Computational materials science opens doors to quicker, cheaper discoveries

It could pass for a video game: a mass of yellow, blue, and green dots that writhe and collide with errant pink flecks. But the scene that plays out on Erik Luijten’s computer screen is actually a simulation of an experimental gene-repair therapy, demonstrating on an atomic level how a synthetic polymer molecule could deliver a healthy strand of DNA to a genetically mutated cell.

“Something as rudimentary as the shape of the polymer molecule can have a huge impact on how the healthy DNA gets distributed in the body,” explains Luijten, associate professor of materials science and engineering and of engineering sciences and applied mathematics. “My job is to figure out how to create those different shapes.”

And how does he do that?
“A bit of experience and a bit of magic,” he says.

Luijten isn’t a biologist—or a magician, for that matter. He’s a computational materials scientist—a “simulator,” he says, as opposed to the more traditional “experimentalist.”

Computational materials science is transforming the way researchers make materials. From skyscrapers to space shuttles, materials science has been responsible for creating the objects that fill our everyday lives. It’s a process that generally requires laboratory experiments, but developing

Researchers find promise in “crumpled” graphene

They’re the building blocks of graphite: ultrathin sheets of carbon, just one atom thick, whose discovery was lauded in 2010 with a Nobel Prize in physics.

Graphene, many researchers believe, could impact everything from electronic devices to high-performance composite materials. It is extremely strong and an excellent conductor, and, with no internal structure at all, it offers an abundance of surface area—much like a sheet of paper.

Until recently, however, working with graphene has been difficult. Like a deck of cards, graphene sheets easily stack into piles, reducing their surface area and making them unprocessable. But researchers at McCormick have now developed a new form of graphene that doesn’t stack. It is made by crumpling the graphene sheets into balls.

“If you imagine a trash can filled with paper balls, you really get the idea,” says Jiaxing Huang, the Morris E. Fine Junior Professor in Materials and Manufacturing (far right). “The balls can stack up into a tight structure. You can crumple them as hard as you want, but their surface area won’t be eliminated.”

The crumpled shape is created by moistening the graphene sheets and placing them in a furnace to evaporate the moisture, says Huang, who adds that their potential is great: “We expect this to serve as a new graphene platform for numerous applications, such as energy storage and energy conversion.”

Left: Jiaxing Huang, Morris E. Fine Jr. Professor in Materials and Manufacturing (far right). Above: Simulation image of a nanoparticle designed for gene therapy purposes. Plasmid DNA (green) is encapsulated by polymers (blue and yellow) to protect it during transport and to facilitate its entry into a cell.
new materials experimentally can be painstakingly slow, particularly in highly regulated industries. Certifying new materials for aerospace applications, for example, can take more than a decade as researchers stage experiments time and time again.

“It’s expensive, it’s laborious, it’s time consuming, and then you make the material and find out it doesn’t work,” Luijten says. “Was your intuition wrong? Was the experiment contaminated? In a computer, on the other hand, everything is perfectly controlled.”

By manipulating millions of pieces of data describing the charge, size, and other characteristics of particles, Luijten and his peers are able to predict how materials will behave in the presence of other materials or under certain environmental conditions such as heat or strain.

The process can also be flipped on its head, says Peter Voorhees, the Frank C. Engelhart Professor of Materials Science and Engineering and professor of engineering sciences and applied mathematics. “We can now say, ‘What kind of properties are you looking for in a material?’ and then go back to the periodic table, pick A, B, and C, and make it on the computer,” he says.

Voorhees uses computational materials science to predict the structure of materials composed of more than one phase. Using computer codes, Voorhees can determine exactly how to process combinations of metals, such as aluminum and copper, to make them as strong as possible—vital information for metal makers, airplane manufacturers, and other industries. The same process allowed Chris Wolverton, professor of materials science and engineering, to help design an ultralight aluminum engine block for the Ford Motor Company, and Greg Olson, Walter P. Murphy Professor of Materials Science and Engineering, to design a high-performance gear steel commercialized through his company, QuesTek Innovations.

Computational materials science can’t replace lab experiments, Voorhees says, but the two can work together to greatly shorten the development process. “The idea is to make the design process two cycles instead of ten,” he says.

While it’s still early, Luijten says the field holds enormous promise for everything from the automotive industry to biomedical engineering to energy harvesting. “We are just at the start of this process,” Luijten says. “We are really thinking outside the box.”

Shape memory alloys: From airplanes to implants

Picture an airplane engine that can change shape during flight, taking the optimal form for a smooth, quiet takeoff and then reconfiguring itself at cruising altitudes to its most fuel-efficient shape. Such things are possible with shape memory alloys, a type of metal that can “remember” its original shape and revert to it under a stimulus such as heat or electric current.

Shape memory alloys can set a device in motion without the added bulk and noise of a motor—an asset in aerospace applications, where each extra gram means added fuel cost. And they’re already being used for some medical purposes, such as stents: unlike a stainless steel stent that must be implanted using balloon inflation, a shape memory alloy stent can self-deploy as it warms inside the body.

Now McCormick researchers are looking at adding something new to shape memory alloys: pores. “One idea is to use this new material in bone and joint implants,” says Cate Brinson, the Jerome B. Cohen Professor in mechanical engineering, who, along with David Dunand, the James N. and Margie M. Krebs Professor in materials science and engineering, is exploring the new material. “Porous shape memory alloys have a lower stiffness, like real bone, reducing atrophy of the surrounding bone tissue and allowing the bone to grow into the pores for stabilization.”

The porous material could also find its way into aerospace in the form of lighter, shape-shifting engines and other lightweight actuation applications. “When you couple this lighter, more flexible material with shape memory alloys’ ability to change shape, there is a multitude of possibilities,” Brinson says.