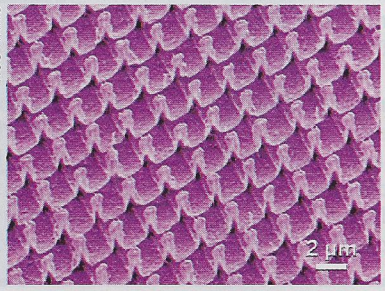
SOFTWARE ENABLES SPEEDIER METABOLOMICS

Scientists at Scripps Research Institute have developed a software program that improves the efficiency of mass spectrometry-based metabolite profiling by making it possible to carry out analyses in a multiplex manner. Software currently available for metabolomics—the study of the chemical end products of cellular processes—is capable of comparing only two sample groups at a time to determine metabolite differences, such as samples from an organism exposed to different conditions. The new program, metaXCMS (metlin.scripps.edu/metaxcms), developed by Scripps's Ralf Tautenhahn, Gary J. Patti, and Gary Siuzdak, along with coworkers, enables comparisons of an unlimited number of sample classes simultaneously (*Anal. Chem.*, DOI: 10.1021/ac102980g). This type of second-order analysis could speed up metabolomics data processing considerably, the researchers report. They demonstrated the software's capabilities by analyzing metabolites in mice exposed to pain from three different causes and showing that histamine levels change similarly in each case relative to histamine levels in pain-free mice. The team also notes that metaXCMS's multiplex capabilities will enable researchers to identify biologically relevant differences in data sets prior to confirming metabolite structures, which is a time-consuming step in metabolomics studies.—SB

PATTERNED POLYMER NANOWIRE ARRAYS

Arrays of polymer nanowires can be fabricated on a large scale from various types of polymers by using a process that combines laser interference patterning and inductively coupled plasma etching, according to a U.S.-Chinese research team (*ACS Nano*, DOI: 10.1021/nn103319p). Numerous methods are available for preparing arrays of semiconductor and other types of inorganic nanowires. But few techniques have been demonstrated for making organic or polymeric nanowires, and even fewer methods have been developed for preparing these materials as patterned arrays. Developing new ways of making such arrays could lead to advances in the fields of organic light-emitting diodes and solar cells. Zhong Lin Wang and Hao Fang of Georgia Institute of Technology and coworkers there and at Peking University exposed polymer films to interference patterns formed by crossing a pair of laser beams. The process, which was applied separately to UV-absorbent and non-UV-absorbent films, generated ablation trenches with patterns and dimensions that could be controlled by tuning the laser parameters and by rotating and reexposing the films. The team then etched the patterned films, leaving behind arrays of polymer nanowires with spacings ranging from nanometers to micrometers.—MJ

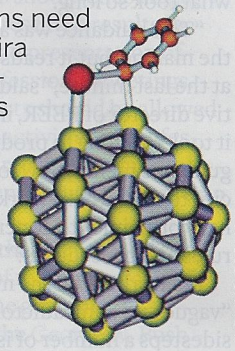


ACS NANO

Arrays of polymer nanowires can be made by patterning and etching a variety of polymers, including a polyethylene-polycarbonate blend shown in this SEM image.

GOLD CATALYSIS REVISITED

Transition-metal complexes with one or more gold atoms need help to catalyze cross-couplings such as the Sonogashira reaction, but gold nanoparticles can go it alone, according to work from a team led by Avelino Corma of Spain's Polytechnic University of Valencia (*Chem. Commun.*, DOI: 10.1039/c0cc04564k). Last year, Antonio M. Echavarren of Spain's Institute of Chemical Research of Catalonia and coworkers questioned several groups' work, including Corma's, on gold complexes catalyzing the Sonogashira reaction, suggesting that palladium impurities were crucial for the process (C&EN, July 26, 2010, page 41). Corma's team has now performed kinetic and theoretical studies that suggest gold nanoparticles catalyze the reaction without help from palladium. The researchers also revisited reactivity they reported was catalyzed by gold complexes and found evidence of gold nanoparticle formation over time, suggesting nanoparticle catalysis. Echavarren says the new work is in agreement with both other groups' work on gold nanoparticles and his team's study. Organometallic chemist A. Stephen K. Hashmi of the University of Heidelberg, in Germany, adds that it's not surprising that the groups find different catalytic behavior because they are dealing with very different gold species. "I think both teams are right," Hashmi says.—CD



AVELINO CORMA

A theoretical rendering of a gold nanoparticle participating in Sonogashira chemistry.

NEW METHOD FOR MONITORING HEPARIN

An analytical method developed by a research team in Germany could improve the use of heparin as a blood anticoagulant (*J. Am. Chem. Soc.*, DOI: 10.1021/ja109699s). The polysaccharide heparin is used as an anticoagulant during surgery, and its effects are reversed by the addition of the polypeptide protamine. The doses of both drugs are controlled according to an assay that measures a quantity called the activated clotting time (ACT). Werner Mäntele and coworkers at Goethe University, in Frankfurt, measured complexes formed by heparin and protamine with light scattering and analytical ultracentrifugation. They found that the two biomolecules form nanoparticles under physiological conditions and that nanoparticle formation is enhanced at heparin-protamine ratios of 1:2, suggesting that an excess of protamine is required to neutralize heparin. The intensity of the light scattering is directly related to the quantity of heparin. Therefore, monitoring nanoparticle formation could serve as the basis for quantitative heparin determination and as a replacement for the ACT assay, the