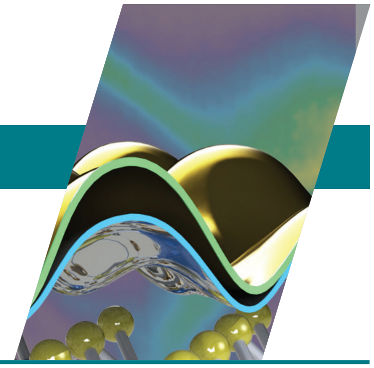
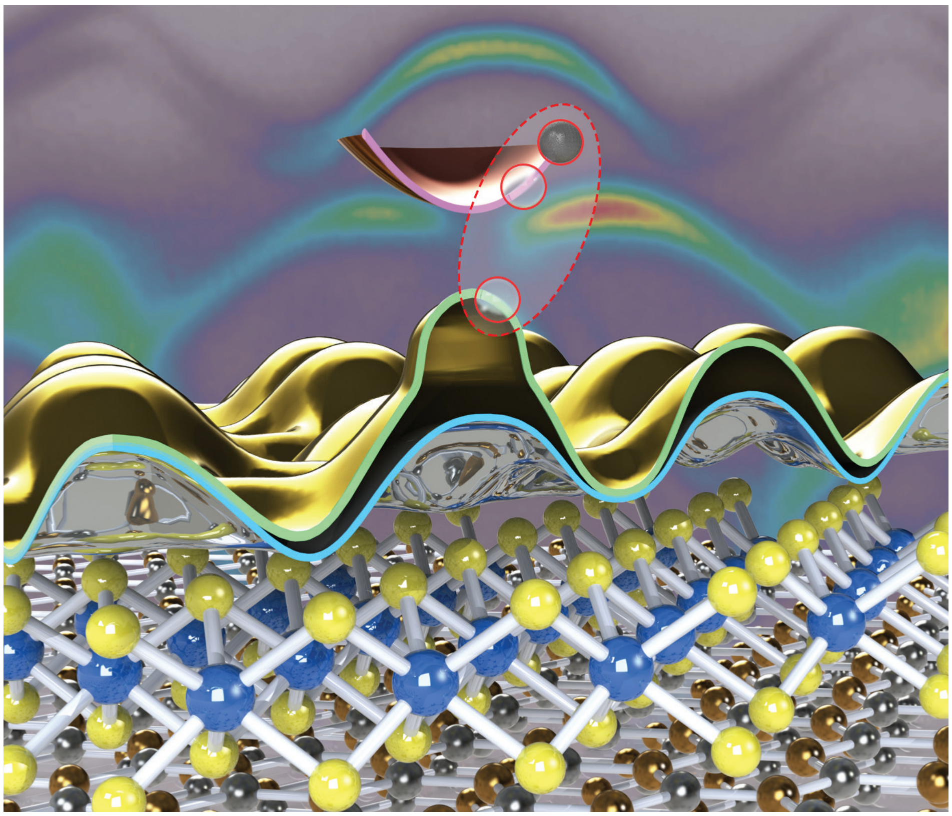
ADVANCED LIGHT SOURCE

MATERIALS SCIENCES

Tuning the Electronic Structure of a 2D Material





Rendering of the atomic structure of a 2D layer of tungsten disulfide, or WS_2 (blue and yellow), on top of layers of 2D boron nitride (silver and gold). Above that is a representation of the WS_2 valence bands (green- and blue-edged metallic surfaces), showing increased splitting. The results of this experiment suggest that the splitting could be due to the presence of "trions," exotic three-particle combinations of holes and electrons, depicted here as transparent and gray spheres, respectively, in the valence and conduction bands (the conduction band is rendered as a pink-edged metallic surface). The background shows the raw WS_2 electronic-structure data, as measured in the experiment. (Credit: Chris Jozwiak/Berkeley Lab)

Scientific Achievement

The electronic structure of a stacked 2D material was tuned by in situ electron doping, resulting in a large increase in the splitting of two valence bands.

Significance and Impact

Stacked 2D materials possess an array of tunable properties that are expected to be important for future applications in electronics and optics.

Mix 'n' match materials

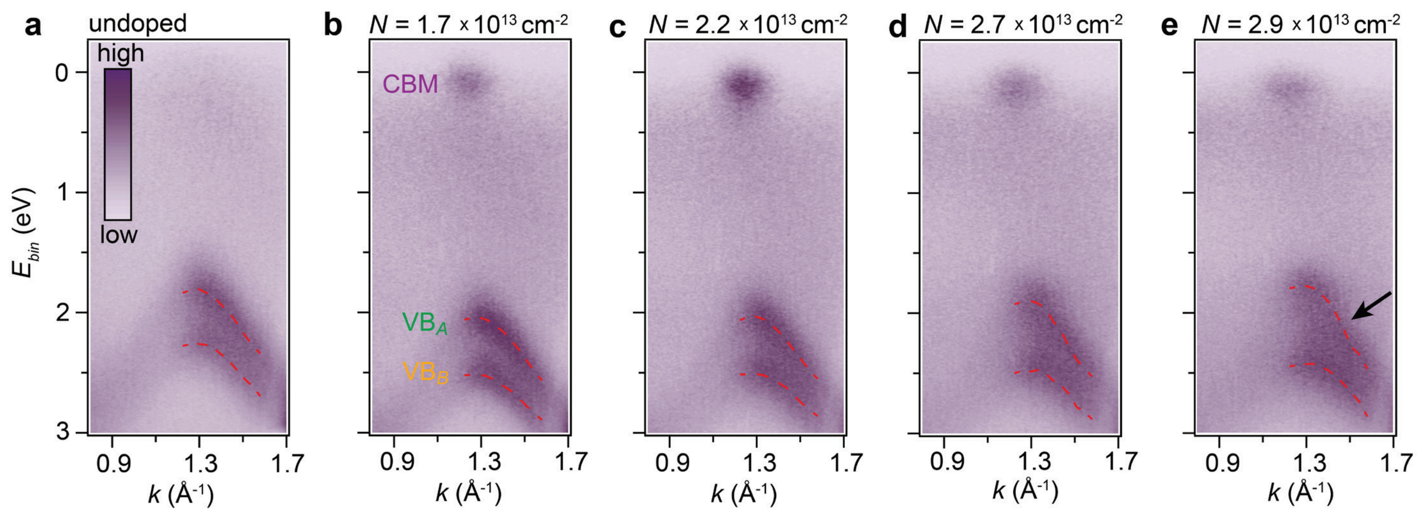
When some atomically thin—or 2D—materials are stacked like Lego bricks in different combinations with other ultrathin materials, new properties often emerge that are potentially useful for next-generation device applications. For example, tungsten disulfide (WS_2) is a semiconductor that belongs to a family of 2D materials (transition-metal dichalcogenides, or TMDs) that have received an enormous amount of interest due to their many advantageous properties that can be tuned by mixing and matching them in stacks with other 2D materials.

In this work, single-layer WS_2 was stacked on a thin flake of hexagonal boron nitride (h-BN), all on a base of titanium dioxide (TiO_2). This heterostructure provided a stable, non-interacting platform that enabled a team of researchers to directly and accurately probe the WS_2 electronic states and excitations, including the effects of interactions between the electrons themselves (many-body effects), at a level of detail not previously possible.

MAESTRO's exquisite sensitivity

MAESTRO (Microscopic and Electronic Structure Observatory), a facility at ALS Beamline 7.0.2 that opened to scientists in 2016, can handle very small sample sizes, on the order of tens of microns, which is key to studying 2D materials. Scientists are continuing to push MAESTRO's capabilities to study even smaller features—down to the nanoscale. The endstation also features the ability to fabricate and manipulate samples for x-ray studies while maintaining pristine conditions that protect them from contamination.

To probe the WS_2 electronic structure, the researchers used micro-focused



The divide between valence bands VB_A and VB_B grows as the sample is doped. N = charge-carrier density. CBM = conduction-band minimum. Arrow in (e) points to a possible kink in VB_A.

angle-resolved photoemission spectroscopy (microARPES), a technique in which a beam of x-rays, focused to 10 μm, is used to kick electrons out of the sample. By analyzing the ejected electrons' direction and energy, the researchers can obtain the material's band structure—a map of the electrons' behavior in the semiconductor. Moreover, the technique is capable of resolving many-body effects and capturing subtle changes caused by the stacking of 2D materials.

Doping splits up the band

Seeing the intrinsic electronic properties of WS_2 was an important step, but the biggest surprise emerged when the researchers increased the number of electrons in the system through in situ surface doping. This led to a dramatic change in the WS_2 band structure, substantially increasing the splitting between two valence bands, from 430 meV to 660 meV, and reducing the bandgap by at least 325 meV. The study suggests that this ability to tune the electronic structure of WS_2 is driven by trions—exotic three-particle combinations of electrons and holes.

The increased valence-band splitting bodes well for the potential use of WS_2 in spintronic devices. WS_2 is also known to interact strongly with light. The new findings make it a promising candidate for optoelectronics, in which electronics can be used to control the release of light, and vice versa.

There is an endless array of possibilities in this world of "2D Legos." Scientists are right now on the brink of being able to study a huge variety of such materials, measuring their electronic behavior and studying how these effects develop at even smaller scales.

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