Profile of George Schatz

As a graduate student at the California Institute of Technology in the mid-1970s, George Schatz took classes given by Richard Feynman on particle physics and quantum electrodynamics covering the abstract and microcosmic basis of physical science. But, less than six years before, Schatz was a hayseed from Sackets Harbor, NY, a town of fewer than 1,000 people. Until college, he had never met anyone with a Ph.D. His transformation into a top theoretical chemist was propelled by his energy and curiosity, with only a few nudges from mentors who revealed to him what might be possible in life. Schatz is best known for his work on the theory of chemical reaction rates as well as his computational modeling of the optical properties of nanoparticles. He was elected to the National Academy of Sciences in 2007.

Schatz grew up in a rural environment where fertilizers and pesticides were common. The noxious fumes from the local paper plant were hard for him to ignore. "We all get exposed to chemicals," he says. The ubiquity of chemistry triggered a decision in the 17-year-old Schatz. "Without ever having talked to anybody, just simply having read books, I decided that this was what I wanted to major in in college."

He attended Clarkson University in Potsdam, NY, which was known for its science and engineering programs. "The good fortune for me was that there were very talented people at Clarkson willing to take me under their wing," he says. Richard Partsch, still a professor at Clarkson, taught Schatz organic chemistry. "When I became a junior," Schatz recalls, "he found me one day and said, 'There are these undergraduate research programs that you can get involved with where you go visit a national lab for a semester. Maybe you'd want to try this.'" So in the fall of his senior year, 1970, Schatz found himself at Argonne National Laboratory working on a project in materials science. "This was a defining point in terms of my career," he says. "And I never would have thought about doing this if it hadn't been for Partsch."

George Schatz

Not Your Usual Chemistry Major

However, his professors left him on his own when it came to choosing a graduate school. He applied to the California Institute of Technology (Pasadena, CA) because of its strong program in chemical physics. He was accepted, and once in Pasadena, he knew he had made the right choice. "There were lots of people who had similar interests to mine," he says. "It was a very stimulating environment." Schatz was a chemistry major, but "I was a weird deal. . . I decided, oh, I'm just going to take physics courses because I really want to know all the fundamentals." He absorbed Feynman's lectures on physics. Ever since, Schatz says, "I've been learning how to use my background in fundamental physics to make applications to chemical problems." For his Ph.D. dissertation, under the supervision of Aron Kuppermann, he studied the mathematics of chemical reactions in the gas phase.

In 1975, Schatz traveled to the Massachusetts Institute of Technology (Cambridge, MA) to work as a postdoc for John Ross, a pioneering theorist specializing in chemical reaction kinetics. "MIT has a completely different culture than Caltech," Schatz says. "I thought I was smart stuff, and I ran into a whole bunch of people who told me that they were not impressed with what I had done at Caltech. In fact, they weren't even sure it was right!" At Caltech, Schatz's research focused on in-depth analysis of ideal systems. "At MIT," he says, "I started thinking about bigger-picture problems, about coupling to many degrees of freedom, to reaction of condensed phases. It was only a year, but it was a very good year for me to retool and think of things in a broader way."

Where Did You Say Northwestern Was?

The mid-1970s were a tough time to look for a job in academia. The universities that had sprung up during the 1960s were fully staffed with young professors. Schatz credits Mark Ratner, now his colleague at Northwestern University (Evanston, IL), for going out of his way to recruit him. Schatz was hired as an assistant professor in 1976. Of Ratner, he recalls, "He talked to some people at Caltech who knew me, and so suddenly I get this letter out of the blue from Ratner which says, we want you to apply for the theory job at Northwestern. And then he actually came to MIT and talked to me." When Schatz filled out the job application, he was not even sure where Northwestern was located. "Northwestern has really grown in quality over the years," he says, "and established itself as one of the premier places, particularly in the area of nanoscience." According to Schatz, this success is largely because of Ratner's efforts to strengthen the theory group in the chemistry department.

At Northwestern, Schatz's theoretical research is complemented by his colleagues in experimental research, such as Richard van Dyne and Chad Mirkin. Strong feedback exists between theory and experiment in nanoscience, and the theorists at times have had to wait for the experimentalists to catch up and to define the direction in which the field is moving. As a student in the mid-1970s, Schatz says, "we realized that if you could make particles where you could control the size, shape, and arrangement, then there would be a lot of interesting applications." But at the time, it was not possible to produce such particles. "So in the end, we set some of our ideas on the shelf. And in the mid-1990s, there were suddenly new technologies for making particles with lithography, and there were methods for measuring their properties with scanning probe and electron microscopy."

The Nano-Engineered World

Schatz considers his studies of how gold and silver nanoparticles absorb light to be some of his most important work. "You can tune the wavelength of absorption throughout the visible range by just changing the size and the shape and the local environment," he says. New computational electrodynamics methods arose in the 1990s, which made a full analysis possible. One practical spinoff of his work was a new type of biosensor

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that could be used to diagnose diseases such as Alzheimer's from a blood sample. To this end, Mirkin and van Dyne attached proteins to the surfaces of the nanoparticles. "It turns out that when you bind a protein to these particles, then you're changing the dielectric environment, and that changes the wavelength at which the particles absorb," Schatz says. When the nanosensors detect a target protein, their absorption peak alters by 30 nm, an easily detectable shift.

Schatz considers problems that range from the atomic level to the mesoscopic, the scale at which bulk material properties take over. For simple problems concerning single particles, he is able to carry out calculations on a desktop computer. But for arrays or groups of atoms or nanoparticles, or systems in which larger geometry has an effect—for example, he has studied how light interacts with metal films that are perforated with different kinds of nanoscale holes—he yokes together many desktop computers. "Computers, fortunately, have gotten cheap in recent years," he says. Or, when he needs thousands of processors operating in parallel, he signs up for a block of time at one of the national supercomputing centers.

In his Inaugural Article (1), Schatz reviews several of his approaches to modeling the optical properties of nanoengineered materials. In some situations, he uses the "top-down" strategy of classical electrodynamics, which treats materials as a continuum. In others, a "bottom-up" approach, modeling the behavior of individual particles, is the best. "Sometimes you miss crucial things," he says, "such as in materials fracture; the top-down theories really don't describe fracture in a meaningful way because they don't know about individual chemical bonds. So then you have to use a bottom-up theory, such as electronic structure, to correctly describe the breaking in the chemical bonds." Often, he finds it necessary to build an ad hoc model combining elements of both.

"Early on in your career, it's very important to be able to go off in many different directions and try things."

Schatz is grateful for the no-strings-attached grants he received early in his career, which he says gave him the freedom to pursue subjects that caught his interest. In 1980, the Alfred P. Sloan Foundation awarded him a fellowship; in 1981, the Camille and Henry Dreyfus Foundation gave him a Teacher–Scholar Award. "Early on in your career, it's very important to be able to go off in many different directions and try things," he says. "It's nice to have some flexible support." When he first began work in nanoscience, the field had no name, and no government agency was offering funding. Yet these two independent foundations saw promise in Schatz and his research, and their investment has certainly paid off.

Kaspar Mossman, *Science Writer*

1. Schatz GC (2007) *Proc Natl Acad Sci USA* 104:6885–6892.