



GERARD 't HOOFT (LEFT) AND MARTINUS VELTMAN at a University of Utrecht reception 14 October. (Photo taken by C. de Laat, University of Utrecht, © C. de Laat.)

anomaly," explains 't Hooft. "You have to be much more careful monitoring which diagrams have anomalies, and if there are any, making sure that they cancel out in an appropriate way. If they don't, the theory will not renormalize. Shortly afterwards, crucial papers on this issue were published by William Bardeen, and by Claude Bouchiat, Iliopoulos, and Philippe Meyer."

In 1972, 't Hooft and Veltman published their results,⁴ and the particle theory community took off like a rocket. That same year, the Science Citation Index, which had had only a handful of references to Weinberg's paper before that year, had 64 citations. His paper later became the most cited paper in the history of particle physics.

With dimensional regularization established, theorists could apply it not only to the electroweak interactions, but also to the strong interactions, says 't Hooft. "The constraints that were quite clear from our work were so rigid that people knew exactly how to make models, not only that of Weinberg and Salam, but also several alternative models. Then it was up to experiments to figure out which one was correct. So, by putting the theory on a firmer mathematical foundation, we had identified the correct set of possible theories."

In 1970, Glashow, Iliopoulos, and Luciano Maiani had extended the gauge theory to involve quarks as well as leptons, and they found that such an extension would require the existence of a fourth quark (the charmed quark) and the existence of neutral currents. The neutral currents of this gauge theory would con-

serve strangeness. Such neutral currents were found in 1973. Then, in 1983, the W and Z particles were discovered at CERN.

The Swedish academy stresses that even though the electroweak theory predicted the existence of the W and Z particles from the start, "it was only through 't Hooft's and Veltman's work that more precise prediction of physical quantities involving properties of W and Z could start." CERN's Large Electron Positron collider has made large quantities of W and Z particles, and comparisons between measurements and calculations have shown "great agreement, thus supporting the theory's predictions," the academy says.

Nobel Prize Goes to Zewail for Developing Femtochemistry

The 1999 Nobel Prize in Chemistry has been awarded to Ahmed Zewail, "for his studies of the transition states of chemical reactions using femtosecond spectroscopy." Zewail is the Linus Pauling Professor of Chemistry at Caltech. "I'm also a professor in the physics department," he wants our readers to know.

By the mid-1980s, the development of ultrafast pulsed laser technology was making available light pulses briefer than 10 femtoseconds. (1 fs = 10^{-15} s.) Tens of femtoseconds is the typical vibration period for molecules, and it's the timescale for making and breaking molecular bonds. Zewail's Caltech group has played a pioneering role in the development of "femtochemistry," the exploitation of

The academy singles out the prediction of the top quark's mass. About 1977, Veltman had shown that the radiative correction to a certain combination of the W and Z masses and the weak mixing angle is sensitive to the square of the top quark mass. As measurements of the W and Z masses and the weak mixing angle were improved, a precise prediction for the top mass became possible—about 180 GeV. That value is consistent with the Fermilab experimental observation of the top quark (see PHYSICS TODAY, May 1995, page 17).

Biographies

Gerard 't Hooft was born in 1946 in the Netherlands and earned his PhD in 1972 at the University of Utrecht. He has been a professor of physics there since 1977.

Martinus Veltman, born in 1931 in the Netherlands, earned his PhD in 1963 at the University of Utrecht. He had gone to CERN in 1961, where he remained until he became a professor of physics at the University of Utrecht in 1966. He became John D. and Catherine T. MacArthur Professor of Physics at the University of Michigan in 1981, where he remained until his retirement in 1997. He now lives in Bilthoven, near Utrecht.

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Femtosecond pulsed lasers have made it possible to catch molecules in the bonding act.

femtosecond laser pulses to resolve the temporal details of molecular bond formation and rearrangement.¹ "It lets us watch the fundamental chemical act as it's happening," Zewail told us. (See the article by Zewail and Martin Gruebele in PHYSICS TODAY, May 1990, page 20.)

Zewail was born in Egypt, near Alexandria. After getting his MS in chemistry at the University of Alexandria in 1969, he came to the US and received his PhD in chemistry at the University of Pennsylvania in 1974. His thesis research, directed by

Robin Hochstrasser, was in solid state spectroscopy. For the next two years, Zewail was an IBM fellow at the University of California, Berkeley, doing optical detection of magnetic resonances with Charles Harris in the chemistry department. He joined the Caltech chemistry faculty in 1976.

Molecular beams

At Caltech, Zewail at first did experiments on gases, liquids, and solids, using nanosecond and picosecond laser pulses. "Then in 1979, even before we had femtosecond lasers, we made the transition to molecular beams," he told us. Molecular beam techniques became crucial to the evolution of femtochemistry in Zewail's laboratory. In the widely used "supersonic expansion" technique for producing the very cold molecular beams one wants, a high-density gas of reactant and carrier molecules is made to expand into a vacuum through a narrow nozzle. After subsequent collimation, one can get a beam with an effective temperature (in its rest frame) of only a few kelvin.

That's important for a number of reasons. At low temperature, few molecules occupy the excited vibrational and rotational states that plague molecular spectroscopy. Extraneous collisions are kept to a minimum. And—particularly important for the femtosecond study of molecular collisions—at these very low temperatures one has, at the start, loosely bound "van der Waals complexes" of the molecules whose interactions one seeks to investigate.

In 1982, Charles Shank and colleagues at Bell Labs demonstrated 30 fs light pulses. They accomplished that by using optical fibers and a diffraction grating to chirp and compress the 90 fs output of a mode-locked colliding-pulse ring dye laser. (See *PHYSICS TODAY*, December 1982, page 19.) By 1984, Erich Ippen's group at MIT, using similar techniques, was producing 16 fs laser pulses and, a year later, Shank's group got down to 8 fs. (That's only about five oscillations of the electromagnetic field in the visible.) And one could tune the wavelength of these femtosecond pulses all the way from the infrared to the ultraviolet.²

"Not long after that, we built our own colliding-pulse dye laser, following Shank's design," Zewail told us. "Nowadays you can buy an all-solid-state femtosecond laser off the shelf. That has made it possible for groups all over the world to apply femtochemistry to an incredible variety of systems—including biology and surface catalysis."



AHMED ZEWAIL

In pre-femtosecond days, molecular beams for the study of chemical reactions generally involved a pair of crossed beams, each carrying one of the species to be collided. "We couldn't resolve the molecular collisions on the relevant timescale," explains Dudley Herschbach (Harvard), "but we got a lot of information about the reactions by looking at the angular and velocity distributions, and the excitation states, of the reaction products long after they had departed the scene." For their work with crossed molecular beams, Herschbach and Yuan Lee shared the 1986 chemistry Nobel Prize (with John Polanyi).

"But we use only single beams in our femtochemistry experiments," explains Zewail. "The relatively slow crossing of colliding beams would smear out the specification of the initial time far too much." Instead, the Caltech group defines the initial time t_0 for the process under study by an intense femtosecond "pump" pulse directed at the single molecular beam. The pump pulse is followed, after a well-defined time interval Δt , by a weaker "probe" pulse designed to see where matters stand at $t_0 + \Delta t$.

Watching the chemical act

If one is simply studying the photodissociation or isomerization of single molecules, one chooses a pump-pulse wavelength that will raise the molecule to the excited state from which it will break apart or rearrange itself. But studying the time evolution of a reaction initiated by a collision between two different molecules in a single beam necessitates a trick to specify t_0 , the collision energy, and the impact parameter.

That's where the van der Waals complexes formed in the supersonic expansion come in. For example, when the Caltech group in 1987

wanted to study the reaction $\text{H} + \text{CO}_2 \rightarrow \text{CO} + \text{OH}$, an important process in the upper atmosphere, they formed a beam containing hydrogen iodide as well as CO_2 . At sufficiently low temperature and high density, the weak van der Waals forces between these molecules create HI-CO_2 "precursor molecules." The experimenters initiated the $\text{H} + \text{CO}_2$ process by a pump pulse at a wavelength that renders the strong bond between H and I repulsive, making them fly apart in close proximity to the CO_2 . The kinematics of the reaction under study are determined—but also limited—by the energy of the pumping photon and the known configuration of the van der Waals complex that holds the reactants together at the start.

To define, with sufficient accuracy, the time intervals between the pump pulse and the sequence of probe pulses that follow, one has to start with a single laser pulse. This initiating pulse can be split into pump and probe components, the latter being delayed by detours through longer optical paths. (A 100 fs delay requires a detour of about 30 microns.) Non-linear optical elements can alter the wavelength of the probe pulse. Probe-pulse wavelengths can be chosen to detect the fleeting presence of some transitional state that will not survive the completed reaction. In the $\text{H} + \text{CO}_2$ experiment, for example, Zewail and company were able to determine³ that the reaction proceeds by way of a relatively long-lived transitional HOCO molecular state that lasts for about 1000 fs.

Potential-energy surfaces

The principal theoretical construct for the description of chemical processes is the molecular potential-energy surface. There's an important symbiosis between the theoretical calculations of these surfaces and their empirical investigation by femtochemistry and other experimental means. In the spirit of the Born-Oppenheimer approximation, theorists separate the rapid motion of the molecular electron clouds from the lumbering response of the nuclei. "Clamping" the nuclei of a molecular system in fixed positions, they solve the Schrödinger equation for the resulting electronic energy states. Repeating this calculation for many different positions of the nuclei, they arrive at potential-energy surfaces over the nuclear configuration space for the electronic ground state and for higher states excited by a collision or the absorption of a photon.

The deep wells, saddle points, hills, and valleys of these potential

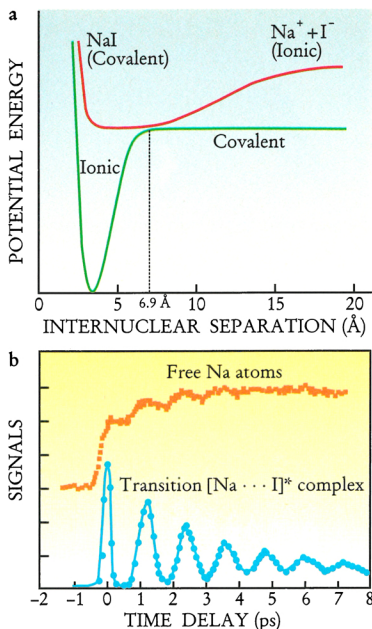
surfaces dictate the confinement or departure of the nuclei, and thus the outcome of the chemical process. For his development of computational techniques that greatly facilitate the calculation of molecular potential-energy surfaces, Northwestern University theorist John Pople shared last year's chemistry Nobel Prize. (See PHYSICS TODAY, December 1998, page 20.)

When the potential energy of a diatomic molecule, at a given electronic excitation level, depends only on the distance between the two nuclei, the potential-energy surfaces are simply curves, as we see in the figure at right. For NaI, a prototypical alkali halide molecule, the figure shows the theoretically calculated ground-state potential curve, with a deep ionic-bonding well at an equilibrium nuclear separation of 2.8 Å, and a nearby excited-state potential curve with a broad, shallow well.

In a 1988 experiment,³ Zewail and coworkers gave a striking demonstration of how femtochemistry can elucidate the dynamics of such a fundamental molecular system. The two NaI potential energy curves come very close to each other when the nuclei are 6.9 Å apart. At this point there's a bonding role reversal, as is often the case at such "avoided crossings": The strong ground-state bond, which is ionic at small separations, becomes covalent, and thus weaker, at separations beyond 6.9 Å. Conversely, the short-distance covalent bond of the excited state becomes ionic, and thus stronger, beyond 6.9 Å. This long-distance creation of an ionic bond in the excited state has been described as harpooning the iodine atom from afar with the sodium atom's valence electron.

The Caltech group's experiment began with a pump pulse that raised NaI molecules in the beam to the excited state. That was followed, at 50 fs intervals for the next 10 ps, by probe pulses at wavelengths chosen to reveal the creation of free Na atoms and of a putative short-lived transition complex of bonding and antibonding states, denoted $[\text{Na} \cdots \text{I}]^*$. The experimental results, shown in part b of the figure, exhibit a remarkably clear and persistent oscillation, with a period of 1.25 ps. The upper data curve signals the liberation of Na atoms, while the lower curve signals the fleeting appearance of the elusive transition complex.

The 1.25 ps periodicity manifests the oscillation period of the NaI molecule in the excited state's broad potential well. Every time the separation approached the 6.9 Å avoided-crossing point, the $[\text{Na} \cdots \text{I}]^*$ transition state would form, and there was a



MOLECULAR DYNAMICS of NaI at femtosecond resolution.³ (a) Potential energy curves for the ground state (green curve) and the experiment's excited state (red) come very close to each other at 6.9 Å and trade bonding characteristics. (b) Probe laser pulses at 50 fs intervals detect 1.25 ps oscillations in the population of liberated Na atoms (orange data points) and a short-lived transition complex (blue).

roughly 10% chance that the molecule would jump down to the covalent branch of the ground-state curve and thus finally dissociate.

But—if the experimental signal is a sum over millions of independent molecules—why don't the oscillations wash out? The answer is that, in such

a femtochemistry experiment, the pump pulse catches all the ground-state molecules at once, all of them very close to the equilibrium 2.8 Å separation at the bottom of the deep potential well. Thus they all start to oscillate in the excited well almost in lockstep, giving us an unprecedented "movie," with angstrom resolution, of a prototypical molecular disintegration in progress.

Femtosecond diffraction

"Now we're looking at biological systems and other very complex processes," Zewail told us, "and we're hoping to apply electron diffraction techniques on a femtosecond scale. Kent Wilson's [University of California, San Diego] group has recently managed to do lattice-dynamics diffraction experiments with picosecond x-ray pulses."⁴ As these diffraction techniques evolve, they should make possible the structural study of crystals and complex molecules on the timescale of their formation.

"Again and again, Zewail's group has shown us how much one can learn by resolving the dynamics of chemical systems on femtosecond scales," says Herschbach. "This inspirational impact is an important aspect of Zewail's contribution."

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A New Way to Guide Light in Optical Fibers

Many of our phone conversations and e-mail communications race to their destinations over optical communication links that rely on total internal reflection to guide pulses of light down hair-width fibers of glass. Despite their prodigious bandwidth, these glass fibers will be hard pressed to meet the heavy traffic demands being placed on them by the exploding use of the Internet. Recently, researchers from the US and UK have demonstrated another way to transmit light waves through narrow channels: By surrounding a hollow core with photonic bandgap structure.¹ Their achievement opens the way for guiding light with little or no loss through an evacuated channel.

A novel form of fiber optics, featuring a hollow core rather than one made of glass, holds promise for communications systems or other applications.

That's important because the interaction of light with glass now limits the maximum power that one can transmit with today's glass-core fibers. It's not possible to have hollow cores with fibers that rely on total internal reflection because the core must have a larger index of refraction than the cladding, and there's no solid material that has an index of refraction less than one.

The recent demonstration is thus