Researchers demonstrate the bandgap engineering of 2D C_3N bilayers

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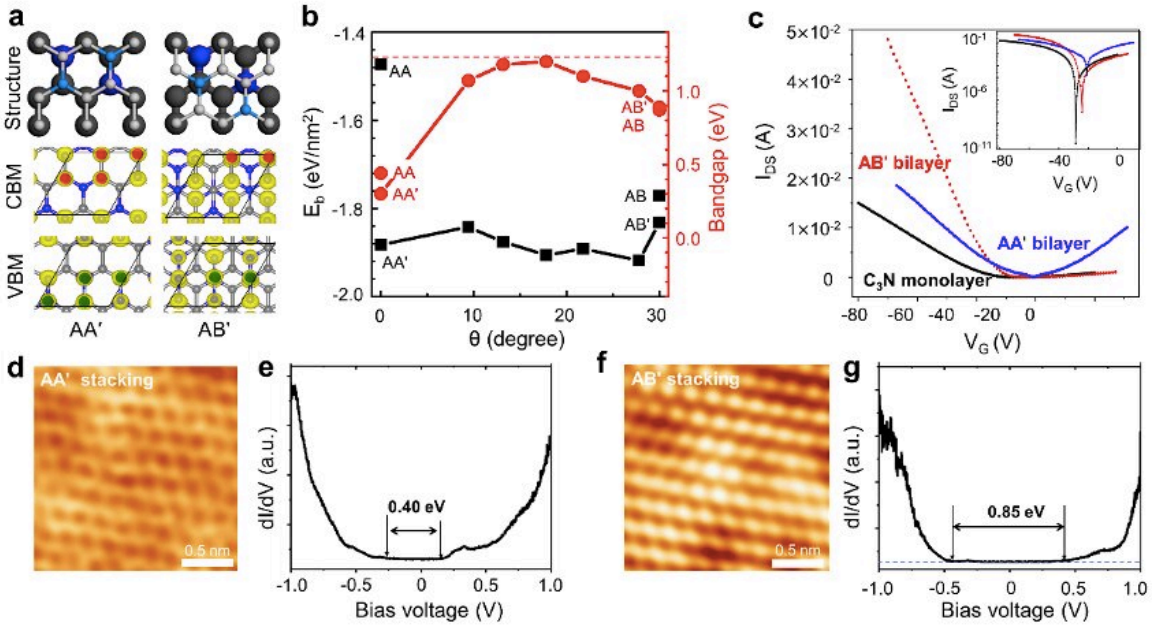


Stacking configuration and bandgap of C_3N bilayer. a, Structure and partial charge densities of the CBM and VBM of C_3Nbilayer with AA' and AB' stacking. b, binding energies (black squares) and bandgaps (red circles) of C_3N bilayers as a function of the twist angle. c, IDS-VG curves of FETs fabricated with single-layer C_3N (black curve), a C_3N bilayer with an AB' stacking (red curve) and a C_3N bilayer with an AA' stacking (blue curve). (T=4K) d, Atomic-resolution image of an AA' stacking area with honeycomb lattice. e, a representative dI/dV spectra showing the electronic bandgap of C_3N bilayer with AA' stacking. f, atomic-resolution image of an AB' stacking area with hexagonal lattice. g, a representative dI/dV spectra showing the electronic bandgap of C_3N bilayer with AB' stacking. Credit: Wei et al.

Silicon-based transistors are rapidly approaching their limits, both in terms of speed and performance. Engineers and material scientists have thus been trying to identify alternative materials that could enable the development of faster and better performing devices.

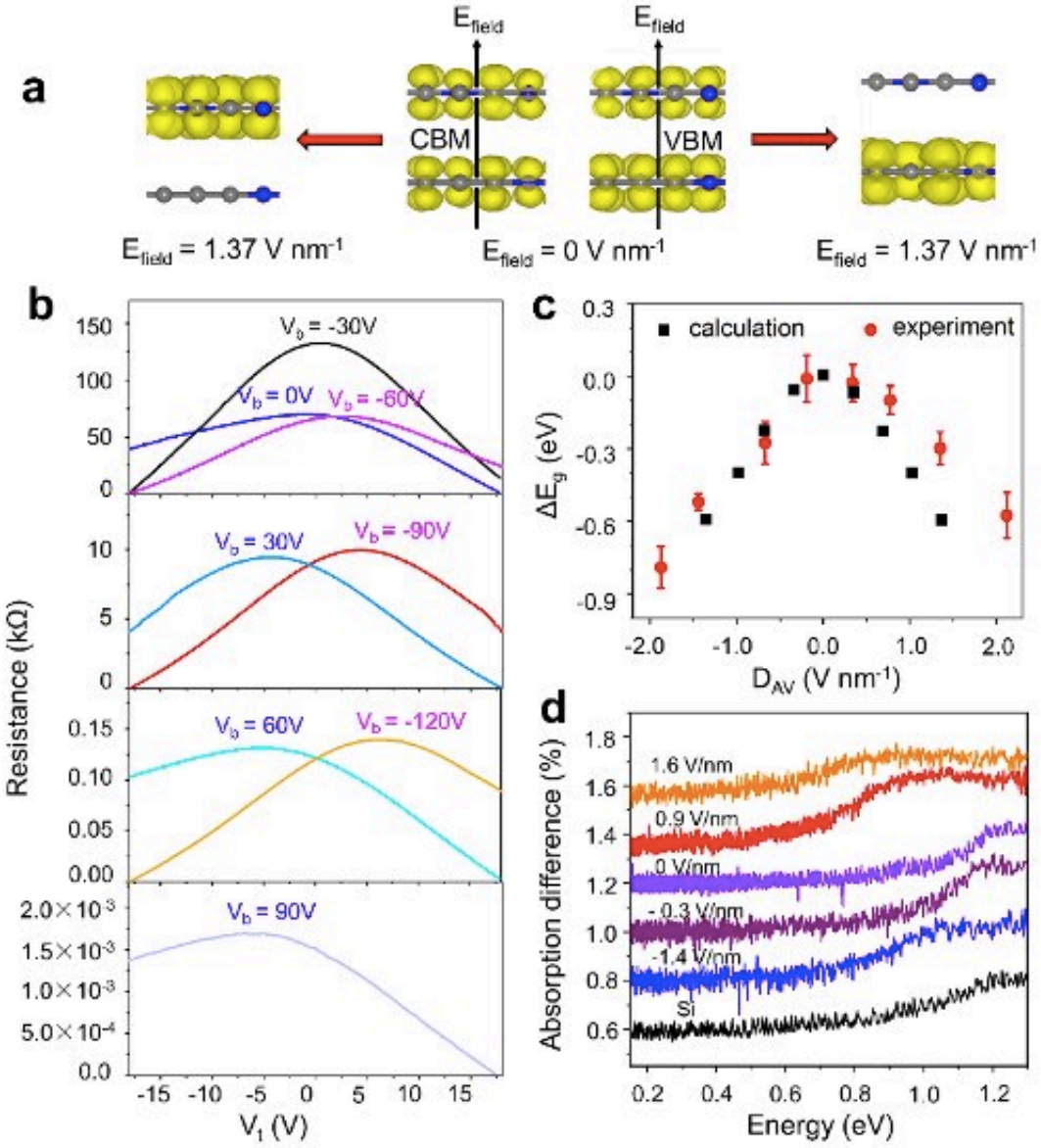
Carbon-based materials are among the most favorable candidates for the development of the next generation of electronics, due to their many advantageous properties, including a high mechanical strength and a good electrical and thermal conductivity. One of the most promising among these materials is graphene, which also exhibits a high flexibility and transparency.

Despite its advantages, graphene has no bandgap, which is an essential requirement for channel materials inside transistors. In recent years, some engineers have thus been conducting studies evaluating an alternative two-dimensional (2D) material that resembles graphene, known as C_3N. C_3N consists of a uniform distribution of carbon and nitrogen atoms, arranged in a graphene-like structure.

Researchers at University of Queensland in Australia, East China Normal University, Shanghai Institute of Microsystem and Information Technology and other institutes in China have recently demonstrated that the bandgaps of bilayers of 2D C_3N can be engineered by changing their stacking order or applying an electric field to them. Their paper, published in *Nature Electronics*, could pave the way towards the development of better performing C_3N-based devices.

"C_3N has attractive properties similar to graphene, but in addition, has a medium sized bandgap," Zhenhui Kang, Debra J. Searles and Qinghong Yuan, three of the researchers who carried out the study, told *Tech Xplore* via email. "We therefore thought that we might be able to tune

the properties of the C_3N monolayer by forming different bilayers and changing its environment by applying an electric field."



Bandgap engineering of C_3N bilayer induced by external electric fields. a, Illustration of charge density separation of the CBM and VBM of C_3N bilayer with AB' stacking under external electric fields. b, Electrical resistance of a C_3N bilayer with AB' stacking as a function of top gate voltage (Vt) at different fixed bottom gate voltages (Vb). c, Experimental measured (red dots) and the DFT

calculated (black squares) variations of the energy bandgap as a function of the average electrical displacement field (DAV). d, Gate-induced absorption spectra of C_3N bilayers at CNPs (δD=0) with different applied displacement fields DAV. Credit: Wei et al.

Kang, Searles, Yuan and their colleagues carried out a series of theoretical calculations and experiments aimed at investigating the potential of C_3N as a material to develop the next generation of electronic devices. They found that C_3N bilayers can have a wide bandgap tuning range, while also exhibiting controllable on/off ratios, high carrier mobilities and photoelectronic detection capabilities.

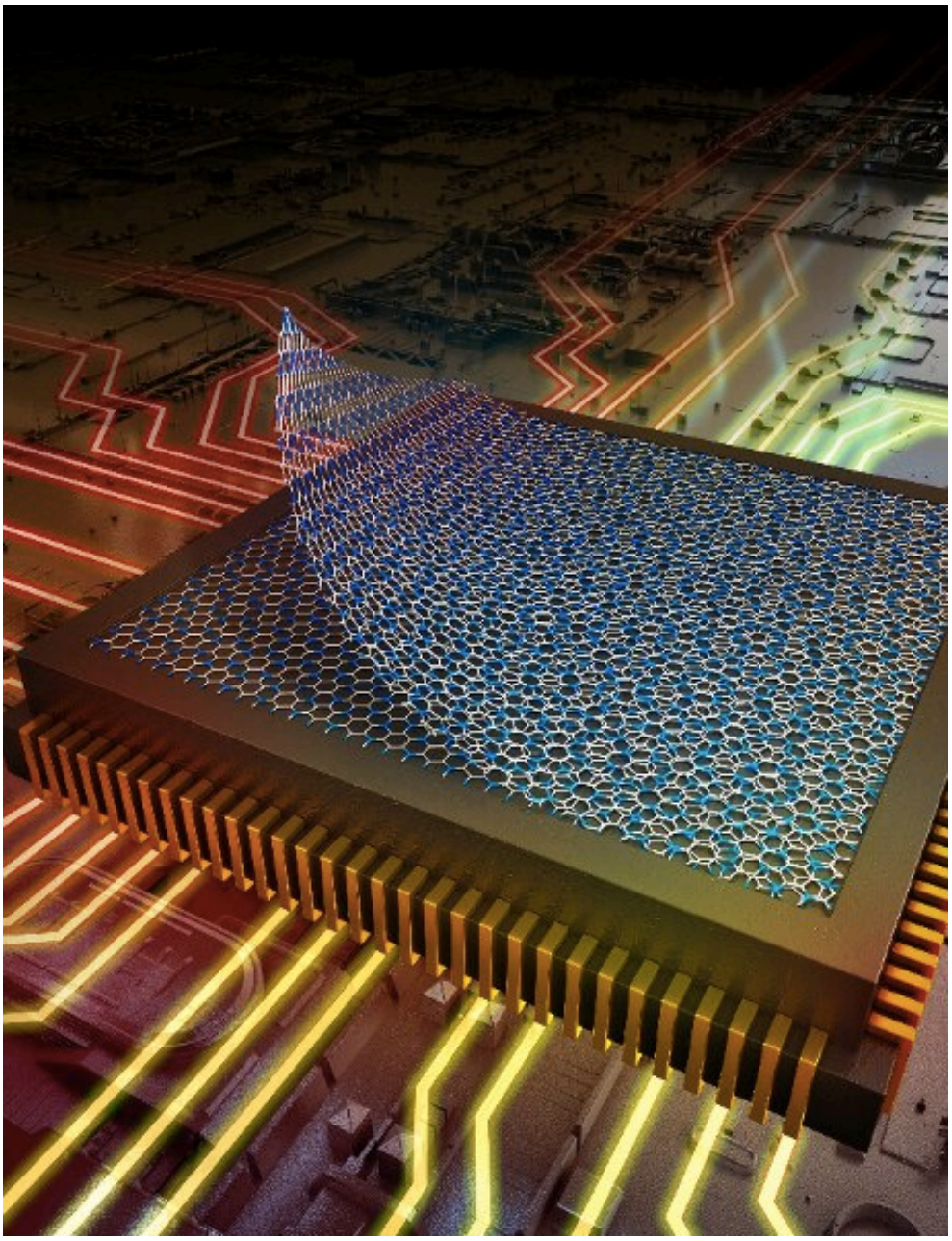
In their paper, the researchers proposed two different strategies for engineering the bandgap of C_3N bilayers. The first strategy consists in tuning the stacking configuration or twist angle between top and bottom C_3N layers.

"Fabrication of layered 2D materials with required twist angles has been achieved using the transfer method or atomic force microscope (AFM) tip manipulation techniques," Kang, Searles and Yuan said. "C_3N bilayers with different twist angles could have completely different bandgaps, varying from 0.3 to 1.21 eV. To the best of our knowledge, this is the bilayer material that demonstrates the largest bandgap tuning range."

The second strategy for engineering the bandgap of C_3N bilayers proposed by the researchers entails application of an external electric field. This strategy has already been widely used to modulate the bandgap of numerous other 2D bilayer materials.

"We found that the bandgaps of C_3N bilayers can be tuned from 0.89 eV

to nearly 0 eV only under a medium applied voltage of 1.91 V/nm," Kang, Searles and Yuan said. "Overall, our results suggest that the C_3N bilayer could substantially change the bandgap, while maintaining other attractive properties. The part of our team who focused on the experimental side of our research was able to synthesize the materials and test them experimentally."



The new structures enable production of various electronic components that can be combined to produce electronics with requirements and capabilities. Credit: Wei et al.

The primary goal of the recent study by Kang, Searles, Yuan and their colleagues was to develop a new 2D carbon-based material that could help to extend Moore's law in a post-silicon era. By uncovering the highly advantageous properties of C_3N bilayers, the researchers demonstrated its potential for the development of better performing, carbon-based field effect transistors (FETs), as well as other electronic and optoelectronic devices.

"The high carrier mobilities and widely tunable bandgap of C_3N bilayers makes them very promising for applications in many research fields," Kang, Searles and Yuan said. "For example, depending on the stacking order, the C_3N bilayer can be either semiconducting or metallic, which means that it could be used for both conducting and channel materials in transistor fabrication. This may be helpful in resolving the problems of contact resistance of different materials in transistor fabrication."

The recent study by this team of researchers could inform the development of better performing carbon-based electronic devices. In addition, the C_3N they fabricated could be used to create more advanced optoelectronics and laser communication technologies. In fact, the team showed that FETs fabricated using AB' C_3N were highly photo-responsive upon near-infrared (wavelength 1550 nm) light illumination.

"The excellent photo-responsivity of AB' C_3N bilayers to near-infrared light makes them suitable for infrared photodetection, which has the advantages of an atmospheric window and 24-hour detection in comparison with other photodetection methods. In addition to a high

carrier mobility, good photo-responsivity, stable chemical properties, low resistivity, and high mechanical strength, our C_3N material is compatible with the well-developed silicon devices."

The 2D C_3N bilayers examined Kang, Searles and Yuan have numerous advantageous characteristics and could soon be used to create a variety of devices. In contrast with other carbon-based materials, these bilayers are highly flexible and transparent, thus they could also be used to create transparent electrodes and wearable devices. In fact, the bandgap of C_3N can also be tuned using a bilayer, rather than multilayers. This results in a thinner material with greater transparency and flexibility.

"Considering that the development of current infrared photodetectors is hampered by the need for high-performance materials, C_3N materials provide a promising option for future infrared photodetector and laser communications," Kang, Searles and Yuan said. "Our future research in this field will focus on the application of C_3N materials in infrared photodetection, sensor and ferroelectric materials. We will also try to fabricate a C_3N transistor with high performance."

More information: Wenya Wei et al, Bandgap engineering of two-dimensional C_3N bilayers, *Nature Electronics* (2021). DOI: 10.1038/s41928-021-00602-z