bacterium *Arthobacter* inhibits angiogenesis and suppresses the growth of Kaposi's sarcoma cells in culture.

SP-PG has an important difference from traditional anticancer therapies: It doesn't devastate normal cells. "Shuji and I share a dream," says S. Zaki Salahuddin, another former Gallo associate now working with Nakamura at USC, and one of the authors of the paper. "The dream is to bring into tumor biology nontoxic drugs." SP-PG's manufacturer Daiichi Pharmaceutical Co. Ltd. of Tokyo has now purified SP-PG and is producing enough of it to complete preclinical trials of the drug by this summer.

UCLA's Miles is excited about what all these findings mean for the future of Kaposi's sarcoma research. "I think the whole thing is really coming together in terms of the LIF receptors and the IL-6 receptors being the receptors for Oncostatin M," he says. "This is really big, and it gives us a lot of different directions to go in." Taken with the potential advances in therapy and the narrowing search for another infectious agent, there is room for cautious optimism about getting a clear picture of the KS puzzle. ■ JOSEPH PALCA

Building a Silicon Surface, Atom by Atom

Almost all of us, mostly in childhood, have played with building blocks, carefully arranging them to create model houses, skyscrapers, or bridges. A more sophisticated version of that playful behavior is now taking place in the field of materials science, where researchers are using the principles of quantum mechanics to assemble imaginary atoms into models of the microscopic structure of real materials. Just last week, this high-tech Lego game reached a turning point.

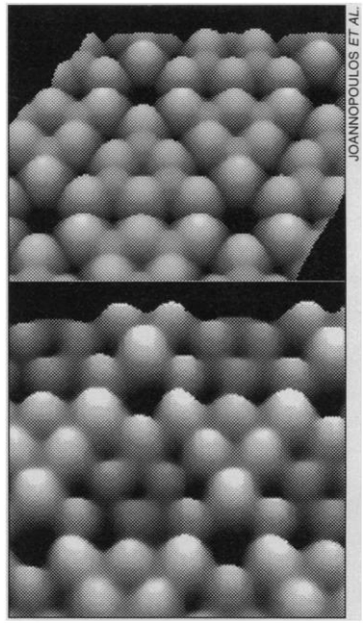
In a photo finish, two groups of physicists reported that by harnessing the power of new parallel computers, they had independently succeeded in modeling the arrangement of atoms known as the 7×7 Takayanagi reconstruction of silicon. This extremely complicated structure, which draws its name from the Japanese scientist who first described it, is the configuration of atoms found on one of the faces of a silicon crystal. The results, published in back-to-back papers in the 2 March *Physical Review Letters*, don't hold any surprises about this well-studied atomic arrangement—except for the unprecedented scale of the models. While comparable earlier efforts at assembling silicon atomic Lego had peaked at about 100 atoms, the two groups in this case, led by physicists John Joannopoulos of the Massachusetts Institute of Technology and Michael Payne of the University of Cambridge, upped the figure to about 700 atoms—enough to reproduce the full complexity of the silicon surface.

Modeling on this scale could eventually offer new insights into how defects and changes in composition alter the atomic structure of materials, and hence their properties. "The excitement here is that you can do ab initio calculations on real material problems now," says Joannopoulos.

The term ab initio—meaning "from first principles"—sums up the challenge both groups faced: They had to calculate the most energetically favorable position for each atom using only the quantum mechanical equations that describe the total energy of a system of atoms. In theory it should be possible to calculate the most stable arrangement of any number of atoms; after all, nature does it every time a solid takes shape. In practice, the calculations are enormously time-consuming. The process starts with a collection of atoms arranged in a ballpark estimate of the structure based on theory or experiment. Next, the computer "jiggles" the atoms around in search of the equilibrium state—the one in which the structure has the lowest total energy. To do this jiggling, the computer calculates the forces on each atom, shifts the atoms slightly in response to these forces, allows the electrons to relax back to their ground state, and finally recomputes the total energy of the structure.

By repeating this procedure over and over again, the computer ultimately arrives at the lowest-energy, most stable structure. Doing this for 700 atoms takes hundreds of hours of computer time—even on parallel computers, which are well suited to such simple, repetitive calculations.

In a task of this magnitude, errors can easily creep in. But because they worked independently and followed different procedures, the Cambridge and MIT groups inadvertently acted as a check on each other's results. Joannopoulos' team ran the calculations on a Connection Machine, which has more than 16,000 simple processors; Payne's group used a different algorithm and ran it on a Meiko i860 Computing Surface, which has only 64 processors, albeit more powerful ones. In spite of the differences, the two groups arrived at virtually the same result for a key parameter: the energy per surface atom. Right before simultaneously submitting their manuscripts, the groups compared their figures and found less than a 3% difference. "We all burst out laughing in relief," remembers Payne.



Fair likeness. *A hypothetical STM image of a computer-modeled silicon surface* (top) *resembles an image of the real thing.*

The surface energy figure, both groups note, is well below the energy per atom calculated for other conceivable arrangements, which explains why the 7×7 reconstruction is the stable arrangement of surface atoms. And, as a graphic demonstration that they have reproduced the surface arrangement that forms in nature, the MIT group produced computer images that show how their theoretical surface would look through a scanning tunneling microscope (STM). In a comparison with an actual STM image of a silicon surface, the computer image holds up quite well.

Reproducing known structures isn't the ultimate goal of such supercomputer calculations, of course. As a first step toward using simulation to open a new, atomic-scale window on materials, Joannopoulos would like to see the calculations extended to larger systems of atoms. Modeling structures of 1000 atoms should be feasible with the same techniques that recreated the silicon surface, he says. And "as you go bigger," Payne says, "you can begin to study more problems." For example, it usually takes systems of more than 100 atoms to model cracks or defects. Once you get into the thousands of atoms, a range of other processes that can affect the physical and chemical character of a material can be examined. Beyond that, some researchers think, lies the possibility that supercomputers could be used to discover completely new materials.

Such feats could make the parallel supercomputer a standard tool of materials research. And when that day comes, predicts Oscar Alehand, a physicist at Bellcore, "These papers will [be seen as] a milestone." ■ JOHN TRAVIS