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Molecular architects: how scientists design new materials

By Gregory McColm

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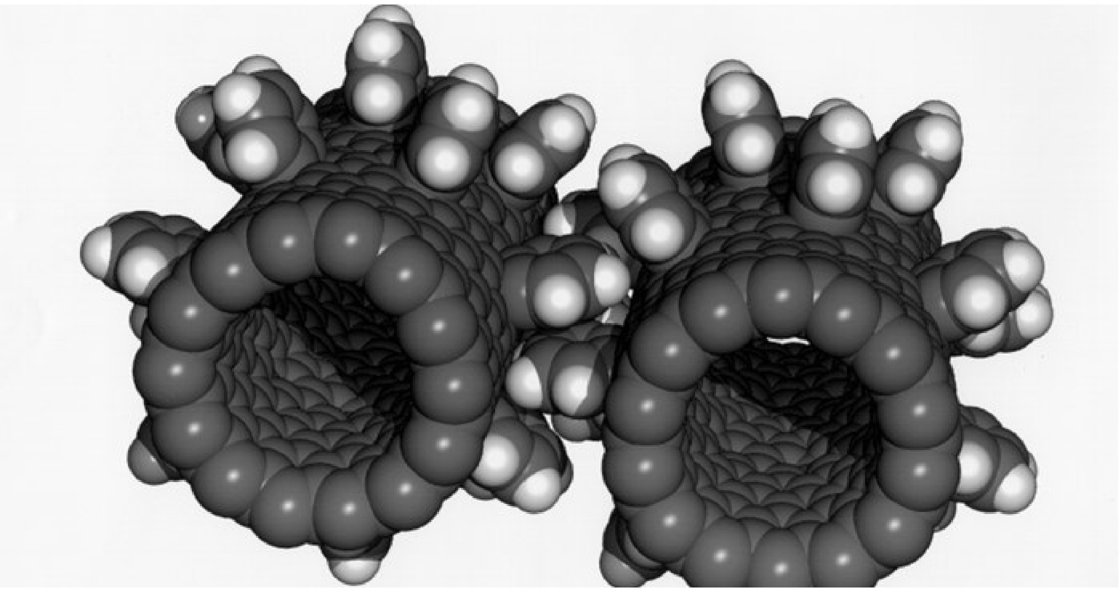
When Thomas Edison wanted a filament for his light bulb, he scoured the globe collecting thousands of candidates before settling on bamboo. (It was years before people were able to make tungsten work properly.) That's our traditional way of getting materials. We picked up stones for axes, chopped wood for housing and carved tools out of bone.



Nano-architects design materials that can work together at very tiny scales, like these interlocking gears made of carbon tubes and benzene molecules. NASA

Then we learned to synthesise new materials out of old ones, like shaping clay into bricks or pots and baking them into stone. Plastics entered our repertoire as a concoction of cotton, acid and wood tar.

A very early materials scientist: Albertus Magnus. Sailko,

Much of the quest for novel materials has moved into science labs. The search is more efficient than when Albertus Magnus (allegedly) synthesised the Philosopher's Stone, but the game is still intelligent serendipity. We try combinations of ingredients, combinations of heating, mixing and other processes, and hope that one of them works. During the last few decades, a scaled-up, highly organized and automated search system called "combinatorial chemistry" has produced new drugs and materials including automotive coatings, hydrogen storage materials, materials for solar cells, metal alloys and organic dyes.

Architects and engineers do not wait on search or serendipity to produce a novel bridge that doesn't collapse under a 10-ton truck. They use established principles, paper and pencil (and software) to produce a design that they can confirm, by computation and deduction, will meet the necessary specifications. Today's chemists and materials scientists are taking a similar approach, pushing forward a materials revolution.

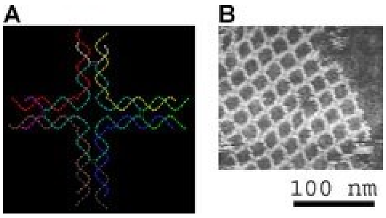
The challenges of design-build planning

One of the great technological challenges of this century is to design novel materials to satisfy given specifications – and then, when the material is synthesised, have it meet those specifications. Just as builders can make a house out of bricks and beams and mortar using a blueprint indicating where the bricks and beams go, scientists conceive of synthesising a material out of molecules using a blueprint indicating where the "molecular building blocks" go.

But there is a problem. Unlike bricks, beams and mortar, people cannot pick up atoms or molecules with their hands and place them in a structure. This must be done indirectly, rather like modern construction: just as we have cranes, pulleys and other devices for manipulating beams, panels and prefabricated modules, we need devices for manipulating the atoms or molecules to get them into place – and then welding them together.

Working with DNA

Let's consider one (very nice) example: DNA. With current technology, DNA is much more easily manipulated than other materials; during the past few decades, we have developed many ways to manipulate DNA molecules. In 1980, Nadrian Seeman looked at M.C. Escher's "Depth," an infinite regular array of fish, and decided to make it – which he ultimately did three decades later. In between, he made a cube of DNA; Paul Rothemunde made a DNA smiley face, Leonard Adleman showed how DNA can compute things and a whole community arose making nano-things out of DNA.



At left, the design of a single tile of a nanogrid made of DNA; at right, the grid as viewed by an atomic force microscope. Strong, 2004, CC BY

Rothemunde's smiley face is a likely harbinger of things to come. It is a sort of nano-textile, with a very long DNA strand, folded back and forth so that it covers a circle. Two hundred short strands – "staples" – hold the long strand together. It isn't just the outline (the long strand with its folds and staples) that is designed in advance. Each DNA strand has its own code, which can be used to control how different DNA strands bond to each other. The codes of the long strand and the staples are computed in advance, and from these designs, strands are synthesised and mixed together to produce the intended structure.

Expanding to more difficult compounds

Meanwhile, chemists and materials scientists are making progress on less controllable materials, like proteins and crystals. For example, a decade ago, Omar Yaghi, Michael O'Keeffe and four colleagues published a manifesto on "reticular synthesis" in nature. They observed that crystals have regular molecular structures, and proposed that chemists should design a structure and then make crystals from the design.

One of the major efforts is making a porous crystal that can serve as a safe and stable storage tank for hydrogen powered cars. (Porous crystals, with nanoscale channels and chambers, are not oddities: you may find some in the catalytic converter in your car or even your cat's litter box.)

Many of our major technological challenges will require new materials with specific properties, whether for a new drug, a solar panel, a computer chip or airplane skin. When we see progress in medicine, energy, computing power and transportation, the materials revolution is an integral part of the scientific process of discovery.

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