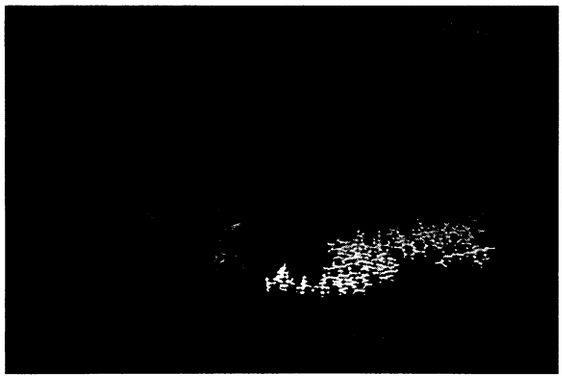
makers, and materials scientists whose labors of love and profit involve thousands or millions of atoms?

To cope with these larger molecules, an entire sub-specialty has grown up devoted to developing "new computational strategies and algorithms," says Almlöf. These strategies link the equations of quantum mechanics and other physical theories that describe chemical phenomena to the number-crunching ways of computers. "Half of what we do is to develop methods [of computation]," concurs Schaefer.

In many cases, Schaefer and his colleagues strike a compromise with experiment, reducing the computational burden by using some laboratory data in the calculations. Workstation programs based on that strategy are already available commercially, and they can calculate stable structures (including such features as bond distances and angles) for 50-atom molecules in as little as 2 minutes, according to an in-depth market analysis of computational chemistry published this year by Charles T. Casale of the Aberdeen Group Inc., a private industry and technology assessment firm in Boston. Meanwhile, by pushing such methods, solid state scientists like Berkeley's Cohen have been extending computational chemistry to the architectures of periodic materials such as crystals, with atomic constituencies numbering in the millions. To do so, Cohen and his colleagues resort to "molecular mechanics" and "empirical force field" calculations. These techniques sidestep computer-choking quantum mechanical computations by portraying molecules as, say, sets of balls linked by springs, which represent the balance of electron-electron repulsions and electron-nucleus attractions.

Such computational advances have given experimentalists a way to keep a critical eye on their laboratory measurements: On finding a mysterious peak in an infrared absorption measurement, for example, researchers can calculate whether it is a plausible one for that molecule. But chemistry by computer is also taking the place of experiment. At NASA Ames, for example, Bauschlicher and his colleagues are using computational methods to investigate the rate of reactions that might occur as fuel burns in rocket engines and other advanced propulsion systems, places too hostile and chemically complicated even for the most bold and capable of chemists. Bauschlicher suspects that his team's ab initio studies of hydrogen atoms recombining into hydrogen molecules, for example, will help designers of engines for the hypersonic National Aerospace Plane (NASP) or the High Speed Civil Transport project (a proposed new generation of supersonic airliners) set optimum lengths for nozzles or combustion chambers.



MOLECULAR SIMULATIONS INC.

Molecular tango. A computer calculates a time-lapse view of a polystyrene molecule adhering to a graphite surface.

The High Energy Density Materials Program—a joint effort of the AFOSR and a team at the Edwards Air Force Base in California—takes computation in a different direction. While Bauschlinger and his colleagues are studying familiar reactions under unfamiliar conditions, the Air Force project aims to come up with entirely new substances that will serve as better liquid and solid rocket propellants. "Our aim is to store as much chemical energy as we can in light chemical compounds," notes Burggraf of AFOSR, the program's manager. And computational chemistry, by suggesting new molecules that might be stable yet release exceptional amounts of energy when they burn, is proving invaluable. "The computational chemists have predicted new systems," Burggraff says. Schaefer of the University of Georgia, for example, proposed rings of oxygen atoms—a form that chemists had never synthesized—as an energy-packing form. Rings of four oxygen atoms turned out to be unstable, says Burggraf. "But there is hope for eight-member rings."

Streamlined discovery. Even the kind of molecular tinkering to improve an existing compound's properties that used to be done at the lab bench is now moving into computers. In one ongoing project, computational chemists at the General Electric Co. in Schenectady, New York, model polycarbonate molecules, the chemical basis of their company's Lexan line of plastics, seeking molecular variants that might hold colors better or be easier to mold. Having chemists synthesize and test hundreds of slightly altered molecules is one route to the desired properties, says Mike O'Mara, GE's manager of chemical research at the company's Research and Development Center, "but it's not a very efficient way to work." Using computers to first edit down the possibilities saves time and money. "The computational approach will lead us to answers faster," O'Mara says.

That prospect is bringing many other industries into the computational fold. "In the last few years, companies specializing in polymers, ceramics, and materials in general have come to believe that theory can now provide good enough information that they can do

A Gem of a Diamond-Beater?

Computational chemists are becoming ever more adept at conjuring up new compounds and structures (see main text). But all this digital artistry still has to face the test of the laboratory. Just last week came evidence that one of computational chemistry's more dramatic predictions—of a material that might be harder than diamond—has been realized.

The quest began 3 years ago, when Northwestern University materials scientist Yip-Wah Chung came across the work of Amy Liu and Marvin Cohen. Liu and Cohen, a materials scientist and a physicist, respectively, at the University of California, Berkeley, had used a supercomputer to predict that a superhard material might be made from carbon and nitrogen atoms (*Science*, 25 August 1989, p. 841). Their calculations indicated that if the atoms were arranged in structures similar to certain forms of silicon nitride (Si_3N_4), the carbon-nitrogen bonds might be stronger than the carbon-carbon bonds of diamond.

At last week's International Conference on Metallurgical Coatings and Thin Films in San Diego, Chung reported that his lab has synthesized a material that may fit the bill. Using a process known as magnetron sputtering, in which an argon-nitrogen plasma interacts with high-purity graphite, Chung and his colleagues were able to coat a number of surfaces with thin carbon nitride films.

The group hasn't yet confirmed that their material has the predicted structure, but they do know that, like diamond, it is an excellent lubricant and extremely wear-resistant. And preliminary tests suggest it may indeed be harder than diamond. For example, nanoindentation, a test using a small diamond point, produced no holes in the films—which could mean either that the coating is harder than diamond or that it is highly elastic. Further tests scheduled at Sandia National Laboratory should settle that question.

If Chung really has made a diamond-beater, Liu and Cohen will breathe easier. Their prediction had faced a certain skepticism, says Cohen, since materials scientists tend to see the hardness of diamond as a natural superlative, "like the speed of light." Says Cohen: "We were hoping for some experimental confirmation. I hope he has it."

–John Travis