Studies provide answers about promising 2-D materials

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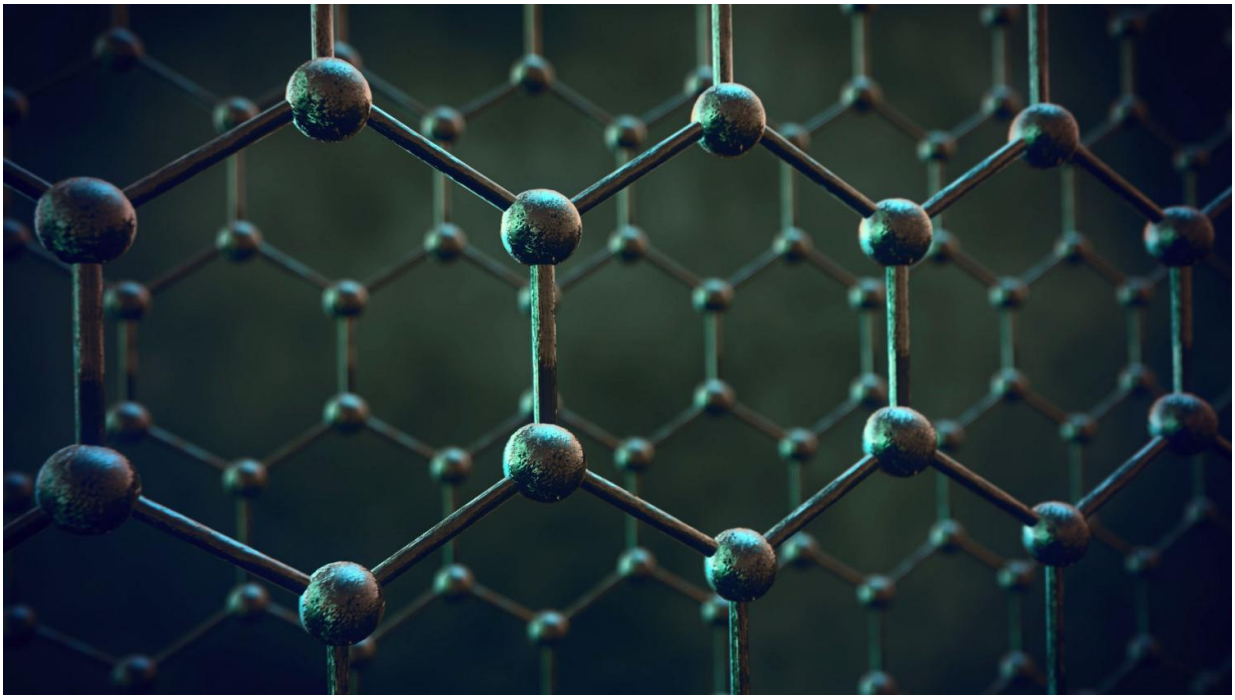

This visualisation shows layers of graphene used for membranes. Credit: University of Manchester

Two-dimensional, layered materials hold great promise for a number of applications, such as alternative platforms for the next-generation of logic and memory devices and flexible energy storage devices. There's still much, however, that remains unknown about them.

Two studies from the lab of Judy Cha, the Carol and Douglas Melamed Associate Professor of Mechanical Engineering & Materials Science and a member of Yale West Campus Energy Sciences Institute, answer some crucial questions about these materials. Both studies were funded with grants from the Army Research Office (ARO), an element of the U.S. Army Combat Capabilities Development Command's Army Research Laboratory, and have been published in *Advanced Electronic Materials.*

In one paper, Cha and her team of researchers, in collaboration with Yale chemistry professors Nilay Hazari and Hailiang Wang, experimentally measured the precise doping effects of small molecules on 2-D materials—a first step toward tailoring molecules for modulating the electrical properties of 2-D materials. In the process of doing so, they also achieved a very high doping concentration.

Doping—adding impurities such as boron or phosphorus to silicon, for example—is essential to developing semiconductors. It allows for the tuning of the carrier densities—the number of electrons and other charge-carriers—to produce a functional device. Conventional doping methods, however, tend to be too energy-intensive and potentially damaging to work well for 2-D materials.

Instead, because 2-D materials are pretty much all surface, researchers can sprinkle small molecules known as organic electron donors (OED) onto the surfaces, and activate the 2-D materials—that is, create surface functionalization. Thanks to organic chemistry, the method is remarkably effective. It also greatly widens the choice for the material being used. For this study, Cha used molybdenum disulfide (MoS_2).

However, to further optimize these materials, researchers need a greater level of precision. They need to know how many electrons each molecule of the OED donates to the 2-D material, and how many molecules are needed altogether.

"By doing so, we can go forward and design properly, knowing how to tweak the molecules and then increase the carrier densities," Cha said.

To make this calibration, Cha and her team used atomic force microscopy at the Imaging Core at Yale's West Campus. For their material, they achieved a doping efficiency of about one electron per molecule, which allowed them to demonstrate the highest doping level ever achieved in MoS2. This was possible only by the precise measurements that were conducted.

"Now that we know the doping power, we are no longer in the dark space of not knowing where we are," she said. "Before, we could dope but couldn't know how effective that doping is. Now we have some target electron densities that we want to achieve and we feel like we know how to get there."

In a second paper, Cha's team looked at the effects of mechanical strain on the ordering of lithium in lithium-ion batteries.

Current commercial lithium ion batteries use graphite as the anode. When lithium is inserted into the gaps between graphene layers that make up graphite, the gaps need to expand to make room for the lithium atoms.

"So we asked 'What if you stopped this expansion?'" Cha said. "We found that local straining affects the ordering of the lithium ion. The lithium ions effectively get slowed down."

When there's a strain energy, lithium is not able to move as freely as before, and more energy is required to force the lithium into its preferred configuration.

By calculating the exact effects of the strain energy, Cha's research team

was able to precisely demonstrate how much the lithium atoms slow down.

The study has broader implications, particularly if the field moves away from lithium batteries in favor of those made from other more readily available materials, such as sodium or magnesium, which can also be used for rechargeable batteries.

"Sodium and magnesium are much larger, so the gap needs to expand much more compared to lithium, so the effects of strain will be much more dramatic," she said. The experiments in the study provide a similar understanding of the effects that mechanical strain could have on these other materials.

ARO researchers said Cha's studies will be very helpful in advancing their own work.

"The results obtained in these two studies related to novel two dimensional materials are of great importance to develop future advanced Army applications in sensing and energy storage," said Dr. Pani Varanasi, branch chief, ARO.

More information: Joshua V. Pondick et al. The Effect of Mechanical Strain on Lithium Staging in Graphene, *Advanced Electronic Materials* (2021). DOI: 10.1002/aelm.202000981

Milad Yarali et al. Near-Unity Molecular Doping Efficiency in Monolayer MoS 2, *Advanced Electronic Materials* (2020). DOI: 10.1002/aelm.202000873

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