Researchers establish theoretical framework for graphene physics

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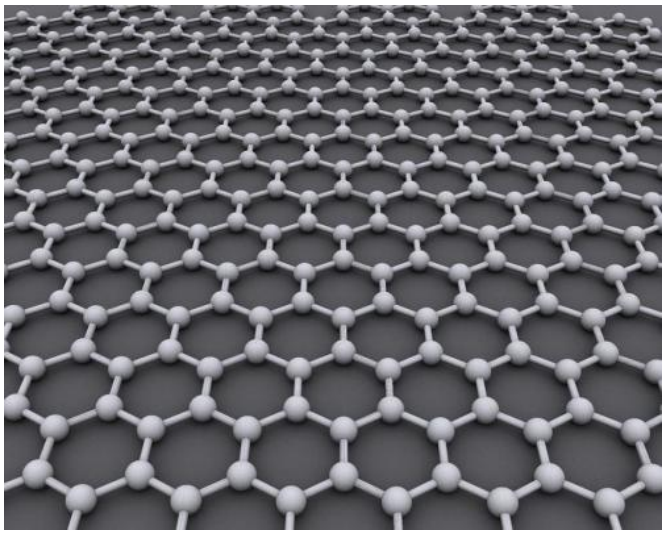

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Since the discovery of graphene about a decade ago, scientists have been studying ways to engineer electronic band gaps in the material to produce semiconductors which can create new electronic devices. A team of researchers from Yale-NUS College, the Center for Advanced 2D Materials and Department of Physics at the National University of Singapore (NUS) and the University of Texas at Austin (UT Austin) have established a theoretical framework to understand the elastic and electronic properties of graphene. The findings were published in February 2015 in *Nature Communications*.

Graphene, a single-atom-thick sheet of carbon atoms arranged in a honeycomb-like lattice, is one of the simplest materials with unrivalled mechanical and electronic properties. The material has been hailed by scientists as an extremely good conductor of electrons due to its strength and its light weight. In 2013, researchers from the Massachusetts Institute of Technology (MIT) discovered that placing graphene on top of hexagonal boron nitride, another one-atom-thick material with similar properties will create a hybrid material that shares graphene's amazing ability to conduct electrons, while adding the band gap necessary to form transistors and other semiconductor devices. Semiconductors, which can switch between conducting and insulating states, are the basis for modern electronics. The reasons behind why the hybrid material performed as such were unexplained until this new theoretical framework was created by researchers from Yale-NUS, NUS and UT Austin.

To fully harness the hybrid material's properties for the creation of viable semiconductors, a robust band gap without any degradation in the electronic properties is a necessary requirement. The researchers concluded that it is necessary to use a theoretical framework that treats electronic and mechanical properties equally in order to make reliable predictions for these new hybrid materials.

Shaffique Adam, Assistant Professor at Yale-NUS College and NUS Department of Physics, said," This theoretical framework is the first of its kind and can be generally applied to various two dimensional materials. Prior to our work, it was commonly assumed that when one 2D material is placed on top of another, they each remain planar and rigid. Our work showed that their electronic coupling induces significant mechanical strain, stretching and shrinking bonds in three dimensions, and that these distortions change the electronic properties. We find that the band gap depends on several factors including the angle between the two sheets and their mechanical stiffness. Going forward, we will continue to theoretically explore the optimal parameters to create larger bandgaps that can be used for a wide range of technologies. "

Pablo Jarillo-Herrero, the Mitsui Career Development Associate Professor of Physics at MIT, whose research team first reported band gaps

in this new graphene hybrid material said, "This theory work has increased the accuracy and predictability of calculating the induced band gap in graphene, which may enable applications of graphene in digital electronics and optoelectronics. If we are able to increase the magnitude of the band gap through new research, this could pave the way to novel flexible and wearable nanoelectronic and optoelectronic devices."

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