

SCIENCE & TECHNOLOGY

digital briefs

NEW SOFTWARE AND WEBSITES FOR THE CHEMICAL ENTERPRISE

WEBSITES

The Materials Research Facilities Network (MRFN) is a National Science Foundation-supported organization established to provide scientists access to advanced instrumentation and research facilities across the U.S. Nineteen Materials Research Science & Engineering Centers (MRSECs) from California to Massachusetts currently belong to the network (www.mrsec.org). Potential users at schools near MRSECs, especially undergraduate and minority-serving institutions, can submit short proposals on MRFN's website requesting the use of state-of-the-art instruments and training from skilled staff at one of the facilities. For instance, researchers seeking to characterize newly synthesized materials can apply to operate a transmission electron microscope or an imaging X-ray photoelectron spectrometer at the University of California, Santa Barbara, and to collaborate with others at that site. Some financial support could be awarded to help defray the costs of instrument fees and travel to and from each research center. **MRFN, www.mrfn.org**

Launched in August, **PharmaValet** is a subscription-based website that enables pharmaceutical companies to search, analyze, and monitor approved drugs from both the U.S. and Canada. Including drugs and patents from FDA's Orange Book and Health Canada's Patent Register, the PharmaValet database

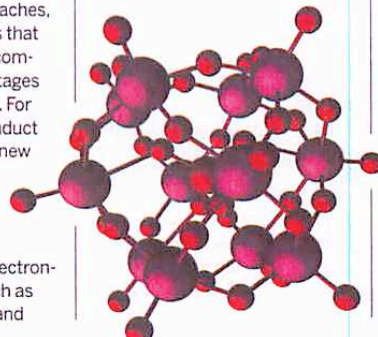
allows users to evaluate a drug's worldwide patent position and to monitor a competitor's portfolio. Pharma users also have access to supplemental data and chemical structures associated with a drug and can carry out searches on a patent's full text, as well as look for publication, approval, and expiration dates. PharmaValet was codeveloped by consulting firm Chemvalet and Multimus Information Technologies, both based in Montreal. **www.pharmavalet.com**

SOFTWARE

Powered by NetBase technology originally developed in MIT's Media Lab, **Illumin8** is a Web-based research tool for innovation professionals "that does the reading for you," says Elsevier, the software's producer. Corporate customers can use Illumin8, which searches the semantic structures of sentences and other unstructured text, to turn information overload into an asset and identify solutions to specific research problems. To begin, users enter any topic, problem, or desired benefit. The software then searches 8 billion Web pages, five patent repositories, and Elsevier's journal content to return products, approaches, people, and organizations that might be helpful to R&D companies at the beginning stages of the innovation process. For instance, a firm could conduct a search on developing a new inexpensive solar cell, and Illumin8 might return information about companies with technology for printing electronics, critical molecules such as poly(3-hexylthiophene), and

experts who have developed a fabrication method for organic photovoltaic systems. **Elsevier, www.illumin8.com**

ADF2009 is the latest version of the Amsterdam Density Functional program for quantum chemical calculations. Released in September by Scientific Computing & Modelling, in the Netherlands, ADF2009 enables chemists to compute the structures, reactivities, and properties of molecules and periodic structures such as bulk crystals and metal surfaces. In addition, users can investigate the thermodynamics of pure and mixed liquids with a COSMO-RS (Conductor-like Screening Model for Realistic Solvents) module. The updated software, which has a graphical user interface for job setup and output visualization, also allows the study of highly coordinated heavy-metal compounds (shown below), as well as the prediction of molecular spectroscopic properties for techniques such as magnetic circular dichroism and resonance Raman spectroscopies. With ADF2009, users have access to the latest meta-hybrid and dispersion-corrected functionals for computations, improved self-consistent-field convergence methods, and a



mobile block Hessian method for calculating vibrational modes. **SCM, www.scm.com**

California-based software firm Wavefunction has released **Odyssey v3.2**, a major upgrade to the Odyssey molecular simulation teaching program for general chemistry classes. This upgrade enables Macintosh users to access version 3 of the Odyssey package for the first time. Distinct versions of the updated software for college and



high school classrooms are also now available. Odyssey includes simulation experiments with step-by-step instructions; an extensive, now-expanded "stockroom" containing hundreds of preconstructed samples of molecular systems geared toward student investigation; and an easy-to-use model kit. For improved lab and classroom use, version 3.2 contains a number of enhancements such as the ability to save snapshots and plots and the tools to change font size and colors for clearer projection. **Wavefunction, www.wavefun.com**

This is the final installment of Digital Briefs. News about new or revised electronic products can still be sent to d-briefs@acs.org.

LAUREN K. WOLF wrote *Digital Briefs*.