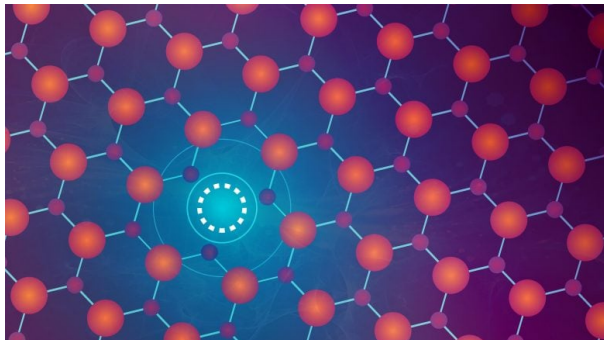


How Chips Are Being Revolutionized by Atom-Thin Materials

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Courtesy of SynEvol
Credit: Kyle Palmer/ PPPL Communications Department

For more than 50 years, silicon computer chips have been a reliable technology. Considering that a human hair is about 80,000 nanometers broad, the smallest features on chips that are now on the market are only about 3 nanometers in size. Our never-ending desire for greater memory and computing capacity in the palm of our hands can be satisfied by shrinking the size of chips' characteristics. However, there's a limit to what can be done with conventional materials and procedures.

In order to develop the next generation of computer chips, scientists at the Princeton Plasma Physics Laboratory (PPPL) of the U.S. Department of Energy (DOE) are utilizing their knowledge of physics, chemistry, and computer modeling. They are working toward methods and materials that will result in chips with fewer characteristics.

"All of the electronics we use today are built with silicon chips, which are three-dimensional materials. These days, a lot of businesses are investing heavily in chips composed of two-dimensional materials, according to PPPL associate research physicist Shoaib Khalid. The materials are actually two-dimensional (2D) materials because they are extremely thin, consisting of only a few layers of atoms, yet actually existing in three dimensions.

Khalid, Bharat Medasani of PPPL, and Anderson Janotti of the University of Delaware examined a transition-metal dichalcogenide (TMD), a 2D material, as a possible substitute for silicon.

Their latest work describes the changes that can take place in the atomic structure of TMDs, the reasons behind them, and the effects they have on the material. It was published in the journal *2D Materials*. Understanding these differences paves the way for improving the procedures required to make computer chips of the future.

The ultimate objective is to develop plasma-based manufacturing methods capable of producing TMD-based semiconductors that are precisely tailored to the needs of the intended use.

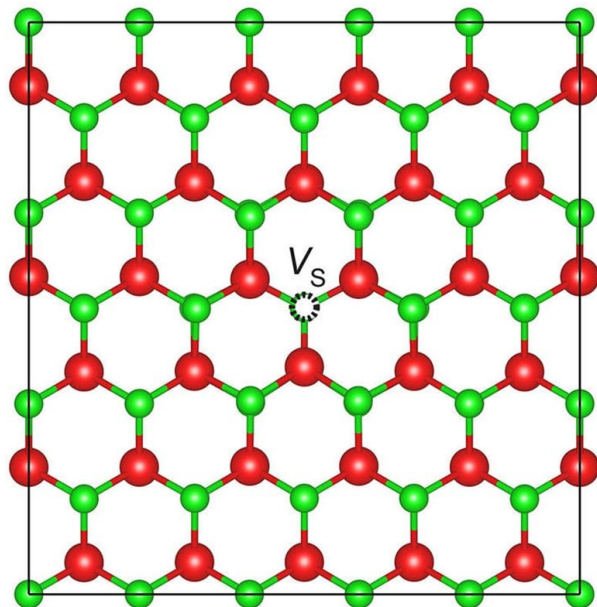
A triple-atom-thick TMD is possible. Imagine it as a little sandwich made of metal. One of the chalcogen elements—oxygen, sulfur, selenium, or tellurium—is used to make the bread. A layer of transition metal, which can be any metal from groups 3 to 12 in the periodic table of elements, makes up the infill. There are five or more atomic layers in a bulk TMD. The atoms are organized in a lattice or crystal form. In an ideal lattice, the atoms are arranged in a precise and regular way. In actuality, the pattern contains a few minor modifications. There could be an atom missing from one place in the pattern or an atom located in an unusual place. Although these changes are referred to as faults by scientists, the material may benefit from them.

For instance, certain TMD flaws can increase the semiconductor's electrical conductivity. Whether a defect is good or negative, scientists must comprehend why it occurs and how it affects the material in order to incorporate or remove it as needed. The researchers can also explain the outcomes of earlier TMD tests by having a better understanding of prevalent faults.

"There are excess electrons when bulk TMDs are made," Khalid stated, adding that the reason for the presence of these extra negatively charged particles remained unknown to the researchers. "In this work, we explain how hydrogen may be the cause of the excess electrons."

Once the researchers calculated the energy needed to generate various types of TMD flaws, they arrived at this result. They examined defects involving hydrogen because this element is frequently present throughout the chip production process and defects involving chalcogen vacancies, which were previously known to be present in TMDs. Because these are the flaws that are most likely to arise because they don't require much energy to happen, researchers are very interested in determining which defects require little formation energy!

Next, the group looked at how each low-formation-energy defect functioned. They were particularly interested in learning how each flaw arrangement may affect the material's electrical charge. The researchers discovered that excess electrons are produced by one of the hydrogen-related defect configurations, leading to the creation of negatively charged semiconductor material known as an n-type. Combinations of positively charged, or p-type, semiconductor material and n-type semiconductor material are used to make computer chips.



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The third kind of defect examined in the research is called a chalcogen vacancy, which is, depending on the kind of TMD, a missing atom of tellurium, oxygen, sulfur, or selenium. The scientists concentrated on providing an explanation for the outcomes of earlier tests conducted on flakes of molybdenum disulfide, the main TMD material. Unexpected light frequencies emanating from the TMD were visible during the testing, which involved shining light on the device. The researchers discovered that the electron mobility associated with the chalcogen vacancy may account for these unexpected frequencies.

"This is a common defect. When they grow the TMD film, they can typically see it in the images captured by scanning tunneling microscopes," Khalid explained. "Our work proposes a strategy for investigating the presence of these vacancies in the bulk TMDs." We explained previous experimental results in molybdenum disulfide and expected a similar outcome for additional TMDs.

The researchers' proposed process entails examining the TMD for faults using photoluminescence testing tools to determine the frequencies of light the material emits. The peak frequency of light can be used to determine the electron configurations of the TMD's atoms as well as the existence of chalcogen defects. The journal article contains information on the frequencies radiated by five types of TMDs with chalcogen vacancies, including molybdenum disulfide. As a result, the findings serve as a foundation for future research into chalcogen vacancies.

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