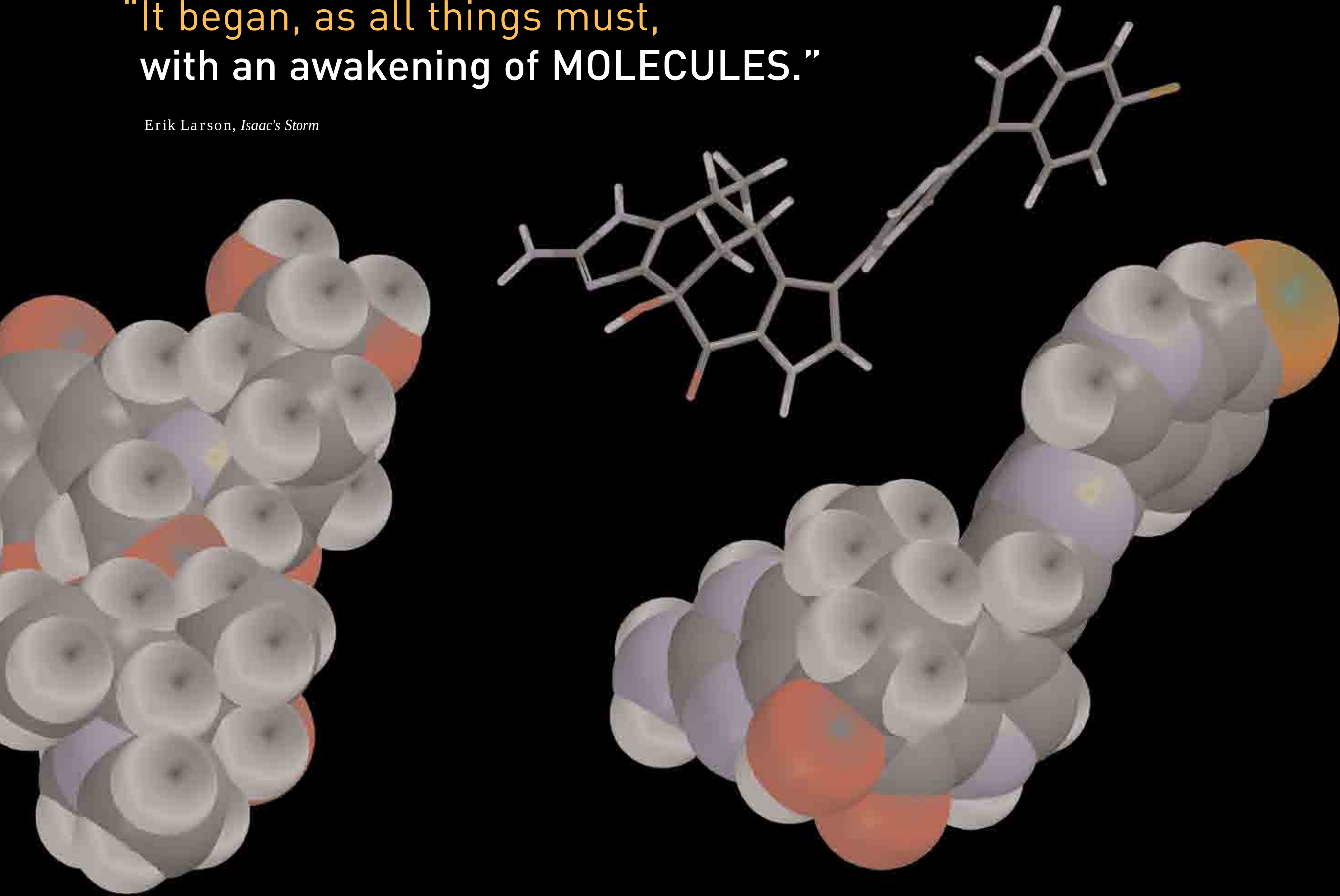
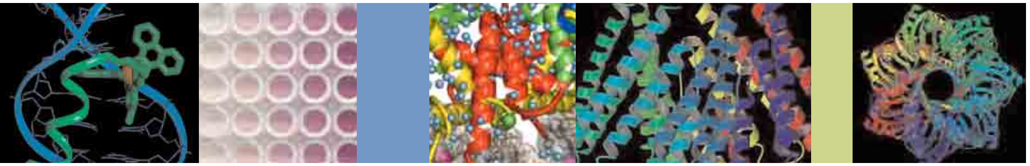
Division of Chemistry and Chemical Engineering
California Institute of Technology

"It began, as all things must, with an awakening of MOLECULES."

Erik Larson, *Isaac's Storm*



Chemistry...



is the science of change.

Chemists and chemical engineers seek not just to understand the world around us, but also to change it. In many ways, chemistry is the "central" science — intellectually positioned between physics and biology, and lying at the core of most modern technologies and health care advances. From the synthesis of new pharmaceuticals to the development of new technologies for energy conversion and environmental protection, the work of chemical scientists affects modern life in countless important ways.

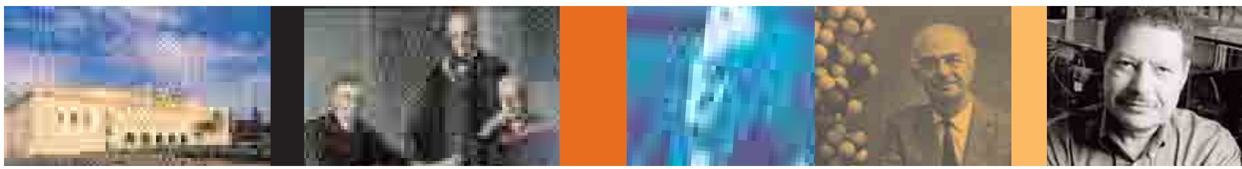
Chemists operate at the level of the molecule, and efforts to understand molecular structure, reactivity, and behavior are the foundation of the field. In addition, chemistry is an innately creative science: the overwhelming majority of known molecules are not found naturally, but were designed and synthesized by chemists.

Division of CHEMISTRY and CHEMICAL ENGINEERING

Chemistry has been an integral component of Institute research since 1921, when astronomer G. E. Hale, chemist A. A. Noyes, and physicist R. A. Millikan joined forces to launch the modern Caltech. In the 1930s, alumnus Linus Pauling (PhD '25) revolutionized the field with his insights into the nature of the chemical bond, work for which he won the Nobel Prize in 1954. Other Caltech alumni and faculty who have made outstanding contributions to the chemical sciences include Edwin McMillan (BS '28, MS '29; 1951 Nobel Prize for his discovery of element 93, neptunium); William Lipscomb (PhD '46; 1976 Nobel Prize for his studies on the structure of boranes); Rudolph Marcus (1992 Nobel Prize for his theory of electron transfer in chemical reactions); and Ahmed Zewail (1999 Nobel Prize for his study of chemical reactions on the femtosecond timescale).

Today, the Division of Chemistry and Chemical Engineering—one of Caltech's six academic divisions—comprises 37 faculty members, 14 of whom have been elected to the National Academy of Sciences or the National Academy of Engineering. In addition, 106 postdoctoral fellows, 255 graduate students, and 72 undergraduate students work and study within the division's varied teaching and research programs. The division offers undergraduate and graduate degrees in chemistry and chemical engineering. Graduate options (majors) in biochemistry and molecular biophysics, bioengineering, and environmental science and engineering are also offered jointly with other divisions.

Chemistry at Caltech emphasizes the design and synthesis of novel and significant molecules of varying shapes, sizes, and complexities; the determination of their three-dimensional structures; systematic explorations of their chemical reactivity; and a theoretical understanding of the fundamental principles underlying chemical bonding and reactivity. Some of the division's research programs are directed at the tailored synthesis of materials with novel optical, electrical, and magnetic properties

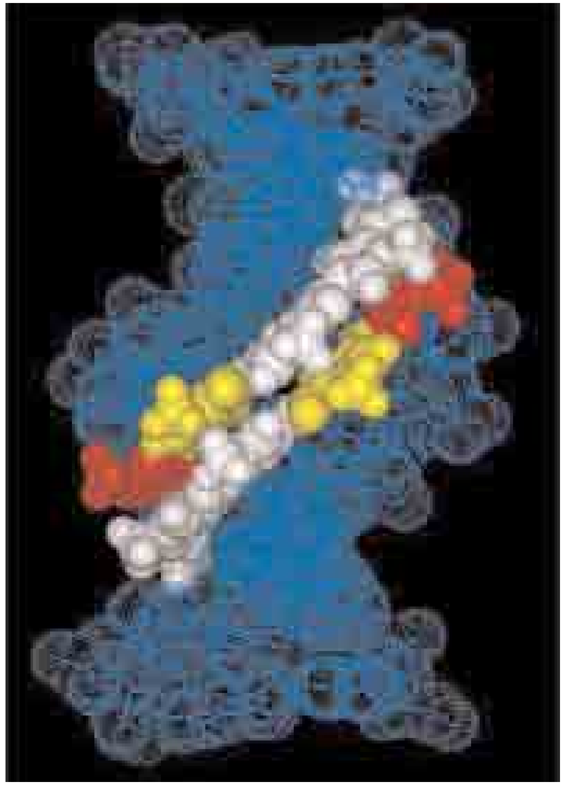


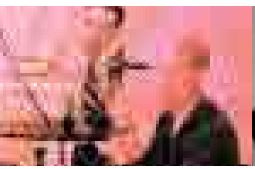
and of sophisticated organometallic compounds with unique catalytic capabilities. Many other programs are conducted at the interface of chemistry and biology, and focus on the molecules involved in life processes, particularly those that store and process genetic information and those that catalyze cellular reactions. Caltech chemists are also developing methods to study fundamental chemical processes with lasers and to visualize molecules on surfaces at near-atomic resolution, and are using supercomputers to examine the hierarchy of complex motions in large molecules and to predict the fate of molecular encounters.

In chemical engineering, pioneering research is being carried out in catalysis; in the flow of non-Newtonian fluids, suspensions, and polymers; in the chemistry and physics of the urban atmosphere; in the relationship between molecular and macroscopic properties of polymers; in the manufacture of ceramics and electronic materials; and in biotechnology and biochemical engineering.

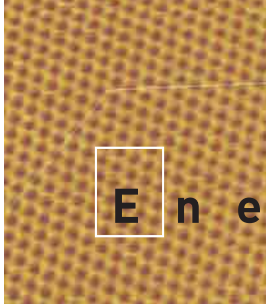
Caltech's practice of unifying the chemical sciences under one administrative umbrella greatly facilitates cooperation in both teaching and research, and fosters fruitful interactions among chemists and chemical engineers. The Institute's relatively small size also encourages cooperation, making it easy for chemical scientists to meet and form research partnerships with biologists, physicists, geologists, and engineers. This singularly collaborative environment has helped make the division's graduate programs some of America's best: both chemistry and chemical engineering consistently rank among the top five programs in the nation.

While continuing to focus on the molecular view of the physical world, the Division of Chemistry and Chemical Engineering has made special commitments to four research priorities: energy, the environment, the molecules of life, and advanced materials.





"The percentage of people at Caltech who do highly original work is, I think, unusually high. It's a small faculty...and there's a certain beauty in relatively small groups thinking in as original a fashion as they can."
— Rudy Marcus



Energy

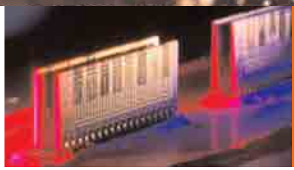
The United Nations projects that by 2050, meeting global energy demands in a sustainable manner will require not only increased energy efficiency and new ways of using existing carbon-based fuels, but also a staggering amount of carbon-free power. One of the chemical sciences' grand challenges is efficiently and economically interconverting the abundant and useful forms of energy: solar, chemical, and electric.

Caltech has a strong tradition of energy-conversion research. Significant advances in the field include explaining the principles of electron flow in photosynthetic reaction membranes, demonstrating the possibility of light-driving multielectron transfer reactions, and achieving record efficiencies in photovoltaic and photoelectrochemical devices. Institute research has also shed light on energy conversion using semiconducting electrodes, and on the catalysis of multielectron transfer processes that enable the energy-efficient formation of fuels from sunlight. Elucidating electron and ion transport mechanisms has enabled Caltech to lead the field in efficient fuel-to-electricity conversion using novel fuel cell materials and structures.

But many of the most fundamental questions in the field remain unanswered. While biological systems readily perform multielectron transfer processes in fuel-forming reactions, no man-made system can even approximate their performance. Similarly, although hydrogenase enzymes evolve hydrogen from water under essentially equilibrium conditions, no comparable electrocatalysts for either fuel or electricity production are on the horizon. The principles of electron transfer rates developed theoretically by Caltech chemist Rudy Marcus have been applied to a broad range of biological and chemical systems, and can help to unravel the mechanisms of photosynthesis in biological systems and to develop new paradigms for energy conversion in inorganic analogs.

Finding an efficient energy cycle with solar energy as input and chemical fuels and electricity as outputs will require research that is inherently interdisciplinary. This research will involve inorganic chemistry, solid-state chemistry, materials chemistry, electrochemistry, chemical engineering, organic chemistry, and biochemistry, as well as homogeneous and interfacial chemistry at solids, liquids, and their boundaries. The coming decade presents the opportunity to launch such a chemistry-centered, interdisciplinary effort—one that will place Caltech at the forefront of the field and ultimately provide a scalable, sustainable energy stream.

right: *a photoelectrochemical cell used to study storage of solar energy in a chemical fuel. Here, hydrogen gas is produced by shining light on the surface of solid silicon immersed in hydrochloric acid.*



Environment

The division's studies of the earth's environment focus on the chemistry of our atmosphere. Atmospheric changes, whether caused by natural phenomena or human actions, influence the biology of the planet—either directly, by changing the composition of the atmosphere, or indirectly, by changing the climate and the biosphere.

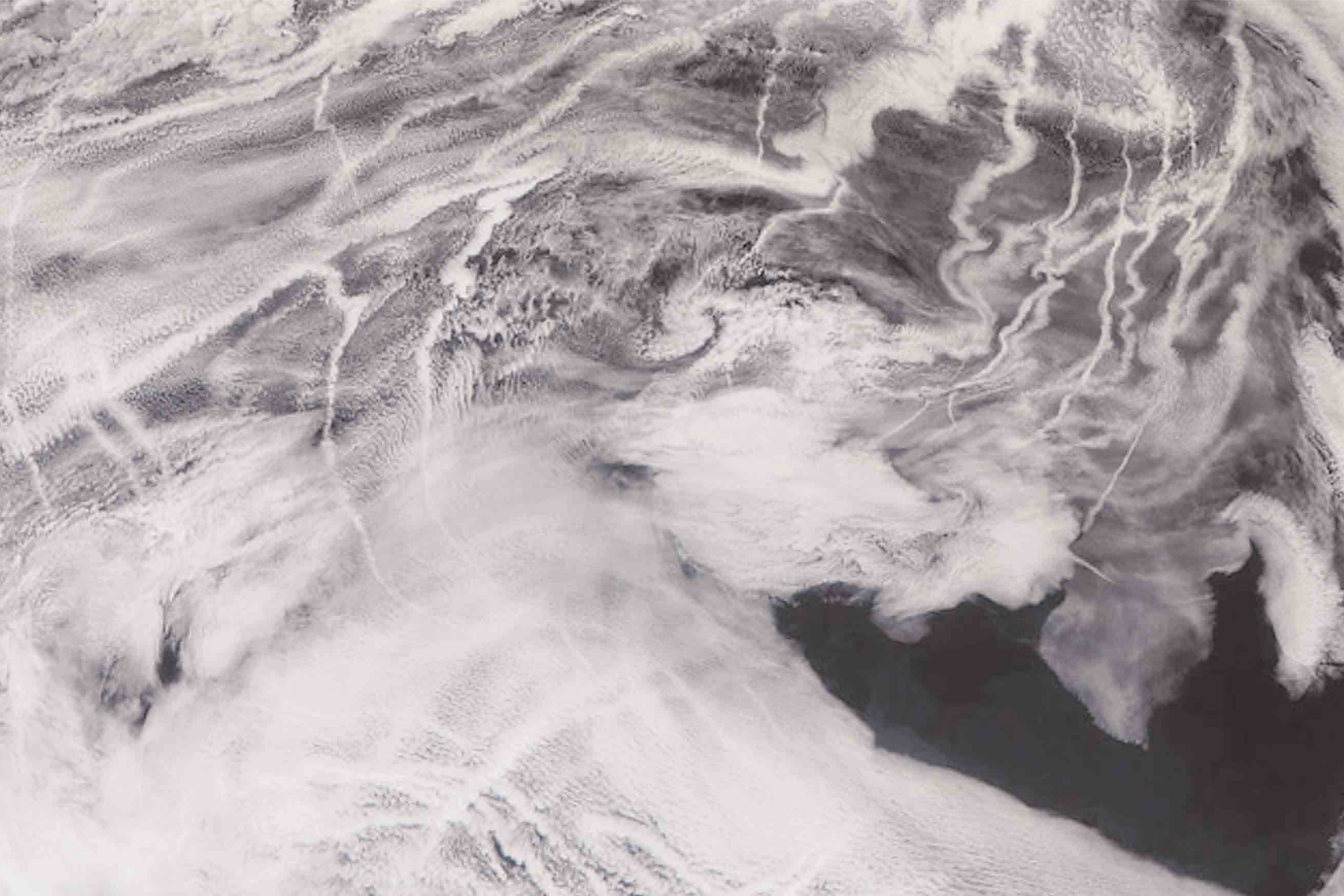
Caltech chemical scientists, along with their colleagues in the Divisions of Engineering and Applied Science and Geological and Planetary Sciences, are tackling environmental problems head-on, using a combination of laboratory studies, atmospheric measurements, and theoretical simulations. Understanding how atmospheric radiative, dynamical, and chemical processes interact is an essential step in predicting how the earth's climate will evolve in the decades to come.

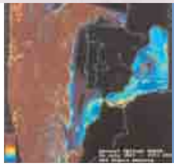
Human-induced changes in the earth's atmosphere are chemical in nature, and influence the earth at all scales, from the urban to the global. The atmosphere's detergent is the hydroxyl (OH) radical, which is formed largely from ozone and water vapor. Changes in OH concentrations, due to human emissions of methane and carbon monoxide, affect the ability of the atmosphere to cleanse itself. Scientists in the division are studying the chemistry of the atmosphere, especially the production and destruction of ozone. Paradoxically, ozone in the stratosphere is essential for human life because it limits the penetration of the sun's harmful ultraviolet radiation, whereas elevated ozone concentrations at ground level are a detriment to human health.

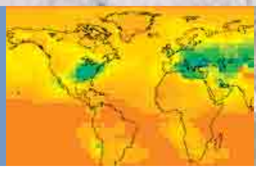
Aerosols—particles in the air—affect the earth's climate in complex ways. Sulfur-containing particles tend to reflect sunlight back to space and cool the earth, while soot-containing particles absorb sunlight and heat the atmosphere. Caltech scientists are studying how atmospheric particles form, especially from hydrocarbon oxidation, and how they evolve in the atmosphere. Faculty in the division have discovered, for example, that nanometer-scale particles in the atmosphere serve as microscopic reactors for organic polymerization reactions.

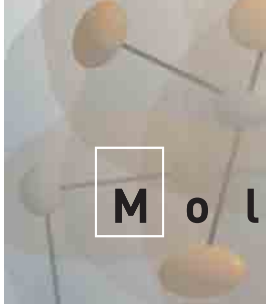
Caltech investigators use a variety of research aircraft to take atmospheric measurements from the lowest 100 meters of the troposphere to high in the stratosphere. Airborne measurements carried out in 2001 off the coast of China established the physical, chemical, and optical properties of Asian dust and pollution, one of the largest sources of particles on Earth.

right: *"ship tracks"—one example of how humans change the environment through burning fossil fuels. Although ships are not significant sources of pollution themselves, their smokestacks do release enough sulfur dioxide to modify overlying clouds.*









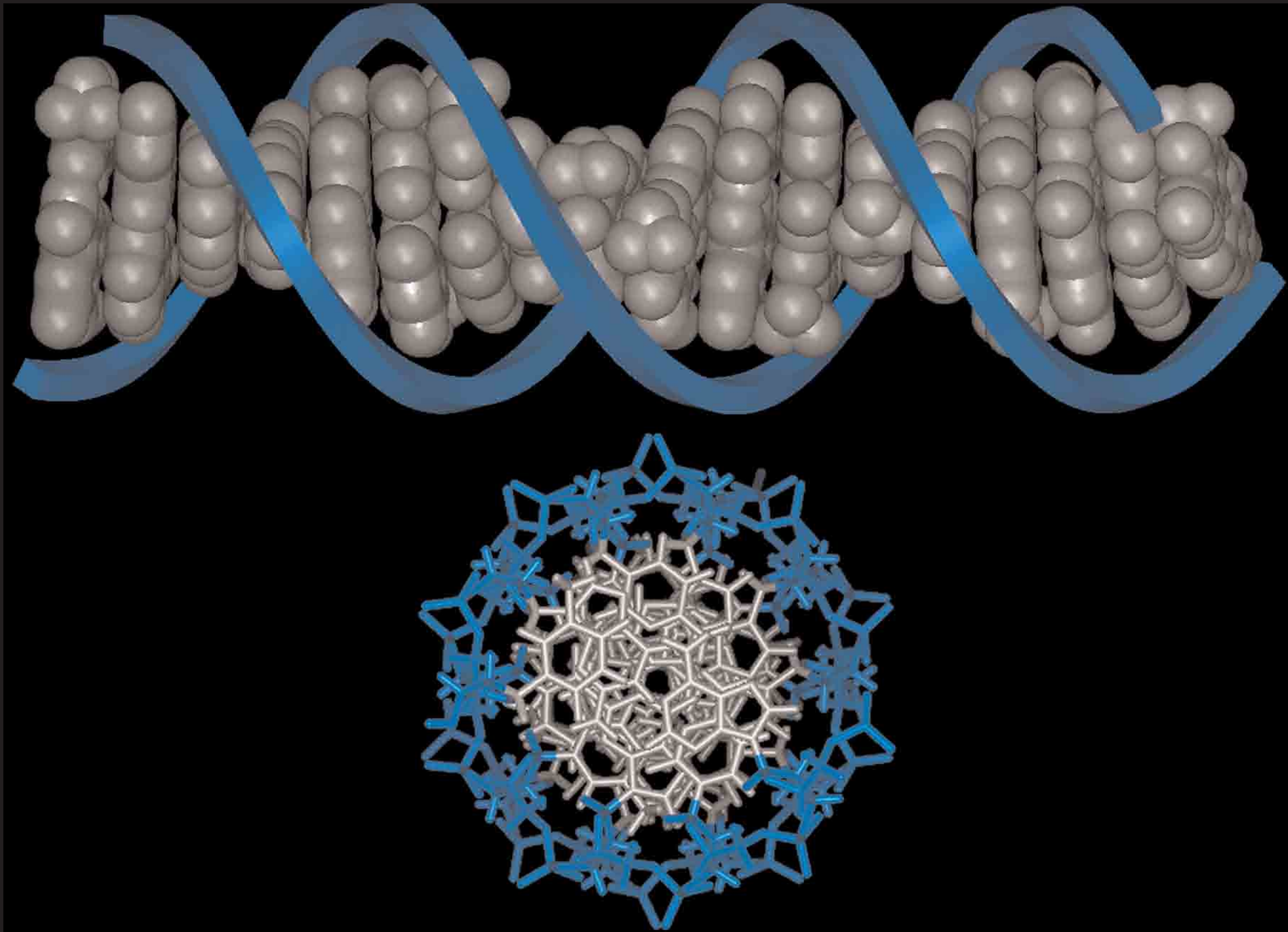
Molecules of Life

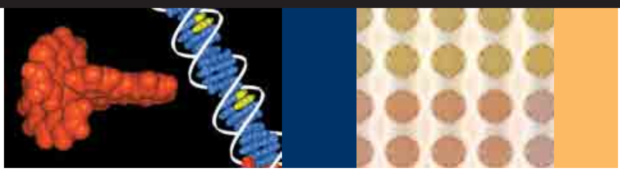
Cells are the basic building blocks of life. Understanding living systems requires understanding the structures and functions of cells' molecular components—the biomolecules that enable memory and thought, regulate genetic development, produce energy from sunlight, metabolize useful substances, and degrade toxins. These biomolecular "machines" offer both substantial challenges and tremendous opportunities for chemists.

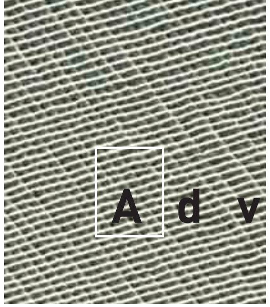
Since biomolecules are the targets of drugs, both beneficial and harmful, the design and development of new pharmaceuticals is very much a chemical undertaking. Another important theme in 21st-century chemical science is understanding systems "beyond the molecule," where assemblies of biomolecules function as a unit to create, process, and store information.

Caltech chemists are providing ever more precise insights into the biochemical processes of all the major classes of biomolecules—proteins, nucleic acids, carbohydrates, and lipids. Several research groups within the division design small molecules that interact with DNA with high chemical specificity, offering new ways to regulate gene expression and new insights into the electronic properties of DNA. Carbohydrates are important regulatory molecules, and chemical methods of synthesis and analysis are being developed to probe the ways in which sugars modulate important biological processes. X-ray crystallography and advanced spectroscopic tools are used to determine the structures of complex proteins, the central action molecules of life. In addition, selection methods and directed molecular evolution are being used to produce new proteins with desirable properties.

right: *two illustrations of double helical DNA, in which the gray spheres represent the stacked base pairs and the blue ribbon is the sugar phosphate backbone. The bottom figure is a view of the DNA duplex down the helix axis.*







Advanced Materials

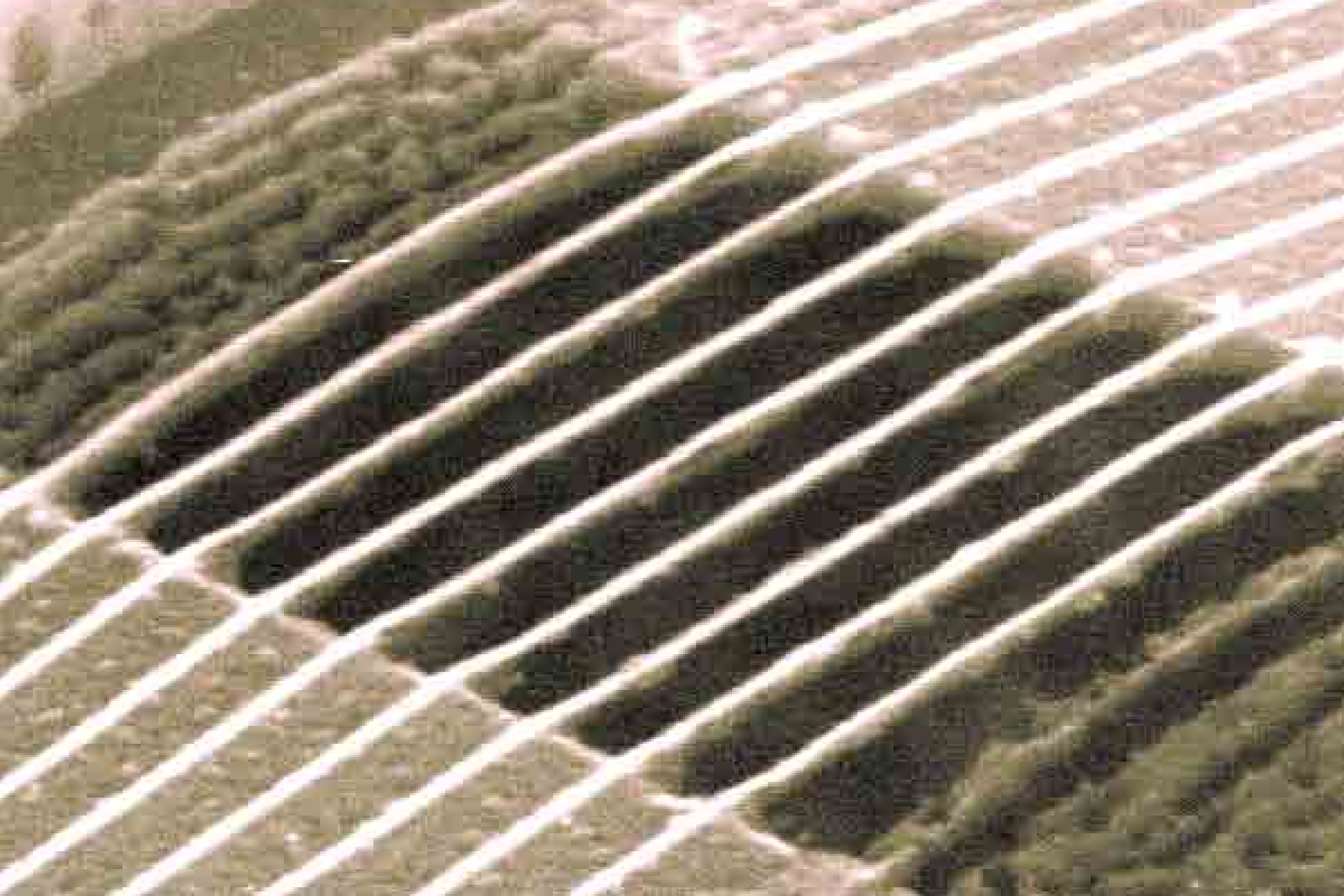
Most of our modern technologies have arisen from an understanding of the very small (atoms and small molecules) or the very large (ordered solids). In fact, the development of a quantitative picture of these two extreme forms of matter was a triumph of 20th-century science. Materials chemistry at Caltech is aiming for a similar level of understanding of "mid-sized" matter—supramolecular complexes, proteins, synthetic and natural polymers, organic/inorganic composites, and nanostructured inorganic materials.

The long-chain character of macromolecular substances allows them to perform an astonishing array of tasks, from holding together high-speed aircraft to carrying genetic information. Such diverse functions require strikingly different molecular architectures. In order to develop new materials and processes, chemists must be able to design and predict the structures, properties, and behavior of macromolecules before experimentation begins.

Molecular materials synthesis at Caltech is highly crossdisciplinary. It draws from fields not traditionally associated with materials, with biology providing much of the inspiration. Some materials chemists are developing novel approaches to directed evolution for creating new, non-naturally occurring enzymes; others are focused on harnessing the machinery of microbial cells to construct atomically precise biopolymers. Still others are designing organometallic catalysts for building new classes of organic polymer materials with remarkable definition of their molecular structures, or are preparing new inorganic mesostructured catalyst materials. In all cases, the goal is to develop new molecular materials with specific applications, among them artificial tissues, thermally stable biocatalysts, mechanical materials, and chemical sensors.

As materials chemistry focuses more and more on the molecular world, new challenges arise. There is a growing need to develop both characterization tools and theoretical models that can give real insight into structural, dynamical, and physical properties of advanced materials molecules. These resources will support projects like the investigation of electron transport in DNA (work that builds upon the Institute's strong tradition of theoretical and experimental work on electron transfer reactions), as well as efforts to characterize the fundamentals of charge transport across organic/inorganic interfaces, to construct molecular electronics circuitry from supramolecular components, and to perform statistical and quantum modeling of the physical and chemical characteristics of molecular materials. These exciting research initiatives place Caltech's Division of Chemistry and Chemical Engineering at the forefront of 21st-century materials science.

right: *a high-frequency nanomechanical resonator made of suspended platinum wires 20 nanometers in diameter. To build the structure, wires were deposited onto precisely grown material and then transferred as an ink onto the substrate—a unique process developed at Caltech.*



"If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generations of creatures, what statement would contain the most information in the fewest words? I believe it is the atomic hypothesis (or the atomic fact, or whatever you wish to call it) that all things are made of atoms—little particles that move around in perpetual motion, attracting each other when they are little distance apart, but repelling upon being squeezed into one another. In that one sentence, you will see, there is an enormous amount of information about the world, if just a little imagination and thinking are applied."

— Richard P. Feynman, from *The Feynman Lectures on Physics: Mainly Mechanics, Radiation, and Heat,* by Richard P. Feynman, Robert P. Leighton, and Matthew Sands (1963).

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Front cover: lemonomycin (left) and dragmacidin F, complex alkaloids that may help address two major health problems of the 21st century. Dragmacidin F is an anti-HIV substance; lemonomycin is a powerful antibiotic against methicillin- and vancomycin-resistant bacteria strains.

Image credits: Arnold Lab—Claudia Schmidt-Dannert, Daisuke Umeno, Matthew Peters (p. 1); Barton Lab (pp. 1, 9); Mark E. Davis (p. 11); Peter B. Dervan (pp. 1, 3); Dougherty Lab (p. 12); James R. Heath (pp. 10, 11); Nathan S. Lewis (pp. 4, 5,11); Douglas C. Rees (p. 1); Brian M. Stoltz (cover, p. 8, insert); visibleearth.nasa.gov (pp. 6, 7)

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"One of the most difficult things to do in science is to ask the right question. You can find people with thousands of questions about the next experiment, or the next observation; but to really ask the right question—that's an art." — Ahmed Zewail there's only **one.caltech**

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