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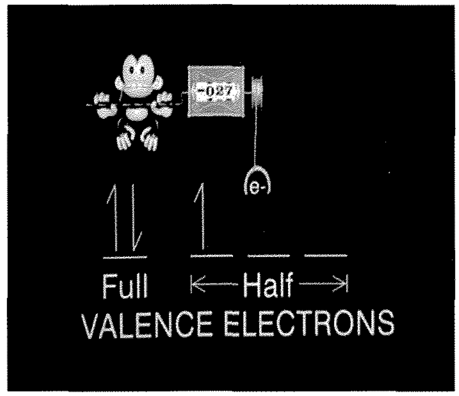
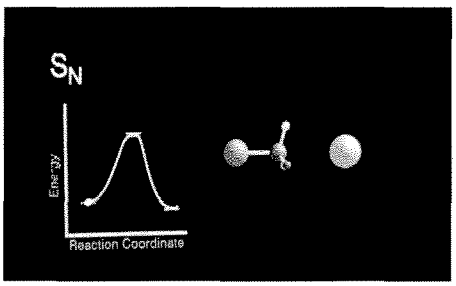
A CAPsule of Chemistry

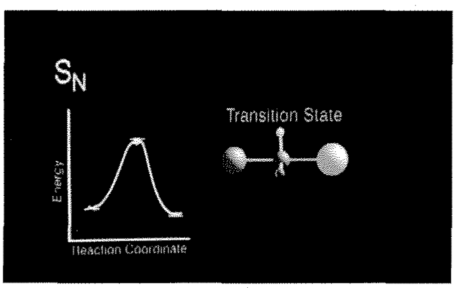
Sodium metal tossed into a pond becomes a dandy Roman candle, and sawdust blown through a Bunsen burner makes a very gratifying flamethrower. But what else do you remember from high-school chemistry? If you stayed awake between pyrotechnic demonstrations, you doubtless recall the instructor drawing a lot of three-dimensional figures on a two-dimensional blackboard. Chemistry teachers are not alone in this respect, of course, but chemistry is all about the spatial relationships between invisible, constantly moving objects. And badly drawn diagrams befuddle rather than elucidate, making the simple complex and the complex incomprehensible. Thus chemistry can appear a lot harder than it really is, and many students never give it a second chance as a result. Caltech's Chemistry Animation Project, or CAP, is using computer animation to help high-school and college students visualize what can't be seen, by producing a set of videocassettes containing scientifically accurate, three-dimensional renderings of fundamental chemical concepts.

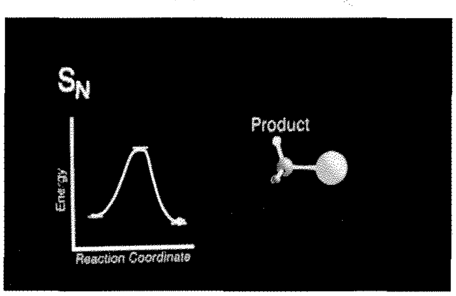
CAP is the brainchild of Professor of Chemistry Nathan Lewis (BS, MS '77), who, by his own admission, "can hardly draw anything." Increasingly frustrated by this pedagogical impediment, he recalls that in 1991, "I asked my Chem 1 classes, 'Can someone please put atomic orbitals on the computer?'" No hands shot up. But surely, he thought, somebody somewhere must have done it. He called all around the country, but no dice. "There were pseudo-three-dimensional things, but if you didn't know what you were looking at, you couldn't figure out what they were." (Not unlike those computer manuals that only make sense if you already know how to do the procedure you're looking up!) So he recruited Andre Yew and J. Alan Low, two SURF (Summer Undergraduate Research Fellowship) students willing to work nights when certain equipment they needed was idle—namely, graphic workstations in the lab of Peter Dervan, the Bren Professor of Chemistry; and video recorders in the lab of William Goddard, the Ferkel Professor of Chemistry and Applied Physics. By summer's end, they had put together a 10-minute videotape of atomic orbitals rotating on a black background. "It was boring," Lewis says. "It was only good for me to use in my class. But I showed it around, and everyone thought it was great! Peo-

Right: The monkey cranks away at a carbon atom's electron (the e^-). The other electrons in the atom's bonding orbitals are drawn as arrows to show how their spins pair up. Below, top to bottom: An S_N2 reaction, in which an iodine atom approaches from the right and kicks out a bromine atom, which exits the molecule to the left. Meanwhile, the remaining atoms, which were originally cocked off to the right of the central carbon atom, flip over to the carbon atom's left, like an umbrella blown inside-out in a storm. The plots at left track the system's energy, which peaks as it goes through the transition state—midway between reactants and products.









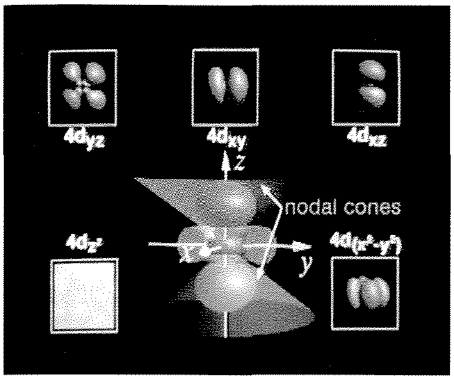
ple wanted to use it, but I didn't want to release it—it wasn't professional quality. So I decided there were two things to do—either abandon it, which is what I fully intended to do, or do it seriously. I'm doing it seriously now."

"Seriously," in this case, has grown to mean eight undergrads (at the moment) and about a quarter of a million dollars' worth of animation software donated by Wavefront, Inc.—the same stuff the networks use. The CAP project owns four Silicon Graphics workstations, overseen by a professional animator, who until recently was Juniko (June) Moody, whose TV credits include the head-butting beer bottles of the Bud Bowl. (Moody recently returned to Hollywood, and Lewis is in the process of hiring a replacement.) The videos include narration and music—light classics that are neither so soothing that the students fall asleep, nor so interesting that they ignore the pictures to listen—and are being dubbed by Complete Post, in Hollywood, to broadcast standards.

But serious doesn't mean stuffy. For example, a segment dealing with ionization energies—the energy it takes to pull an electron off an atom—features an organ-grinder's monkey. The monkey cranks the organ, which is actually a force meter, to tighten a rope attached to the electron. An odometer-like dial on the organ registers how much force the monkey has exerted. If he can't crank hard enough, he hyperventilates and sees stars when he stops. Other segments have flying calipers that measure atomic radii, and periodic tables whose squares turn colors and become bars whose heights are proportional to whatever property is being illustrated.

Of course, Caltech has a tradition of putting science on the small screen. *The Mechanical Universe*, starring Professor of Physics and Applied Physics David Goodstein, debuted on KCET, a Los Angeles PBS affiliate, in 1986, and eventually delivered a full year's worth of physics with calculus. And Project MATHEMATICS!, still in production under the guidance of Professor of Mathematics, Emeritus, Tom Apostol, is an ambitious series of half-hour videos that, among other things, brings the Pythagorean theorem to animated life. Lewis's aim is more modest. "Physicists have an agreement on how the subject should be taught," he explains. "Chemists don't. If I were presumptuous enough to make a series of 20 half-hour tapes that supposedly went through the chemistry curriculum, nobody would ever use it. So we make 10- or 15-minute modules—things the teachers can use in any order they want, and yet still help the students visualize the concept."

Visualization is the key word here. "When we do a simple nucleophilic sub-



Above: The $d_z{}^2$ orbital (center) as it really looks. The wave function is negative in the red regions, and positive in the green ones. The blue "nodal cones" are where the wave function changes sign. Below: These cheat sheets on the communal bulletin board help maintain consistency from video to video. The colors were chosen in accordance with longstanding conventions, modified to be visible on screen against one another.

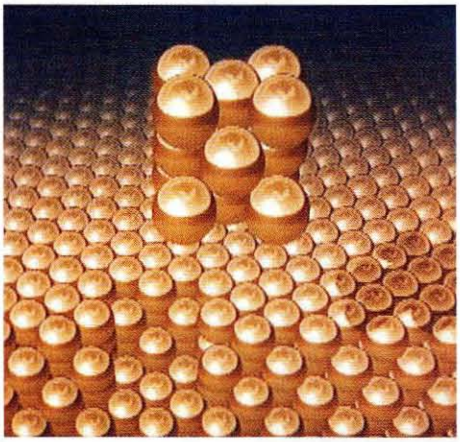
stitution reaction—an S_N2 reaction—it's fine to say the iodine comes in and the bromine leaves. Well, which path does it take? Where are all the other atoms? No chemist—except maybe now Ahmed Zewail [the Pauling Professor of Chemical Physics]—has ever measured this." But accurate depictions are crucial, because visual memories stick. "In most textbooks, people's images of even simple things like atomic orbitals are wrong, it turns out. The textbooks don't draw the whole wave function. When we integrated the $d_z{}^2$ orbital to the 90 percent probability level to find the electron, it didn't look like what was in any freshman chemistry textbook. Somebody even told me it was wrong! We checked and double-checked, and it's not wrong. So the image that you see, as opposed to the function somebody writes down, is the thing that's going to last in these kids' minds."

To get the images right, each video is plotted as meticulously as any stunt sequence Steven Spielberg ever filmed. The production teams—generally two SURF students per video—are survivors of Lewis's Chem 1 class and so know from experience where the ground turns treacherous, and can suggest how graphics in motion could have kept them from getting lost in the swamp. Lewis gives each team a set of concepts to be covered, and the students—"sometimes ignoring my ideas, sometimes using them"—brainstorm on how to present them. CAP's resident graphic artist, Teri Stachura-Seitz, turns these skull sessions into detailed storyboards that give a shot-by-shot, movement-by-movement outline of the video. Says Lewis, "Teri doesn't have a scientific background, by design. And if she can't understand what is being done in such a way that she can logically draw it, we have failed. We have to start over again. And we do that process many times." (Stachura-Seitz, who has a BFA from the Milwaukee Institute of Art and Design, also does the cover art for the video sleeves, and is working for Project MATHEMATICS! as well.)

Once the students have worked out how to depict the material, they use software donated by Biosym, Inc., to calculate the atoms' behavior based on quantum-mechanical first principles, followed by a set of Newtonian, billiard-ball-type calculations that imbue the atoms with "lifelike"—i.e., room-temperature—motions. The results are fed into the animation software, which generates the graphics. Marrying computational chemistry to an animation package designed for TV commercials requires certain adjustments. For example, Lewis remarks, "We have to format the chemistry codes for a program that's really meant to wrap the label around the soda can. But we can make carbon atoms look like strawberries, no problem! Just click on the strawberry texture."

The animation package gives the atoms pretty colors and nice, smooth motions, but there's a lot more to achieving a usable product, says Lewis. "It's not just putting the coordinates in. It's getting motion paths that look right, it's getting the lighting to look right, it's rendering to make things look good in three dimensions. And that's what our animator does. This will vary from buffing up an already good polish, to sanding and a rough polish and the whole thing, depending on what the students do." The production teams have to coordinate—"If we make carbon green here and yellow in the next video, teachers won't be able to lift frames from one to another." (Lewis hopes that teachers will edit the videos on their own VCRs, distilling his offerings into tapes that suit their own needs.) And visuals that are truly stunning on a high-resolution graphics-workstation monitor may look like mud on real-world AV equipment. So CAP checks out all their tapes on what Lewis calls "the world's worst TV"—a 13-inch portable whose color balance is shot, picked up at a garage sale for $7.00 by Todd Allendorf (BS '92. Allendorf went on to a stint at Magic Box, a Hollywood animation studio, and now designs 32-bit CD-ROM video games.)

The work is so labor-intensive, says Lewis, that "no team has ever finished a 10-minute video in a summer. Usually it's two summers. Sometimes it's a summer and an academic year. We make about 30 minutes of broadcast-quality animation a year—that's a *heroic*



Gold's face-centered cubic crystal structure is put on display in this unit cell of gold atoms, which levitates out of the background metal in "Crystals."

amount." Attracting students who are visually oriented as well as computer-literate helps, too. One, senior Scott Townsend, took a year off from Caltech to go to film school before returning to the project. Others are Hollywood-bound computer-science majors, who, following Allendorf's example, hope to parlay their CAP demo tapes into jobs.

(All this computer expertise comes in handy in other ways. The project has a home page on the World Wide Web—http://bond.caltech.edu/—where people will be able to find information about the videos. The page doubles as an on-line discussion group where teachers will be able to tell other teachers what worked for them.)

Now in its third year, CAP has hit its stride. The first two modules—Townsend and Yew's "Atomic Orbitals," and "VSEPR" (valence-shell electron-pair repulsion theory, which predicts the shapes of molecules by counting their electrons), by Mark Huber and Corinna Garcia, are slated to come out just in time for Christmas. (Three years from inception to release isn't bad. David Goodstein—who is also editing the CAP scripts—began working on *The Mechanical Universe* five years before its premiere.) Two more modules—Allendorf's "Crystals," and "Stereochemistry," by Michael Medaglia, Huy Lee, and David Zito—are too late for stocking stuffers, but should be available for Twelfth Night. Three more—"Molecular Orbitals," by Anthony Molinaro; "Diels-Alder Reactions," by Tim Uy and Anil Roopnarine; and "Nucleophilic Substitution," by Chris Bryant and Sean Upchurch—should be done by summer. Others—more crystals, trends in the periodic table, and a whole series on bonding—are in the pipeline. Lewis figures that another couple of years will suffice to cover most of the fundamentals.

Lewis wants to get the videos into the hands of as many teachers as possible. The distribution and pricing details have yet to be worked out, but he plans to sell them at Blockbuster Video prices—"you know, $19.95"—although probably not at Blockbuster Video stores. (That price includes permission for the teacher to make unlimited copies.) And while he doesn't expect to see them on the Movie of the Week, and probably not even on PBS, he's optimistic that teachers will actually use them, based on the reactions to the rough cuts he's been showing around. "Even the ones that we think don't look good and are boring, people say they would love to have."

"What's really neat about this is that students are doing it for other students," says Lewis. And it doesn't have to end with chemistry. "We've got a unique facility, because it's fairly user-friendly. With a little bit of training, an astronomer or a geologist could walk in and have students show earthquake strain propagation, or vector fields like the airflow over a wing, or the wind patterns that lead to weather changes. A lot of the other disciplines are excited about using visualization as a teaching tool." □ *—DS*