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## **Computer-based carbon nanotechnology prophecy**

As device sizes approach atomic dimensions, much of our intuition fails to anticipate the behavior of nanometer-sized structures, governed by quantum mechanics. Fundamental consequences of energy quantization range from the unexpected behavior of semiconductor materials such as silicon and carbon, which may turn metallic or magnetic, or change their color with decreasing device size.

Even advanced experimental techniques, ranging from atomic resolution electron to scanning probe microscopy, and various spectroscopic techniques, provide only limited information about the atomic and electronic properties of nanostructures, since they either significantly perturb the individual systems, or average over large ensembles.

A viable alternative to experimental observation is the use of large-scale supercomputers to model and predict the behavior of nanostructures on length and time scales eluding observation. The reliability of first-principles calculations is currently rivaling that of experimental observations. No surprise that nanotechnology designers are increasingly turning to large-scale computations to guide product development. To some degree, unexpected results of computer simulations in the nanotechnology domain fulfill the same mission as prophecies of old, namely guiding the evolution towards a brighter future.

Supercomputing does not come cheap. The installation cost of the World's fastest supercomputer, the 40-Teraflop Earth Simulator in Yokohama, Japan, is a whopping US\$500 million. The annual maintenance fee, US\$50 million. The Earth Simulator was initially conceived to model the behavior of the Earth, from weather and climate predictions to those of threatening earthquakes. With the change in the economy came a change in mission, to save the economy. In collaboration with the Japanese team, the Michigan State University Computational Nanotechnology group currently uses

up to 70% of the Earth Simulator's muscle to anticipate intriguing phenomena in nanostructures. In the epoch of global collaborations, our Nanotechnology project is open to scientists from all over the World, to further fundamental understanding of nanoscale phenomena and their utilization for the benefit of humanity. Our recent calculations have focussed on the behavior of carbon nanotubes, which are considered as pioneering materials of Nanotechnology by many, ever since they gained popularity in the 1990's. Nanotubes, consisting of graphite monolayers seamlessly wrapped to tubes with a diameter of between 1-20 nanometers, are now being produced and marketed by several dozen companies [1]. Besides transporting electrons without loss of energy, in the so-called "ballistic" regime, nanotubes were predicted to conduct heat better than any other material. The atomic-scale perfection makes nanotubes inert to environmental influences. This is important, when considering nanotubes as building elements of superstructures like the mile-high "megacity pyramid" in Tokyo Bay or the rope of the "space elevator". While being hundred times stronger than steel, nanotubes exhibit an unusually high melting temperature of 4,000 degrees Celsius, suggesting them as components of choice when considering performance under extreme conditions.

Unexpected behavior of nanostructured carbon materials, discovered in our group, suggests their use as high-temperature superconductors, high-temperature magnets, materials with a negative thermal expansion coefficient, nonvolatile computer memory, and even a nanoscale counterpart of velcro. The unexpected thermal contraction, in contrast to the common thermal expansion, results from the simple fact, that even stiff nanotubes bend and twist on large length scales, thus reducing their end-to-end distance in a very similar way to a whip on the macro-scale. The hollow tubes may be filled with fullerenes such as the C60 "buckyball", suggesting the use of the resulting "peapods" as nonvolatile computer memory, as a nanoscale counterpart of the oriental abacus.

The enormous strength and resilience of nanotubes suggests their possibly unique application in nanoscale velcro-like interconnects for nanoscale electromechanical system (NEMS) components. The advantages of nano-velcro, formed of nanotube-based hooks, over

other bonding systems is the unexpected stability of the connection, since the energy required to open the bond amounts to roughly twice the energy involved in breaking the nanotube. While providing an overall strong connection, individual hooks may open and close under the extreme stress induced by differences in the thermal expansion of the connected components, providing the bond with a unique "self-healing" functionality.

While the above applications may sound intriguing, the behavior of carbon nanostructures under extreme conditions is truly amazing. In contrast to silicon-based computer chips, which require an extremely high purity for correct operation, electronic components based on carbon nanotubes appear to be much more defect tolerant. Computer simulations indicate an unusual self-healing behavior, when nanotubes with atomic defects are exposed to light and high temperatures. Other simulations suggest that light could be used to detach particular atoms from nanotubes, as a surgical tool especially suitable for nanotechnology.

Nanostructured carbon is gradually surfacing in commercial products, such as the new generation of flat-panel TV displays using carbon nanotube electron emitters, manufactured by Samsung, or in the cathode material of lithium-ion batteries currently available on the market. When taken at face value, the prophecy of computer simulations projects a bright future and new applications for carbon nanostructures, which await with a plethora of quantum surprises.

[1] Commercial nanotube manufacturers are listed on the web in the "Nanotube Yellow Pages", at <http://www.nanoten.com/ntyp.html>.