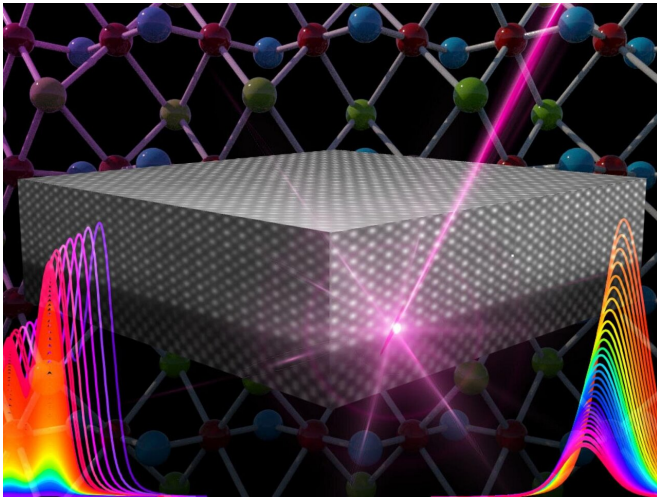


# Surprise finding uncovers new capability for semiconductor material

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Credit: Environmental Molecular Sciences Laboratory

Scientists have taken a common component of digital devices and endowed it with a previously unobserved capability, opening the door to a new generation of silicon-based electronic devices.

While [digital circuits](#) in computers and cell phones are becoming smaller and processors are going faster and faster, limits are approaching, and scientists worldwide are working to extend or go beyond today's technology, known as complementary metal-oxide semiconductor or CMOS technology.

In a research article published in July 2019 in *Physical Review Letters*, the scientists explain how they created a metal oxide—the "MO" in "CMOS"—equipped with an additional important function. Instead of simply being a passive element of the on-off switch in a CMOS transistor, the new metal oxide activates electrical current flow all by itself. The finding could one day help move computing into an era often called "beyond CMOS."

The oxide material creates current in nearby pure, "undoped" [silicon](#), the workhorse semiconductor of the electronics industry. The conductivity in silicon takes place in a very thin region just nine [atomic layers](#) thick. You'd need to stack 100,000 such layers equal to the width of a human hair.

This capability—to induce current in silicon—marks a major step forward for a material that has previously been thought of as being of limited value; it has performed the on-off duties of an insulator very well but it hasn't been considered for the crucial current-creating capacity on which all transistors rely.

"The fact that an oxide, long used only as a passive element in semiconductor devices, can also be an active element is new and intriguing," said Scott Chambers, one of the authors and a scientist at the Department of Energy's (DOE) Pacific Northwest National Laboratory (PNNL).

## Semiconductor measurements at odds

The result is so unexpected that the scientists who did the work, at PNNL, the University of Texas (UT)-Arlington, and elsewhere, spent months trying to understand what mistake they might have made, before confirming through a battery of tests that their unexpected results were sound.

Several measurements of the intricate semiconductor structure, known as a heterojunction, demonstrated the scientists' mastery: The boundary between the metal oxide known as strontium titanate and the silicon was crisp. Atomic row by atomic row, the heterojunction prepared at UT-Arlington by a process known as molecular beam epitaxy seemed nearly perfect.

Except, that is, for some surprising spectral lines, the result of probing the sample with X-ray light. The spectra showed unexpected characteristics for a near-flawless structure.

The team at PNNL checked and re-checked its X-ray measurements. Perhaps there had been contamination of one of the ingredients. Maybe someone failed to open the oxygen valve wide enough during the oxide film growth. Maybe the instruments weren't operating properly. Or maybe they had created different materials than the one they intended.

But everything checked out.

"The data we had were contradictory and seemingly bizarre," said Chambers. "By most measures we had created a material that was near perfect, but another important measurement seemed to indicate that our material was a mess."

It was then that Chambers decided to take a serious look at another possibility—that all the measurements were accurate and that the layered structure central to transistors, and computer chips, and other digital devices of all types was not flawed. Rather, could there be something previously unknown that would explain the mysterious measurements?

Indeed, there was.

Noodling over the X-ray spectra, Chambers realized that the results could be explained by the presence of unexpected electric fields created by a flow of electrons across the junction between the silicon and the strontium titanate.

### Wayward oxygen atoms

It turned out that a very small number of oxygen atoms from the strontium titanate had made their way into the silicon. The team had unintentionally doped silicon with oxygen, resulting in electron transfer from the silicon to the strontium titanate, and the creation of an electrical current of "holes" (missing electrons) in the uppermost atomic planes of the silicon.

It wasn't an easy puzzle to solve. To do so, the team had to develop a new way to understand its measurements. Input from high-energy electron diffraction, X-ray crystallography, and high-resolution transmission electron microscopy all

indicated the material was near perfect, but measurements from X-ray photoelectron spectroscopy (XPS) seemed to indicate otherwise.

XPS works by shining high-energy light—in this case x-rays—on a material and then measuring what happens, as judged by the energies and intensities of the electrons that are emitted.

Scientists can learn a lot by hitting a sample with x-rays. Think of what happens in a crowded tavern when a rock band starts playing. Some patrons will clap, others will head for the exits, and some might pick up their instruments and join in. For scientists hitting a sample with x-rays, analyzing the electrons that come out is important for understanding what atoms are present, what chemical bonding environment they're in, and what the overall energy landscape is within a material. However, ferreting out the energy landscape from the raw data is a major challenge.

Chambers developed a set of hypotheses and a conceptual way to interpret the XPS results in terms of the presence of large electric fields in the material. He then turned to PNNL colleague Peter Sushko, an expert modeler of complex solid materials, to write a computer code to solve the equations associated with the concept and determine the properties of the electric fields.

Sushko developed an algorithm that assigns millions of possible electric field values to the different atomic layers and simulates the spectra that would result for each set. One particular set fit the team's experimental spectra exactly: The team had shown that the strange XPS data were consistent with the presence and strengths of electric fields that would give rise to a hole current in the silicon, just as Chambers suspected.

"We discovered that the energy landscapes which came from correctly interpreting our XPS using this new algorithm were precisely what would need to be present to generate the conductivity we were observing," said Chambers.

"Peter's computer code allowed us to find that unique set of electric field values that explains all our data—truly a needle in a haystack. The crucial

data in an experiment like this can be gathered in a few hours, but it took a year of thinking and analysis to interpret them," he added.

The results were corroborated by Chambers and corresponding author Joseph H. Ngai of UT—Arlington using completely independent methods.

### **No MOSFET revolution—yet**

Chambers and Ngai do not expect this finding to immediately revolutionize the semiconductor industry or the fabrication of MOSFETs (metal-oxide semiconductor field-effect transistors). But this fundamental science opens a new door in the "beyond CMOS" world, and the algorithm the team created to understand the results gives scientists a new tool to probe layered structures of all kinds, not just those for an oxide on silicon.

Provided by Environmental Molecular Sciences Laboratory

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