

TOOLS

Chem Computing Made Simple

The days when chemists had to synthesize a molecule before they could plumb its nature are long gone thanks to computational chemistry, which makes it possible to predict the properties of molecules. But computational chemistry software is challenging for students and researchers to use, says physical chemist William Polik of Hope College in Holland, Michigan.

So he and student Jordan Schmidt have written WebMO, a simple, Web browser-based interface for using popular chem software packages such as MOPAC and Gaussian. You draw the molecule's structure, and the output—including the molecule's transition states and infrared and nuclear magnetic resonance spectra—appears in an easy-to-understand format. "I see this as lowering the barriers to using computational chemistry," says Polik. Download the free program here; a more sophisticated version costs \$995 for academics.

www.webmo.net

RESOURCES

Deconstructing *Salmonella*

They're best known as the bane of the summer picnic, but *Salmonella* bacteria also cause typhoid fever and infest animals ranging from chickens to reptiles. Get the latest on the genomics of this nauseating group of bacteria at Salmonella.org, a University of Illinois site aimed mainly at specialists. Salmonella.org offers genome sequences from several strains of the bug and keeps tabs on worldwide sequencing projects. Also available are a list of *Salmonella* genes, a strain finder, a directory of researchers, and practical advice on reducing your odds of getting sick.

www.salmonella.org

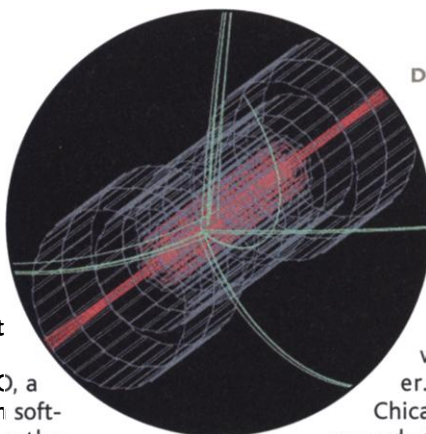
A Day at the Lake

Although this gaudy turquoise lake (right) looks inviting, you wouldn't want to dip a toe into its seething water, which has a pH lower than battery acid. Tiwo Nua Muri Koohi Fah on the Indonesian island of Flores is one of the planet's 80 or so volcanic lakes, bodies of water trapped within a crater. Find out more about these intriguing lakes—some of which may replicate the torrid, chemical-rich conditions under which life first appeared—at this site created by hydrologist Greg Pasternack of the University of California, Davis.

Researchers can study papers by Pasternack and colleagues on the classification of volcanic lakes or scour a bibliography with more than 200 entries. Aimed at a broader audience is the collection of links profiling 15 lakes—from Crater Lake in Oregon to Cameroon's Lake Nyos, which in 1986 belched a pall of carbon dioxide that smothered more than 1800 people. Hoping to forestall another catastrophe, scientists are working to "degas" the water by venting the carbon dioxide.

NETWATCH

edited by MITCH LESLIE



DATA

Hunting Quarks Online

In a first for the field of particle physics, Fermi National Accelerator Laboratory has unveiled a Web tool[†] that lets anyone search 4 years' worth of data from the world's most powerful atom smasher. Between 1992 and 1996, the Chicago-area facility's D0 experiment recorded trillions of collisions between streams of protons and antiprotons, leading to the discovery of the top quark. Such data are not usually publicly released. However, physicists and students stalking still-hypothetical subatomic particles can now search the D0 database for the spoor of their ghostly quarry using a Web interface called Quaero. (Data from the current run of the accelerator may be posted in a few years.)

While waiting for search results—usually available within an hour—check out what's happening inside the lab's accelerator with this page[†] of real-time graphics. Above, a spray of particles emanates from a head-on collision between matter and antimatter.

[†]quaero.fnal.gov/quaero

[†]www.fnal.gov/pub/inquiring/live_events/index.html



Science ONLINE

Epigenetics, the topic of this week's special issue, is also the focus of a new set of features on *Science's* Functional Genomics Web site. Included are a collection of Web resources on topics such as chromatin, DNA methylation, and gene silencing, as well as an archive of epigenetics research papers and reviews published in *Science* over the past 5 years.

www.sciencegenomics.org/resources/res_epigenetics.shtml

Send great Web site suggestions to netwatch@aaas.org