NEW

FRONTIERS FOR TWO-DIMENSIONAL MATERIALS

Unleashing the potential of graphene and other nanomaterials can change the world

By Ty Burke
Photographs by Hadas Parush

Twenty years ago, a pair of researchers at the University of Manchester made a remarkable breakthrough in their lab using an everyday adhesive. While attempting to isolate a layer of carbon that was as thin as possible, they looked through a microscope at the grey, slightly shiny residue from a graphite crystal left behind on a piece of Scotch tape. What they saw was graphene, the first two-dimensional material ever discovered, a eureka moment that eventually led to the Nobel Prize in Physics.

Stronger than steel but lighter than paper, graphene conducts electricity more efficiently than copper wire. Virtually transparent, it also conducts heat better — and is thinner — than any other material. These attributes give graphene almost limitless potential, once we figure out how to use it more effectively.

A form of carbon that's derived from graphite, graphene is the same substance used in a regular pencil. If you lightly trace the tip of a pencil across a sheet of paper, you leave layers of it behind. These one-atom-thick layers can be stacked like Lego to make a nanomaterial that is strong, lightweight and conductive — and that could unlock all kinds of novel applications.

Already a strong candidate for several innovative technologies, graphene could one day be used to make a mobile phone so bendable that you could wrap it around your wrist like a watch, then seamlessly reform it into a rectangle. It could improve the efficiency of solar panels and batteries, enabling electric vehicles to travel tremendous distances on a single charge. It even has the potential to be used in biosensors that could detect cancerous tumours earlier and deliver targeted therapies directly to them before it's too late. But we can't do these things yet. To make the most of graphene, we need a fuller understanding of how it works on a molecular level.

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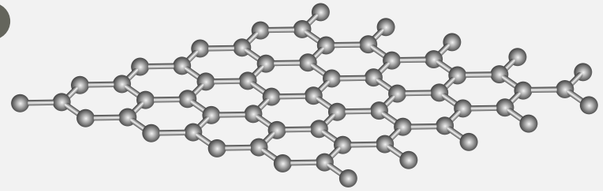
Graphene is just one example of a two-dimensional material. These materials are made of ultra-thin layers just a single atom thick, and they can have all kinds of exciting properties. They have the potential to transform numerous industries, but it is difficult to understand exactly how they work, and even more difficult to harness their potential. Researchers like María Camarasa Gómez are confronting this challenge.

The Spanish physicist, who operates at the confluence of quantum mechanics and theoretical chemistry, joined the quantum theory of materials research group at the Weizmann Institute of Science in August 2021 as an Azrieli International Postdoctoral Fellow. Led by principal investigator Leeor Kronik, the group aims to predict the properties of materials based only on their atomic composition and the laws of quantum mechanics.

GRAPHENE 101

A form of carbon that's derived from graphite, graphene is the same substance used in a regular pencil. If you lightly trace the tip of a pencil across a sheet of paper, you leave layers of it behind. These layers (1) are one atom thick. Electrons move through them as though in a two-dimensional plane. Each carbon atom in these layers is bonded to three other carbon atoms via sigma-type covalent bonds. The atoms share four electrons equally between them, and this creates a hexagonal latticework with the appearance of honeycomb. Because the atoms share electrons with each other, their chemical bonds are especially strong. As a result, graphene is among the strongest materials known to science. Moreover, these layers can be stacked like Lego (2) to make a nanomaterial that is strong, lightweight and conductive. The research that María Camarasa Gómez and her colleagues are doing to better understand the properties of graphene and other two-dimensional materials could unlock all kinds of novel applications.

1



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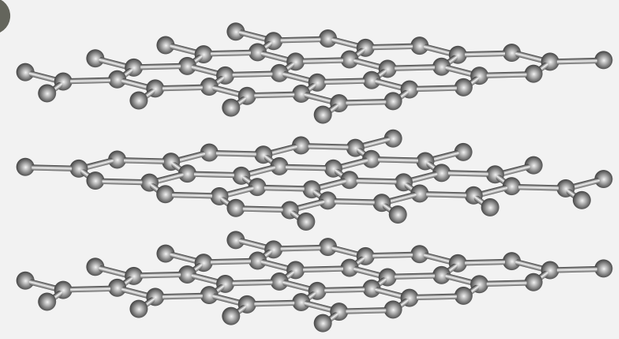

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To understand the properties of any form of matter, one must first learn how the electrons in that substance interact. Understanding the electronic and optical properties of materials in general, and those of two-dimensional materials in particular, is complex because of the need to describe how the material is perturbed from its lowest energy state. Many-body perturbation theory is one of the main ways to do this. It is highly accurate but can require a great deal of computational power and time — it can take weeks to get results — which forces researchers to consider whether each computation is feasible. Yet Camarasa Gómez is now developing variations on existing computational methods that could allow hypotheses about two-dimensional materials to be probed much more efficiently and quickly.

"We primarily use density functional theory, which is reliable but has logistical constraints," explains Camarasa Gómez, who completed a PhD in computational condensed matter physics at the University of Regensburg in Germany in 2020. "So we are developing new computational methods to study the optical and electronic properties of two-dimensional materials that are both fast and reliable and can be used daily without so much energy consumption. Instead of using 100 computers to complete this task, you might be able to use just 10."

At the quantum level, physics and chemistry intersect. Both seek to understand the properties of individual atoms. Density functional theory (DFT) is used by researchers in both disciplines to build this understanding through mathematical simulations of the quantum mechanics of atomic systems. Camarasa Gómez came across DFT in her PhD studies, then learned about Kronik's work at Weizmann and decided she wanted to collaborate with him.

Normally, a system's energy is calculated using a partial differential equation that can get very complicated when a system has many electrons and nuclei. This is called the many-body problem. DFT works around it by focusing on the density of electrons. This greatly reduces the complexity of the equation and makes simulating an atomic system much less computationally intensive. All of which means that researchers can more readily probe their hypotheses.

The quantum theory of materials research group at Weizmann is both applying DFT and developing approaches that stem from the central equation of DFT. Called the Kohn-Sham equation, it was formulated by Lu Jeu Sham and Walter Kohn in the 1960s. Kohn won the 1998 Nobel Prize in Chemistry for his leading role in DFT's development, but it was largely quantum physicists who used this equation in the decades after it was published. It was not until the 1990s and, more so, the 2000s that DFT became a mainstay of quantum chemistry.

Weizmann's quantum materials research group began to develop DFT-based approaches to compute electronic and optical properties more than a decade ago. First, they focused on very simple molecules, followed by more complex molecular crystals, and then three-dimensional semiconducting solids like silicon.

"Existing techniques were already pretty accurate for predicting, for example, the structural and mechanical properties of a material, but for electrical and optical properties, there was often a systematic failure," says Kronik. "What I mean by this is that calculations were nowhere near what we expected. You could make a prediction, but it would be wrong, so it's not much of a prediction."

Two-dimensional materials are a new frontier for DFT. Graphene is the best known of these materials, but Camarasa Gómez's work will be used to characterize the properties of around 10 to 15 other substances, representative candidates from various families of materials.

"Almost any property you can think of appears in an exotic way in some 2D material," says Kronik. "Clearly, we want to be able to predict their electrical and optical properties. That is precisely where María's work comes in, and she already has some very nice results. Being able to make predictions about these materials could help us understand experiments that are presently perplexing. It can help us figure out new materials to suggest to experimentalists to synthesize, or to tell them about the predicted properties of an existing material. But we can't do that for electrical and optical properties unless we have relatively inexpensive methods we trust.

"At some level, it is the long-standing dream of chemistry to be able to make predictions based on atomic composition alone," adds Kronik. "At a more practical level, one encounters many phenomena in the study of materials that people measure in experiments but still defy explanation."

"If we can control one layer of a material like graphene, and then put another layer on top, computational methods could help us simulate how they will interact," Camarasa Gómez elaborates. "There could be unexpected electronic or optical properties. The ability to control or 'tune' these properties — for example, enhancing conductivity — is what would enable a wide variety of applications."

Many of these applications are still on the distant horizon, and Camarasa Gómez compares our current state of knowledge to the famous image of an elephant surrounded by blindfolded scientists. Each scientist reaches out to touch the elephant, but no individual can see or feel the entire animal. One touches its leg and says that it is a tree. Another touches its tail and says that it is a snake. "The approximations we are making with density functional theory are a little like this," she says. "We don't know everything and only ever have partial information. We obtain results about certain systems, under certain conditions, but it will take the effort of many people to fully understand what we are looking at." ▲●■