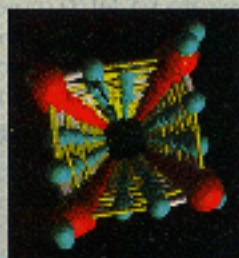


## CONCENTRATES

## Ice nanotubes, computationally

Molecular dynamics simulations suggest that water molecules trapped inside single-walled carbon nanotubes could form a variety of new ice phases that aren't seen in bulk ice [*Nature*, 412, 802 (2001)]. The simulations also suggest that, under the right conditions, the confined water may exist at a solid-liquid critical point at which the two phases lose their distinct identity. This state would allow the liquid to be continuously transformed into the solid without the distinct freezing event that occurs in conventional bulk matter. The simulations indicate that the water molecules, when cooled under axial compression, can form "ice nanotubes" having a square, pentagonal, or hexagonal cross section, depending on the diameter of the host carbon nanotube. The structure of the square ice nanotube (shown) and that of its precursor liquid phase resemble each other, which explains why the liquid phase can transform continuously into the solid phase on cooling, according to chemist Kenichiro Koga of Fukuoka University of Education, in Japan, and his colleagues Guang Tu Gao, Hiideki Tanaka, and Xiao Cheng Zeng at other labs.



## More efficient silicon LEDs

A new, more efficient silicon light-emitting diode (LED) comes from the lab of Martin A. Green and colleagues at the University of New South Wales, in Australia. Silicon LEDs would mesh naturally with silicon-based electronics, unlike traditional LEDs made from other semiconductors, which require inconvenient adaptations. But silicon doesn't emit light easily. Over the past few years, researchers have reported some silicon LEDs, but those devices have had power conversion efficiencies on the order of only 0.01 to 0.1%. The Australian group's LED has an efficiency of 1%, which is close to the efficiency of traditional semiconductor LEDs of a decade ago, they say [*Nature*, 412, 805 (2001)]. The group uses technology they developed earlier for silicon-based solar cells to wring as many photons as possible out of the device. They fashion the surface of the LED

into a series of inverted pyramids, which reduces reflection, increasing light output. Their design also reduces parasitic recombination, where dopants or impurities quench excited electrical carriers before they can be converted into light. For example, they prepare the LED on very pure substrates made by a method known as float-zone growth.

## New routes to Se compounds

Lithium aluminum hydride reacts with elemental selenium to yield LiAlHSeH, a new selenizing reagent that could allow the easy preparation of a wide range of selenium-containing compounds [*J. Am. Chem. Soc.*, 123, 8408 (2001)]. Such compounds are of interest as potential chemotherapeutic agents. Hideharu Ishihara, Mamoru Kakeeni, and coworkers at Gifu University, in Japan, prepare the selenizing reagent

and then, without isolating it, use the reagent to make compounds such as dialkyl selenides in high yields in a one-pot reaction. Previous syntheses of dialkyl selenides required many steps, the chemists note. They also report the synthesis of a variety of other compounds, including dialkyl diselenides, glutaric selenoanhydride,  $\gamma$ -seleno butyrolactone, selenoamides, and the first *N,N*-dialkyl diselenocarbonylates (shown).

## Who's tops in science?

Chemical Abstracts Service (CAS) and ISI have launched new online resources for tracking highly cited research papers and scientists. CAS Science Spotlight (<http://www.cas.org/spotlight>) identifies the 10 journal articles, 10 journals, and 10 patent families in CAS

databases that were most cited in the prior two years. It also lists the 10 papers and patents for which researchers most often requested full text through the online ChemPort Connection portal during the prior quarter. Bibliographic data and abstracts are accessible free of charge, as is full text from participating publishers. The most cited article in 2000 was written by University of Geneva molecular biology professor Ulrich K. Laemmli and concerns cleavage of structural bacteriophage proteins [*Nature*, 227, 580 (1970)]. The new <http://www.ISI HighlyCited.com> website will ultimately feature the 250 or so scientists who have received the most citations in each of 21 disciplines ISI combed through 19 million articles and other records from 1981-99 to generate the list of influential researchers, whose names the

firm has chosen not to rank. The database will expand to include additional years and names. The free site includes the researchers' biographical information and listings of their publications and websites.

## Novel arenes forcibly stacked

Disk-shaped aromatic molecules that stack into columns are considered prototypes for molecular-scale wires since they form a path of conjugation (for charge to migrate) that is insulated by a sheath of substituents. But the association between the aromatic surfaces is weak, so various efforts have been made to strengthen it by hydrogen bonding and other interactions. Chemistry professor Colin Nuckolls and students Mark L. Bushey and Aousin Hwang of Columbia University as well as physics professor Peter W. Sapiens of the State University of New York, Stony Brook,

have now explored how substitution effects can be used to position functional groups into conformations that are more favorable for forming hydrogen-bonded stacks [*J. Am. Chem. Soc.*, 123, 8157 (2001)]. The researchers prepared what they believe are the first examples of benzene rings with secondary amides at the 1, 3, and 5 positions and substituents at other than hydrogen at the 2, 4, and 6 positions (shown,  $R = C_6H_5$ ,  $R' =$  various groups). These arenes self-assemble into columns with hydrogen bonds between the amide groups to form liquid-crystalline or other highly ordered phases. Liquid crystallinity is important in these systems because it provides responsive materials that are fluid and self-healing, Nuckolls notes.

