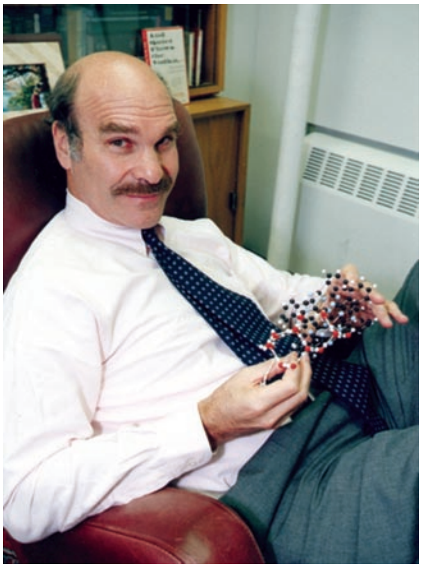
# Biography of Mark A. Ratner

Mark Ratner describes himself as a theoretical materials chemist. Arguably the youngest of the chemical sciences, materials chemistry is concerned with how chemical interactions control and determine the properties of materials. Throughout his career, Ratner has aimed to develop models to define a theoretical language for how the molecular structures of a material are manifested in its physical properties. His work has focused on several areas including charge transport (1, 2), ion transfer (3), nonlinear optical behavior (4), and quantum dynamics (5, 6). Electron-transfer reactions, so fundamental to life, underlie biological processes such as photosynthesis, cytochrome p450 reactions, and cellular respiration as well as materials processes such as electrochemistry and corrosion. "It's one of the most important reactions in chemistry, which is why I've spent 30 years on it and will spend the rest of my life on it," he said.

Born in Cleveland in 1942, Ratner graduated from Harvard University (Cambridge, MA) in 1964 with an undergraduate degree in chemistry. He obtained his Ph.D. in chemistry from Northwestern University (Evanston, IL), did postdoctoral work in Aarhus and Munich, and taught chemistry at New York University (New York) from 1970 until 1974. Later he served as a visiting professor with the National Sciences Research Council at Odense University (Odense, Denmark). Currently, Ratner is Morrison Professor of Chemistry at Northwestern University, where he served as department chair from 1988 until 1991 and as associate dean of the College of Arts and Sciences from 1980 until 1984. He was nominated to the National Academy of Sciences in 2002.

## Molecules as Electronic Devices

As Ratner tells it, one of his most important contributions to science came early in his career in 1974, when he and his graduate student Ari Aviram published a paper in *Chemical Physical Letters* in which they introduced the idea that molecules could act as electronic circuit components (7). The idea received little attention at the time but has since been recognized as a major contribution to the field of molecular electronics (8). This seminal paper suggested that single molecules can perform some functions of electronic devices. Aviram and Ratner proposed that if an electron-rich "donor" group



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and an electron-deficient "acceptor" group, spatially separated by a nonconjugated bridge, could be placed in a single molecule, the electronic asymmetry created would lead to an equivalent asymmetry in the electrical conduction through the molecule. That is, the molecule would act as a molecular rectifier. Importantly, these molecules could replace or perhaps complement semiconductors in electronic applications. Although not yet at the stage of commercialization, this approach has many advantages, and the trend is clear. The size of the molecules, between 1 and 100 nm, makes them cheaper, more efficient, and more precisely reproducible than the smallest possible silicon circuits (9).

## Israeli Connection

Throughout his career, Ratner has spent extended periods of time in Israel and has worked with many distinguished scientists, including Joshua Jortner and Abraham Nitzan from Tel Aviv University (Tel Aviv) and Raphael Levine, Robert Gerber, and Ronnie Kosloff from the Hebrew University of Jerusalem (Jerusalem). "Nitzan has influenced me more than any other scientist," Ratner said. "He has taught me how formal theory integrates with the real world; he is a master at that." In collaboration with Nitzan, Ratner has employed dynamic percolation theory to investigate the dynamics of molecular materials and charge transport and relaxation in materials systems (3, 10). Dynamic percolation theory is a relatively simple mathematical model of a disordered system that relates concentration of conductor sites within a theoretical lattice structure to the flow (or percolation) of charge, particularly ionic diffusion. Below a threshold concentration, or the percolation threshold, the substance is an insulator, and above that concentration it is a conductor. Over the past 10 years, Ratner and Nitzan have examined the properties both of electron transfer within molecules and electron transport in molecular wire junctions (11, 12). In such junctions, single molecules or small groups of molecules conduct electrical current between two electrodes. Because of the very small size of the structures, both the molecular electronic structure and the connection between the molecule and the electrodes strongly influence the current–voltage characteristics of the junction.

## Survival of the Fittest

Ratner's Inaugural Article (13), published in this issue of PNAS, tackles one of the most daunting challenges in computational chemistry: how to determine a protein's folded tertiary structure based on its primary amino acid sequence. A basic statistical calculation tells us that 20 amino acids can produce an astronomical number of sequences. Take any 2 of the 20 amino acids and you can produce 400 possible sequences; put 3 together, and you produce 8,000 sequences, and so on. The number quickly escalates, especially when you consider a peptide made up of hundreds or thousands of amino acids. Only a few of the possible structures actually exist in nature, but this calculation underscores the complexity of the problem.

Ratner and colleagues approach this sequence-to-structure problem by using an evolutionary algorithm computational method. Conventional approaches to the computation of protein structures include the solving of Newton's equations using molecular dynamics and the random sampling and selection of new geometries based on energy criteria using Monte Carlo methods. However, both of these approaches can fail to find energy minima, especially for structures that are dense and compact.

This is a Biography of a recently elected member of the National Academy of Sciences to accompany the member's Inaugural Article on page 7215.

With their approach, Ratner and colleagues select structures in a manner analogous to Darwinian natural selection. In the Darwinian process, populations compete for resources; the ones that survive and evolve are the ones that compete most successfully. Likewise, Ratner compares several candidate structures based on their energy, on analogies to other known structures, and on a combination of these two criteria. Much like Darwin's "survival of the fittest," the structures that best fit the criteria are favored for continuation in the next generation of computations. This evolutionary method is especially efficient for complex problems that are difficult to attack with conventional methods such as molecular dynamics and Monte Carlo simulations. By using this approach, Ratner's team was able to find several previously unknown stable structures for two peptides: unsolvated met-enkephalin (Tyr-Gly-Gly-Phe-Met) and Ac-(Ala-Gly-Gly)$_5$-Lys+H$^+$.

## Popular Science

Ratner, who is married and has two grown children, credits several people in addition to Nitzan with serving as role models. The most important of these, Ratner said, was his father, who came to the United States from Poland "with nothing" and demonstrated how to live a life of service to others. "He spent his time setting up schools to train people who didn't have job skills, chairing hospital and school boards, things like that," he said. Ratner points to his students and his faculty colleagues at Northwestern as his greatest inspirations and teachers. He credits his doctoral advisers, Sighart Fischer and Ludwig Hofacker, and his postdoctoral mentor, Jan Linderberg, for showing him how theory can be useful in understanding nature. In addition, he names several scientific heroes, including Rudolph Marcus, who won a Nobel Prize in chemistry for his work on chemical kinetics, and Josef Michl of the chemistry and biochemistry department at the University of Colorado (Boulder), a friend of 30 years and an unending source of ideas and imagination.

**Ratner identifies the area of artificial photosynthesis as crucially important.**

Another person whom Ratner credits with influencing him is scientist and science writer Roald Hoffmann, who won a Nobel Prize in chemistry for theories concerning the course of chemical reactions. Hoffmann, a professor at Cornell University (Ithaca, NY), writes poetry and books explaining chemistry to the general public. "It's his appreciation of the role of science in society and the way he conveys these concepts to the public that I find very important," Ratner said.

Ratner has written some popular books of his own, including two recent books he coauthored with his son, Daniel Ratner (executive vice president and chief technical officer of Driveitaway.com), that clarify aspects of the complex field of nanotechnology for the general public. In *Nanotechnology: A Gentle Introduction to the Next Big Idea* (14), Ratner and Ratner explain some of the many applications of nanotechnology. In one section they describe molecular motors, organic molecules combined with metal atoms, which are capable of moving molecules many times larger than the device itself. Such devices may one day be able to deliver drugs directly to cells. In their latest book, *New Weapons for New Wars: Nanotechnology and Homeland Security* (15), Ratner and Ratner describe ways in which nanotechnology-based sensors can be used to detect food, water, or air contaminated with biological weapons, as well as nanotechnology-based remediation technologies that could heal environmental damage ensuing from terrorism. On a more technical level, Ratner and his colleague George Schatz have written two textbooks on quantum mechanics in chemistry (16, 17).

Ratner says ultimately he would like to be able to design nanoscale self-assembled structures. "Right now, we can determine the structure of a molecule, but we don't know as much about how to design a molecule to have a certain structure," he said. In the area of electron transfer, Ratner identifies one major theme as crucially important: the process of artificial photosynthesis, or photovoltaics, with the ultimate goal of "trying to find a way to capture energy that is environmentally friendly and useful." According to Ratner, this type of work is usually done in a wonderfully intuitive fashion by brilliant people with strong intuitions. However, such "Edisonian approaches get us only so far," he said. "By developing appropriate theoretical models, I would like to make it a little bit less intuitive."

Emma Hitt, *Freelance Science Writer*


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