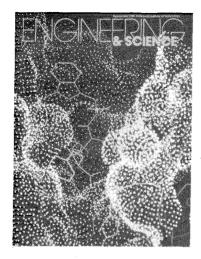
## In This Issue



## On the Surface

On the cover — an inhibitor (yellow) binds to the active site of the enzyme thermolysin in a computer simulation. The blue dots represent the enzyme's surface as seen by the solvent (water), and the yellow tetrahedron at center right is a zinc atom. Thermolysin is a model for an enzyme that could be blocked by drugs to control hypertension, and the CLT inhibitor, as just such a drug (another view is on page 2), should bind tightly to the cleft in the enzyme's surface.

William Goddard and Barry Olafson predicted the optimum structure of this inhibitor theoretically; experiment has shown them correct. With high-speed computer techniques, theoretical chemists can calculate the forces on all the 3,500 atoms of a molecule like thermolysin in solution and predict optimum structures of molecules to bind to it. As Goddard explains in "Theoretical Chemistry Comes Alive," these new techniques have brought theory into its own in helping to understand how and why chemical processes work and in developing new materials with desired properties. He enthusiastically predicts a



revolution in what has been considered an empirical science.

His article. which begins on page 2, was adapted from Goddard's

Seminar Day talk last May, in which theoretical chemistry did indeed "come alive" for his alumni audience. Goddard is also a Caltech alumnus, having received his PhD in engineering science (with a minor in physics) in 1965. (His BS in engineering is from UCLA.) Although he did graduate work here with Pol Duwez in materials science, his interests were already turning to theory, and he became a research fellow in chemistry in 1964. Appointed assistant professor of theoretical chemistry in 1967, he became full professor in 1975.

During the 1970s Goddard's research began to concentrate on the properties of semiconductor and metal surfaces, and since 1978 he has been professor of chemistry and applied physics. Last year he was named to the first Charles and Mary Ferkel Chair in Chemistry and Applied Physics.

## On Semantics

When Jean Weigle died in 1968, some of his friends established a memorial fund to bring lecturers of outstanding talent to Caltech's biology division. They hoped "to preserve the nearly extinct species of the scientist who is indifferent to the organizational aspects of science and is wholly devoted to the beauty of the scientific endeavor as a way of life." (E&S, January 1969)

The 1985 Jean Weigle Memorial Lecture was given last May by Gunther Stent. Before delivering his talk on "Meaning

in Art and Science," Stent reminisced about the late 1940s at Caltech, when he was a research fellow, and Weigle, a physicistturned-biologist, had just arrived. Both worked with Max Delbrück, another physicistturned-biologist, in the "nascent discipline, which, a few years later, came to be styled 'molecular biology."



Before coming to Caltech in 1948 in the exciting years of Delbrück's Phage Group, Stent received his PhD in physical chemistry from the

University of Illinois (BS 1945). He left in 1950 for UC Berkeley. where he has been professor of molecular biology since 1959 and chairman of molecular biology and director of the virus

laboratory since 1980.

Stent's article, which begins on page 9, was originally written for a Nobel Symposium, and it is reprinted here with permission of the Royal Swedish Academy of Sciences. It reflects his current thoughts in a debate about the relationship of art and science that has been running since his first article on the subject in 1972. Stent has also edited Delbrück's Mind From Matter? lectures, which Delbrück gave in the last years of his life, and which will appear in October as a book published by Blackwell Scientific Publications. Inc. E&S will print a chapter from the book in November.

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