and engineering of these technologies are well understood today, but the pathway to their development will depend on



What holds the parts together, isn't rivets, or welds, or bolts, **but molecular adhesion and bonding.**

This model of a molecular gear set, created at the NASA Ames Research Center, uses carbon nanotubes with teeth added via a known benzyne reaction. Building such nanomachines has been a challenge.

organization and investment, and on all sorts of detailed technological developments. And as all engineers know, these factors are less than predictable.

It's interesting to note that in nanoelectronics, the Moore's law trend, the exponential decline in size and the increase of components on a circuit, have been smooth. But what's delayed nanomachines is that there isn't the same kind of smooth path. The technology has to be built up—not scaled down—starting at the molecular level.

The reason comes down to surfaces: In electronics, charge flows through the interior of a device, and rough surfaces are OK. In machinery, motion depends on having smooth surfaces for bearings, and at the nanoscale, this means having all the atoms in the right place. Lithography just can't do that.

Atomically precise fabrication in the molecular sciences has come a long way, up to millions of atoms, but it has a long way to go before building nanomachinery at this level. The problem isn't scale, but materials.

J.T: It's interesting because in this issue **Yan Wang** of Georgia Tech has written an article about a CAD system his team is working on that would allow engineers to create materials specific to their design.

K.E.D: His work and the kind of work I'm outlining here ultimately fit together. And when you consider nano- and macroscale together, you end up needing multiscale and multiphysics modeling.

J.T: What needs to happen to advance the state of nanomechanical systems?

K.E.D: What's most needed today is focused research organized around system-level objectives. We need to develop a field of molecular mechanical systems engineering. It's a matter of research, organization, and funding, based in the molecular sciences, but going in new engineering directions.

Some of the roots are in molecular biology, but this field is organized as a science, a branch of biology. But small groups organized around studying and imitating biology don't build the kinds of components needed for a mechanical engineering technology that builds toward more and more advanced nanomechanical systems.

J.T: How would nanoscale production machinery work?

K.E.D: To a remarkable extent, it will work like macroscale production machinery, the kind used to assemble components to make larger components. As components get larger, later in the process, assembly becomes entirely conventional.

The picture is of nanoscale machinery making nanoscale parts and of those parts being put together to make microscale parts by microscale machinery, and parts on the centimeter-scale assembling centimeter-scale components, and so on.

At the bottom, at the start, the key is to apply nanoscale mechanical systems to move things—molecules—and put them together. This is entirely parallel to what we see in factories, but what holds the parts together isn't rivets, or adhesives, or welds, or bolts, or snap fittings, but molecular adhesion and bonding. Different in many details, but the same function. Also, the smallest parts at the start of assembly, instead of being cut from bar stock or injection molded or stamped out of sheet metal, will be reactive molecules of the kind used in chemical synthesis.

Considering these earliest steps in the process, the best parallel today is continuous-motion assembly machines, the machines used to assemble things like the mechanisms of plastic spray bottles. These assembly machines process a continuous stream of parts and some of them produce as many as 50 assembled products per second. The assembly isn't done with little arms. Instead, the parts are carried and transferred by spinning disks with gripping fixtures around the circumference. What's most like "programming" is in the shape of the cam surfaces that guide some of the motions.

This principles of these continuous-motion assembly machines could be applied on a nanoscale, then the nanoscale products would be handed off to larger machines. These would naturally be organized much like a factory, with parts passed from machine to machine and conveyors moving them along. The final products used by people would be on the familiar human scale, like today's products, even though the parts they are made from would be much smaller, and the properties of the small parts can result in high performance on the macroscale.

This kind of manufacturing process is somewhat like additive manufacturing or 3-D printing which is also about building small bits of materials together under programmable control to make any of an unlimited range of larger objects.

J.T: So the end product would be something you could see and touch. What is an example?

K.E.D: Well, some examples of potential products are photovoltaic arrays, cars, computers, spacecraft, and small medical devices that can work at the level of cells—a list would go on and on. Bottom-up atomically precise manufacturing is a general-purpose manufacturing technology.

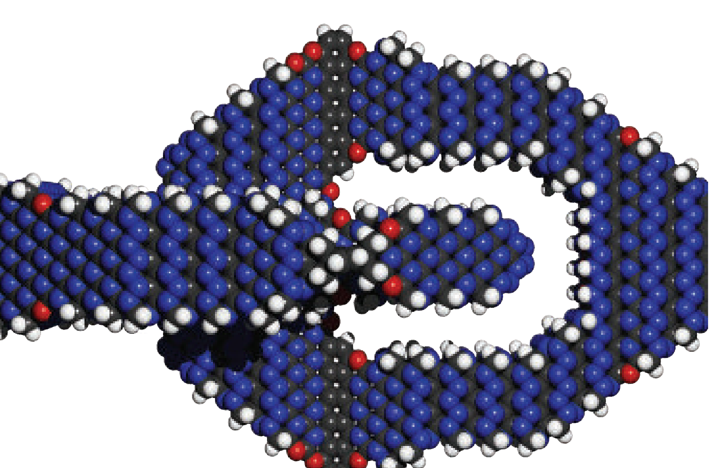
Think of the very general applications of computers. They have totally transformed areas as different as photography, music, scientific equipment, and mail. At the heart of a cell phone are sets of small, fast devices that transform patterns of information at the smallest bits. Using nanoscale devices to build up from molecules is similar in many ways, and will also have very general applications and products.

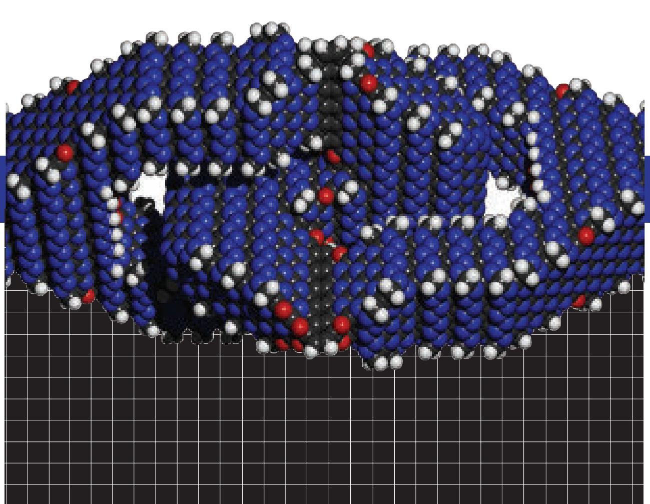
J.T: How should mechanical engineers think about nanomachinery?

K.E.D: Scaling laws tell us that machine-parts that move at equal speeds with similar shapes and patterns of motion will have the same dynamics (and stresses and strains), except for a scale factor in space and time. This means that much of mechanical engineering translates directly to the nanoscale.

At the very bottom, the atoms do matter. They can't be scaled. The meshing teeth of the smallest machines will be on the atomic scale, just rows of atoms. Bearings are a special case, because ordinary lubricants won't work. Instead, properly structured surfaces can slide over one

A universal joint (below) and bearing (opposite) designed with atomic precision.
(Images copyright: Institute for Molecular Manufacturing, imm.org)





another, in direct contact, with the "bumpiness" of individual atomic interactions adding up in a way that results in smooth motion. This phenomenon is called "superlubricity" and has been demonstrated in a lab.

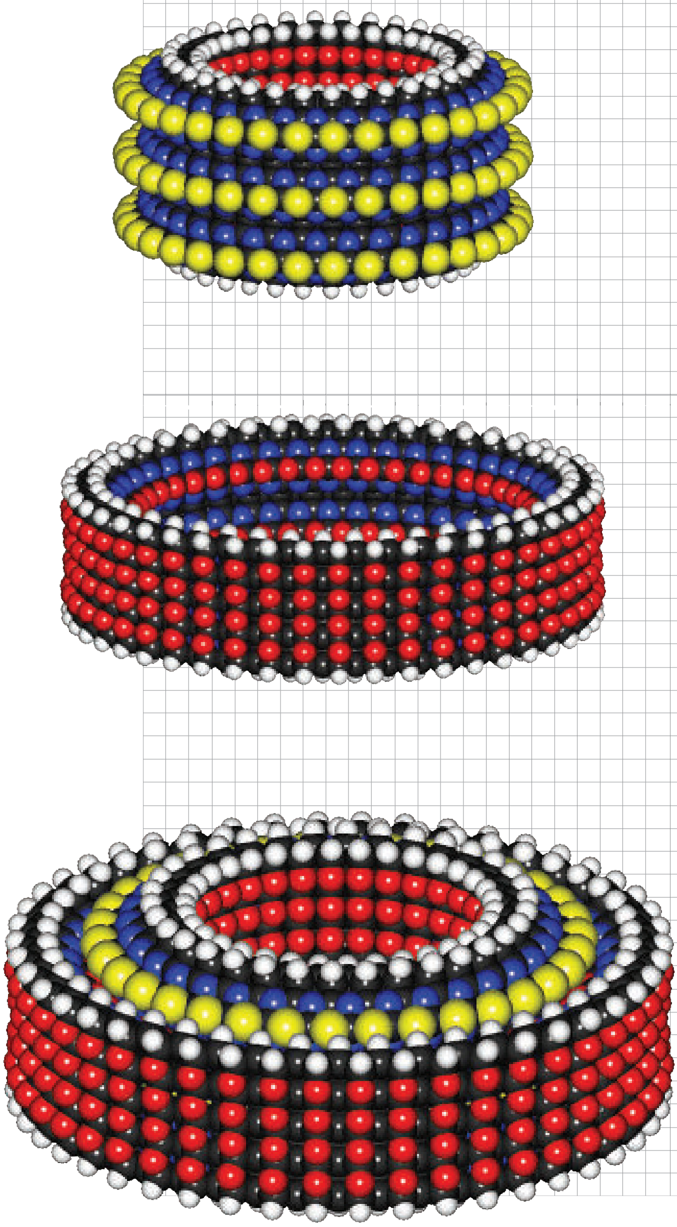
Thermal fluctuations are a special concern at the nanoscale, but they're statistically predicable and are part of standard dynamic models. In mechanical engineering terms, thermal motion amounts to an especially well-understood source of vibrations—but ones that are impossible to damp!

Today, however, the modeling software used to describe and test atomically precise machines machine designs comes straight out of the molecular sciences, and it doesn't directly support abstractions at the component level. The description is very fine-grained.

Traditional CAD would then apply at scaling levels not too far above the nanoscale. At much less than a micron non-atomistic solid models become realistic. Atomistic models can establish elastic properties, friction properties, and so on, and these can then be used to parameterize conventional models. Likewise, atomistic machine designs can be characterized as lumped components, in terms of properties like gear ratios, torque, elastic compliance, friction, and so on.

Mechanical engineers today can work with the existing atomistic models, and can make an enormous contribution to understanding the potential of advanced nanomachinery. In these models, they can build parts and machines, and after testing in simulation, they can calculate performance parameters, then try to come up with better designs. This could make a great area for online competition.

There's a lot to learn in this area of technology, even before we can actually build the machines. I hope that today's mechanical engineers will learn about nanomachinery and help explore this new domain. It's important, exciting, and fun. **ME**



At the very bottom, the atoms do matter. They can't be scaled.
The meshing teeth of the smallest machines will be
on the atomic scale, just rows of atoms.

Properly structured surfaces **can slide over one another,** with the **individual atomic interactions** resulting in smooth motion.