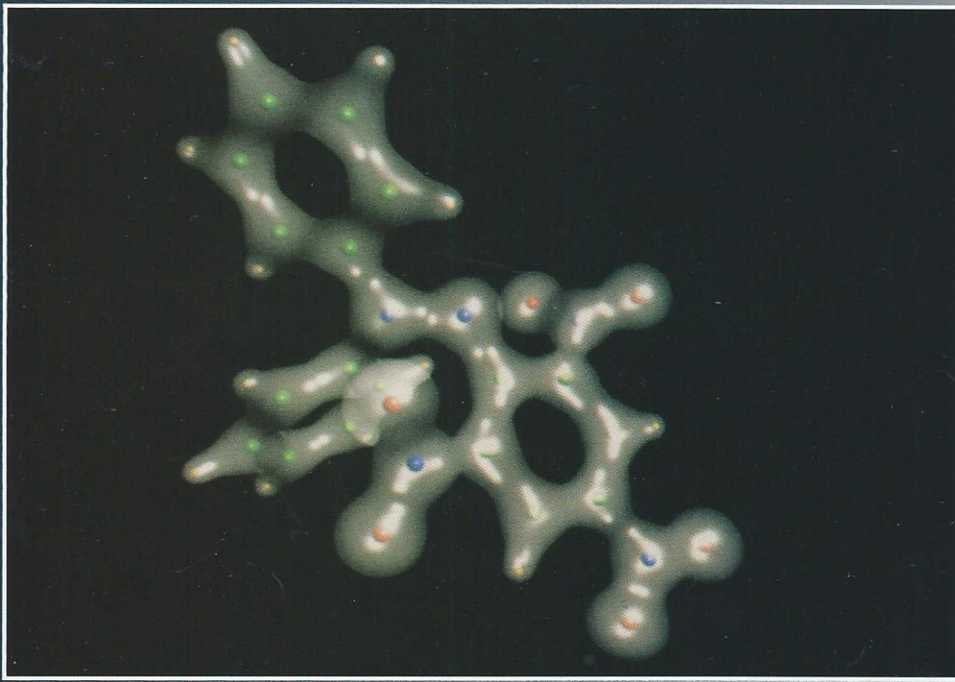
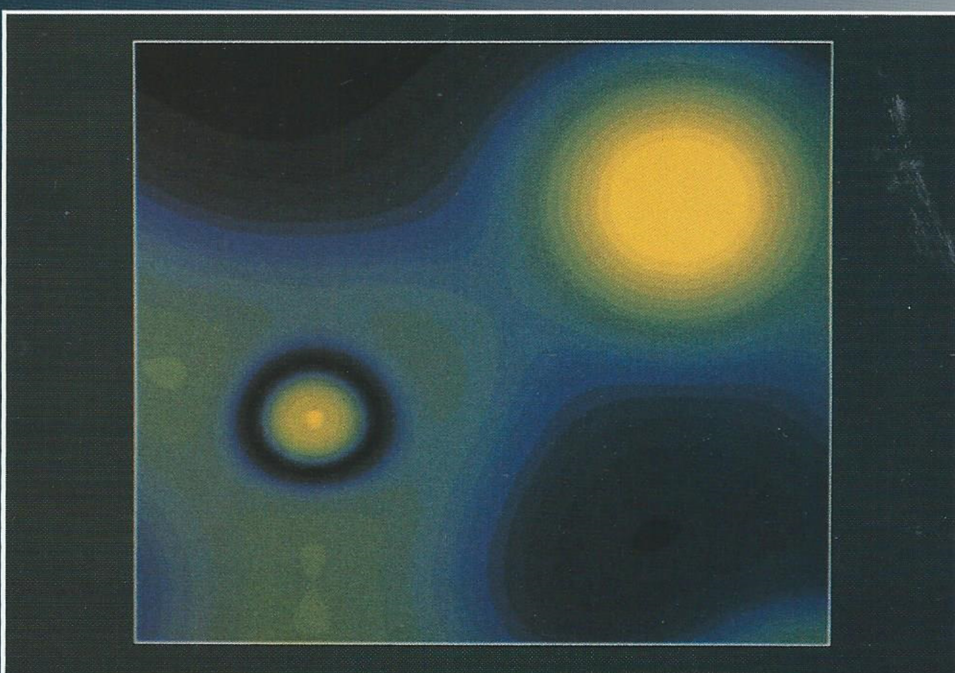
The Imagined Becomes a Reality...





Breakthroughs in Computational Chemistry

Advanced theoretical and numerical approaches combined with the power of Cray supercomputers now allow computational chemists to tackle complexity found in technologically meaningful problems.We are at the beginning of a new era of industrial chemistry: computational chemistry and experimental chemistry are becoming partners. In the partnership, computer graphics are essential for interpreting the wealth of data obtained from calculations and communicating the theoretical results to experimentalists. These graphics can trigger the imagination of both theoretical and experimental chemists and lead to new insights into and control over chemical processes, something impossible to achieve in any other way.

In the image at upper left, the electron density in a complex organic molecule, the α, α-diphenyl-β-picrylhydrazyl (DPPH) radical, is calculated with a fully quantum mechanical approach by B. Delley and E. Wimmer on a CRAY X-MP/48 supercomputer. In any atom, molecule, or solid, quantum mechanics can associate each point in space with a certain value for the electron density. Here, all points with the same intermediate density are connected to form a three-dimensional contour surface.

Catalytic effects play an important role in a variety of chemical processes, yet scientists' in-depth understanding of them is in its infancy. For example, metal atoms such as copper act as catalysts in the initial reaction of silicon in synthesizing polymers. Scientists wondered why the chemically similar silver atoms are not active. Recently, fully quantum mechanical calculations have been performed for both copper and silver atoms on silicon surfaces by scientists from Northwestern University, Dow Corning Corporation, RCA Laboratories (Switzerland), and Cray Research, Inc., using CRAY X-MP/48 and CRAY-2 supercomputers.

The results provide clear evidence for the differences between the catalytic activity of copper and silver. The image at lower left shows the charge density of a copper atom on a silicon surface in a plane perpendicular to the surface. Increasing electron density is represented by color-coded contours, where blue refers to low density and yellow to high density. The insight gained from these calculations and their graphical representation will stimulate chemists to develop new ways to think about catalytic processes, which ultimately will lead to new and better catalysts and once again make the imagined reality with Cray supercomputers.

Credit: Top: Image generated with the OASIS image synthesis package written by Gray Lorig of Cray Research, Inc.
Bottom: Image created with UNIRAS software.

Making the Imagined a Reality. . .

Making the imagined a reality has become commonplace using Cray supercomputers. Previously insolvable problems in the aerospace, petroleum, and automotive industries and in science, engineering, and graphics are being solved today using the power and flexibility of Cray supercomputer systems. In each discipline the Cray supercomputer is used to simulate a real-world process in less time and at less cost.

To support these applications, a wide range of graphic software systems is offered for Cray supercomputers by third-party vendors. Device-independent line-drawing systems like GK-2000 and DI-3000 from Precision Visuals, Inc., TEMPLATE from Megatek, Inc., and DISSPLA from ISSCO, Inc., are being used now on many Cray supercomputers.

Systems for CAD/CAM and pre- and postprocessing like PATRAN from PDA Engineering and MOVIE.BYU from Brigham Young University support a variety of engineering design activities. In those cases where photographic-quality scene generation is the objective, the designers, artists, scientists, and movie-makers are turning to Cray systems to do what could not otherwise be done.

If your application or graphics task requires extraordinary computer power . . . the problems you **can** do are much smaller than the problems you **would** like to do . . . if you need a general purpose powerhouse to run a variety of simulation, engineering, or scientific codes . . . you need a Cray supercomputer!

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