Forget carbon nanotubes. Too difficult to control, researchers say. The material that scientists are heralding as the future of nanocomputing is one that, without even knowing it, we’ve had access to our whole lives.

To scientists, graphene may be an exotic, two-dimensional honeycomb of carbon atoms with high mobility and useful quantum properties. But to the rest of us, it’s a thin cousin of our pencil shavings. Until recently, many scientists didn’t believe a one-atom-thick version of graphite could be separated. Then they discovered that, by folding and refolding an ordinary piece of graphite-laced scotch tape, they could pull off an ultra-thin slice and produce a material that may revolutionize computing by 2020.

The year 2020 may seem like the distant future, but not for semiconductor industries with perpetual fears of falling behind Moore’s Law. “It takes about 15 years for a new technology to come to the market,” Dr. Bhagawan Sahu, research scientist at the Southwest Academy of Nanoelectronics (SWAN), pointed out. “Why not start today, so we don’t run into problems in the future?”

Based on rising costs versus performance of semiconductor production and excessive heat generation, industry projected the downfall of the current silicon transistor technology in the coming decades. Using a roadmap laid out by the Semiconductor Research Corporation (SRC) — the industry group that funds SWAN, with member companies like AMD, Freescale, Intel, IBM, Micron and Texas Instruments — Sahu is leading several projects that tackle aspects of future computing devices.

In 2007, with computing support from the Texas Advanced Computing Center (TACC), Sahu dedicated more than a million hours of computing time on the Lonestar system to simulate the electronic properties of graphene and other emerging materials systems from first principles.
computing hours on TACC’s Ranger system, the most powerful supercomputer for open science research in the world today, to further his study of graphene. From simulations to prototypes, and, perhaps by 2020, to a new model of computing based on graphene, the SWAN team’s research is paving the way for the creation of devices thousands of times smaller, faster and more efficient than silicon-based microprocessors.

No one knows yet whether graphene will prove equal to the hope it has engendered, but the material has certain intrinsic quantum properties that make it a better option than silicon. “The question is always, ‘How small can you shrink your device?’ Graphene is a flat surface just one atom thick. That’s about as small as you can get,” Sahu said. “Also, the mobility of the electrons inside graphene is a few orders of magnitude larger than any other material at room temperature, and it’s relatively insensitive to impurities in the system.”

Importantly, graphene, in the form of graphite, is abundant, available throughout the world, and, by virtue of the “scotch tape method,” theoretically easy to produce. (The large-scale production of graphene-based devices by the scotch tape method is not feasible however, so scientists at SWAN are exploring other production methods as well.) These characteristics differentiate graphene from silicon systems that leak charge at small length scales and rely on expensive, high-tech production methods.

Last fall, researchers at Delft University in the Netherlands produced the first prototype of a transistor made with two layers of graphene. Their results agreed with Sahu and his colleagues’ graphene simulations on TACC’s Lonestar and were published in the February 2008 issue of Nature Materials magazine. “We were very excited. We looked at their numbers and they were getting what we predicted, and we said, ‘This is a direct proof.’ For graphene to replace silicon, an electrically induced gap or a high resistance state is needed, and that’s what we demonstrated numerically.

“But it is still a charge based system,” Dr. Sahu said, his voice softening. “And whenever charges move, it has associated power consumption. After 2020, we are looking beyond charge.”

This brings Sahu to an area of research that tries to exploit the quantum spin states of electrons to create a circuit. “Spin is a concept which is difficult to understand,” Sahu explained. “It is not that something is spinning — it’s an intrinsic degree of freedom an electron carries, other than charge, called angular momentum.” Just as the earth spins around the sun, it also spins on its axis — both motions are manifestations of macroscopic angular momentum. Because there are two orientations for electron spin, up and down, spin “is the most natural, two state system, where
zero and one represent high and low resistance states. Spin-based devices are expected to play a major role beyond 2020,” Sahu said.

Graphene based switch (Picture Courtesy: Max Lemme, IEEE ELECTRON DEVICE LETTERS, VOL. 28, NO. 4, April 2007). In the future, the gate material could be a multiferroic and source and drain could be a magnetic metal.

After some investigation, Sahu and his team discovered that graphene could act as a spin-like system. When sliced with the electron beam lithography technique, graphene naturally takes two forms: armchair and zigzag, which describe the shape of the graphene ribbon’s edge. The spin of the electrons associated with the zigzag edges of the ribbon are ordered by a fundamental quantum mechanical force, called exchange, in such a way that those on one side are all up, while those on the other side are all down. The effect of the spin order — the energy gap — can potentially be tuned with an electric field, Sahu’s team predicts, by joining a hybrid structure of armchair and zigzag ribbons together, establishing a natural barrier to the flow of current. “Then we do not need to put metal contacts with graphene to create a potential barrier, as is done in current transistors,” Sahu added.

As his team pushes deeper into theoretical territory, new ideas for spin-based devices have emerged. Most recently, they’ve determined that graphene paired with a multiferroic material (one that combines charge and spin into a single phase) might have an advantage in future spin-based computing devices. The idea has generated tremendous interest in the field. In fact, Science magazine’s Dec. 21, 2007 issue selected the field of multiferroics as a “Breakthrough of the year” and an “Area to watch in 2008.”

Sahu is collaborating with Dr. Leonard Kleinman, Professor of Physics at UT-Austin, and Prof. Banerjee, to study the feasibility of combined multiferroics and graphene-based devices for SWAN using Lonestar. “There’s no guarantee that graphene will replace silicon, but hopes are high because of its novel electronic properties. And combining graphene with magnetic metals to inject spins and then tune them by multiferroic materials — that’s another hope for the future,” Sahu said.

“TACC’s role comes, at this stage, as a savior. The kinds of computations we do to understand these effects require very big machines and TACC is equipped with the biggest,” Sahu exclaimed. “TACC is doing a great job of providing computing resources to the scientific community.”
“We’re at a stage in this research where a lot of the work can’t be done experimentally, but requires a lot of simulation and modeling to determine what the most promising paths are,” said Dr. Jeff Welser, director of the SRC’s Nanotechnology Research Initiative (NRI). “From a computational standpoint, doing the simulations at the atomic and quantum level is extremely challenging work. We need very high performance computing capabilities to run these algorithms and that is why we look for facilities like TACC that have that capability,” Welser said.

Using TACC’s high-performance computing systems, Sahu can execute complex simulations that were impossible only a few years ago. “TACC’s role comes, at this stage, as a savior. The kinds of computations we do to understand these effects require very big machines and TACC is equipped with the biggest,” Sahu exclaimed. “TACC is doing a great job of providing computing resources to the scientific community.”

With the clock ticking to 2020, Dr. Sahu and his colleagues at SWAN continue to explore novel materials and transistor designs with high-performance computational simulations, each 0 and 1 pointing the way to a better, safer and more energy-efficient computing future.

Aaron Dubrow
Texas Advanced Computing Center
Science and Technology Writer
Feb. 13, 2008