

Chemistry professor's interest in molecules leads to storage of gases

Omar Yaghi

Some professors' offices look like libraries, with books, journals and dissertations all lined up on shelves. Others are more nest-like, with stacks of papers circling a desk and chair in the center of the room. Omar Yaghi's office, on the second floor of the University of Michigan Chemistry building, has the usual piles of paper and rows of treatises, but there's also something gallery-like about the room. Colorful, computer-generated drawings hang beside a large window overlooking an atrium, and track lights cast bright spots onto shelves filled with three-dimensional, geometric figures that resemble abstract sculptures. They're not sculptures; they're models of chemical structures, but Yaghi admires their beauty as others appreciate fine art.

It was the aesthetic aspects of chemistry, rather than the utilitarian, that first lured him into the field, the 40-year-old professor recalls. But his urge to understand the molecules he found so attractive eventually led him to develop materials with very practical applications: storage of hydrogen, methane and other economically and environmentally important gases.

"I didn't set out to solve any big problems," Yaghi admits. "I was drawn to chemistry mostly because of the beauty of the molecules." Browsing through a college catalog one day, he came across pictures of cage-like chemical structures similar to buckyballs – the carbon compounds named for visionary engineer and architect Buckminster Fuller because of their resemblance to the geodesic domes he created. Yaghi "fell in love" with the structures and decided on the spot that he wanted to learn how to design and make chemical structures of various shapes.

Making them, however, was not as easy as admiring them, Yaghi soon discovered. "You have to know how atoms link up together, and you also have to go into the lab and get them to do what you think they should do," he says. "And we all know how difficult it is to get nature to do what we want." But that's just what Yaghi has devoted the past 15 years to doing, and in the process, he's developed a whole new branch of science that he calls reticular chemistry. Reticular means "networked," and the molecules Yaghi creates are netlike structures with large, open spaces or pores. But it's the way they're made, as much as the forms they take, that characterizes this new realm of chemistry.

"The basic idea in reticular chemistry is to design molecular building blocks that will assemble into predetermined structures," he explains, pointing to drawings of some of his lab's creations – open frameworks shaped like honeycombs, stars, pyramids, paddlewheels and other symmetrical constructions. "Before our work, it was really very difficult to logically design large chemical structures like these; we just left it to nature, with all its uncertainties, to produce whatever it would give us. That approach has served humanity for a long time and has yielded some of the

most important materials we have today. But what we're trying to do now is understand how nature makes materials and then, based on that understanding, influence nature to produce certain things that we deem interesting and useful."

Yaghi's curious, creative nature is one key to his success, but that's not all there is to it, says Harvard University chemistry professor Charles Lieber, who has followed Yaghi's career from the start. "He brings quite a bit more intellectual depth to his work than most of the people who've worked in this area," Lieber says. "Some of them have just mixed things together and gotten things out. He's used a much deeper understanding of molecular chemistry to really design the things he wants to create. It's hard to predict just where the applications will come, but I'm confident that, down the road, something will be revolutionized by his work, because he's making new materials that have interesting properties. And all revolutionary advances in technology have been driven by advances in new materials."

Other scientists may be sold on Yaghi's approach now, but in the beginning, he struggled to find support. Fresh from a postdoctoral fellowship at Harvard, he was an attractive candidate when he went searching for an assistant professorship in the early 1990s. But when he told prospective employers about the research he wanted to do, they got skittish.

"The general feeling was, it was too risky," Yaghi recalls. "For me, it wasn't worth doing if it wasn't risky and challenging."

Arizona State University took a chance on the innovative young chemist, then only 26, and their gamble paid off.

"In the first six months that I was a professor, I succeeded in doing one of the things that I said I would do," says Yaghi, recalling how he coaxed that first porous network to assemble just the way he had predicted it would. He leans back in his chair and smiles, a little crescent of a smile that holds unbridled delight in its curve.

With that early success, Yaghi could have thumbed his nose at the skeptics who doubted he could deliver on his promise. Instead, he felt grateful to them, in a way.

"The skeptics just made me more determined to follow through on my ideas and get my work published," he says. "I tell my students all the time that it's important to listen to what the skeptics are saying, but you also have to have enough confidence in your own ideas that you don't get derailed."

There are few skeptics, if any, in the audience at Rackham Amphitheatre on fall afternoon in 2004 when Yaghi delivers a lecture to students, faculty and an assortment of his collaborators and former mentors who have flown in just for the event. A month earlier, Yaghi, who has been at U-M since 1999, was named the Robert W. Parry Collegiate Professor of Chemistry, and the lecture commemorates that honor.

He starts his talk by reflecting on lessons learned from his mentors, one of the most valuable being that science begins with doubt. Not only begins with it, but is permeated with it at every step.

"Just when you think you've figured something out, you often find that you actually haven't," says Yaghi. "You do one more experiment and realize, gee, it's not as simple as you thought." The constant doubt could be disabling if it weren't for another fact of scientific life that Yaghi learned from his postdoctoral advisor: "Research is an exercise in optimism."

Research is also an exercise in enjoyment, if Yaghi's attitude is any indication. Whether he's lecturing an audience of distinguished scientists or casually chatting with students on the sidewalk outside the Chemistry Building, Yaghi acts like a guy who's having the time of his life. And why shouldn't he?

"Why not have a good time when you're doing exactly what you want and enjoying what you do so much that it doesn't feel like work?" he says. "When you discover a new compound and you look at it for the first time, it's just fascinating, because you're the first to see how nature reveals itself. That's what makes it so much fun and so exciting."

It's satisfying, too, when those discoveries lead to solutions for vexing problems, such as how to store large amounts of hydrogen in fuel cells that can be used to power cars, cell phones, laptop computers and other devices. Hydrogen seems like an ideal fuel because when burned, it produces only water -- none of the polluting nitrogen oxides, carbon monoxide and volatile organic compounds that gasoline gives off when it's combusted. Hydrogen is so promising, in fact, that the federal government is doling out \$350 million in grants for research aimed at establishing a hydrogen economy. Two Michigan research groups are getting more than \$5 million of that pot. One is led by Yaghi and includes assistant professor of chemistry Adam Matzger; the other is headed by Ralph Yang of the Department of Chemical Engineering.

That's where Yaghi's honeycombs, pyramids, paddlewheels and the like are set to play starring roles. They're all examples of materials called metal-organic frameworks, or MOFs (pronounced moffs). On the molecular level, MOFs are scaffolds made up of metal hubs linked together with struts of organic compounds. By carefully choosing and modifying the chemical components

used as hubs and struts, Yaghi and his team can define the angles at which they connect and design materials with the properties they want.

The idea is to provide places for hydrogen to attach to the structures, and one way of doing that is to lengthen the struts, creating more surface area. But that approach can produce molecules with big, empty centers – wasted space with nothing for hydrogen to hold onto. A way to overcome that problem, Yaghi's team has discovered, is to nestle the frameworks together, something like chain mail, which makes the structures more compact without sacrificing the amount of surface area available for hydrogen bonding.

Complicated as the chemistry may sound, MOFs are remarkably easy to make.

"You just take Coke bottles and sun block and mix them together," Yaghi likes to joke. That's not far from the truth. "We take a solution of terephthalic acid, which is in most plastic bottles, and mix it with a solution of zinc oxide, which is in sun block, and out comes a very lovely nanomaterial."

So far, Yaghi's group has cranked out more than 500 MOFs, and they're exploring and tweaking the materials' properties, trying to reach the initial goal the government has set for hydrogen storage capacity: six percent by weight. So far, the storage capacity of the Yaghi lab's star MOF is only around two percent, but Yaghi has plenty of strategies up his sleeve for increasing the uptake.

"I have no doubt that we will get to six percent," he says. "But even with our humble nearly two percent, we're quite competitive with batteries that are used in laptops and cellular phones, and I think that's where the first applications for hydrogen storage will be."

Yaghi is also working with BASF and a number of other large companies to develop MOFs for storing methane. He flashes a sequence of slides on a screen behind the podium to show his Rackham audience a demonstration that he uses to sell industry representatives on the virtues of MOFs.

The first slide shows an aluminum canister sitting on a balance; the second is a graph of methane uptake at various pressures. "We introduce methane into an empty can at different pressures and measure the uptake," Yaghi explains. "Then we do exactly the same experiment when the can has been completely filled with MOF material."

On the graph, the lines for the empty can and the MOF-filled can both slant upward, showing, as you would expect, that methane uptake increases at higher pressures. But the line for the MOF-filled can is quite a bit above the one for the empty can. In other words, says Yaghi, "If you have

MOFs in the tank, you can store almost double the amount, even at very reasonable pressures and room temperature."

He smiles that little smile of delight again, as if his capacity for enjoying the work he does is edging ever upward like the lines on the graph.

Back in his office, Yaghi's expression turns serious when he muses on the rewards – and the challenges – of his chosen field.

"Going into chemistry requires dedication and passion," he says. "For me, at first it was pure passion; now it's passion, dedication and commitment." Sure, it can be enjoyable and exciting, says Yaghi, "but I don't want to give the impression that it's a profession where it's all fun. Science must interface with society, and that means that you can't just enjoy the excitement of discovery, but you must also consider how to bring what you discover to benefit other people. You must find a balance."

Striking that balance as gracefully as Yaghi seems to do it takes more than knowledge and skill. You might say it's a real art.

Video of Prof. Omar Yaghi discussing MOFs Image of: video camera

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