2D Semiconductor Engineering is Transformed by Isotopes

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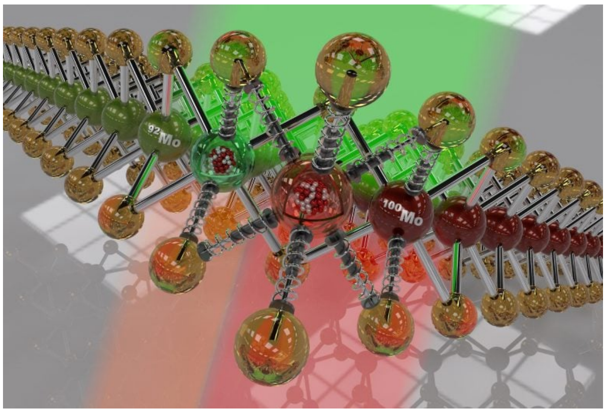

Courtesy of SynEvol
Credit: Chris Rouleau/ORNL, U.S. Dept. of Energy

Recent studies have shown that even minute variations in the isotopic composition of thin semiconductor materials can affect their optical and electrical characteristics, potentially paving the way for innovative and cutting-edge semiconductor designs. Scientists from Oak Ridge National Laboratory, part of the Department of Energy, spearheaded the research.

Electronic gadgets and systems are becoming increasingly sophisticated and advanced on a daily basis, partly because to semiconductors. For this reason, scientists have been researching ways to enhance semiconductor materials to affect their ability to transmit electrical current for decades. Isotope manipulation of materials' chemical, physical, and technical properties is one strategy.

Isotopes are members of an element's family that have the same number of protons but differ in mass due to differences in neutron counts. Traditionally, the goal of isotope engineering has been to improve so-called bulk materials, or 3D materials, which have consistent properties in three dimensions. However, recent work conducted by ORNL has improved the field of isotope engineering in which a layer of only a few atoms thick is limited to current in two dimensions, or 2D, inside flat crystals. The ultrathin structure of the 2D materials may enable exact control over their electrical properties, which makes them promising.

"When we substituted a heavier isotope of molybdenum in the crystal, we observed a surprising isotope effect in the optoelectronic properties of a single layer of molybdenum disulfide. An effect that opens opportunities to engineer 2D optoelectronic devices for microelectronics, solar cells, photodetectors, and even next-generation computing technologies," ORNL scientist Kai Xiao said.

Using molybdenum atoms of various weights, Yiling Yu, a researcher in Xiao's team, created isotopically pure 2D crystals of atomically thin molybdenum disulfide. Yu saw little changes in the color of light that the crystals released when they were stimulated by light, a process known as photoexcitation.

"The light emitted by the molybdenum disulfide containing heavier molybdenum atoms was surprisingly shifted towards the red end of the spectrum, in contrast to the expected shift for bulk materials," Xiao stated. A change in the material's optical or electrical structure is indicated by the red shift.

Working with theorists Volodymyr Turkowski and Talat Rahman at the University of Central Florida, Xiao and colleagues recognized that in the constrained dimensions of these ultrathin crystals, the phonons, or crystal vibrations, must be scattering the excitons, or optical excitations, in unanticipated ways. They found that for heavier isotopes, this scattering causes the optical bandgap to move towards the red end of the light spectrum. The term "optical bandgap" describes the lowest energy required for a substance to either emit or absorb light. Researchers can make semiconductors absorb or emit different colors of light by varying the bandgap, and this tunability is crucial for creating new devices.

Alex Puretzky of ORNL explained how localized strain in the substrate can produce subtle changes in the color that crystals develop on it. In order to validate the anomalous isotope effect and assess its extent in relation to theoretical forecasts, Yu cultivated molybdenum disulfide crystals that contained two distinct molybdenum isotopes.

"We created a two-dimensional material using two isotopes of the same element, but with different masses, and we joined the isotopes laterally in a controlled and gradual manner in a single monolayer crystal," Xiao stated. "Our work was unprecedented in this regard." Because of this, we were able to see the intrinsic anomalous isotope impact on the 2D material's optical properties without being interfered with by an uneven sample.

The study showed that optical and electrical properties of atomically thin 2D semiconductor materials can be affected by even minute changes in isotope masses; this finding serves as a crucial foundation for future investigation.

It was previously thought that in order to create devices like photovoltaics and photodetectors, two distinct semiconductor materials needed to be combined in order to create junctions that would capture excitons and separate their charges. However, by simply altering the material's isotopes, we can really use it to build isotopic junctions that will trap excitons," Xiao stated. "This research also indicates that we can design new applications by tuning the optical and electronic properties through isotope engineering."

Xiao and the group intend to work with the specialists at ORNL's Isotope Science and Engineering Directorate and the High Flux Isotope Reactor on upcoming research. These resources are able to supply a range of highly enriched isotope precursors for the growth of distinct isotopically pure 2D materials. After that, the group can look into the isotope influence on spin characteristics in more detail in order to use it in quantum emission and spin electronics.