Excitonic dark states shed light on TMDC atomic layers

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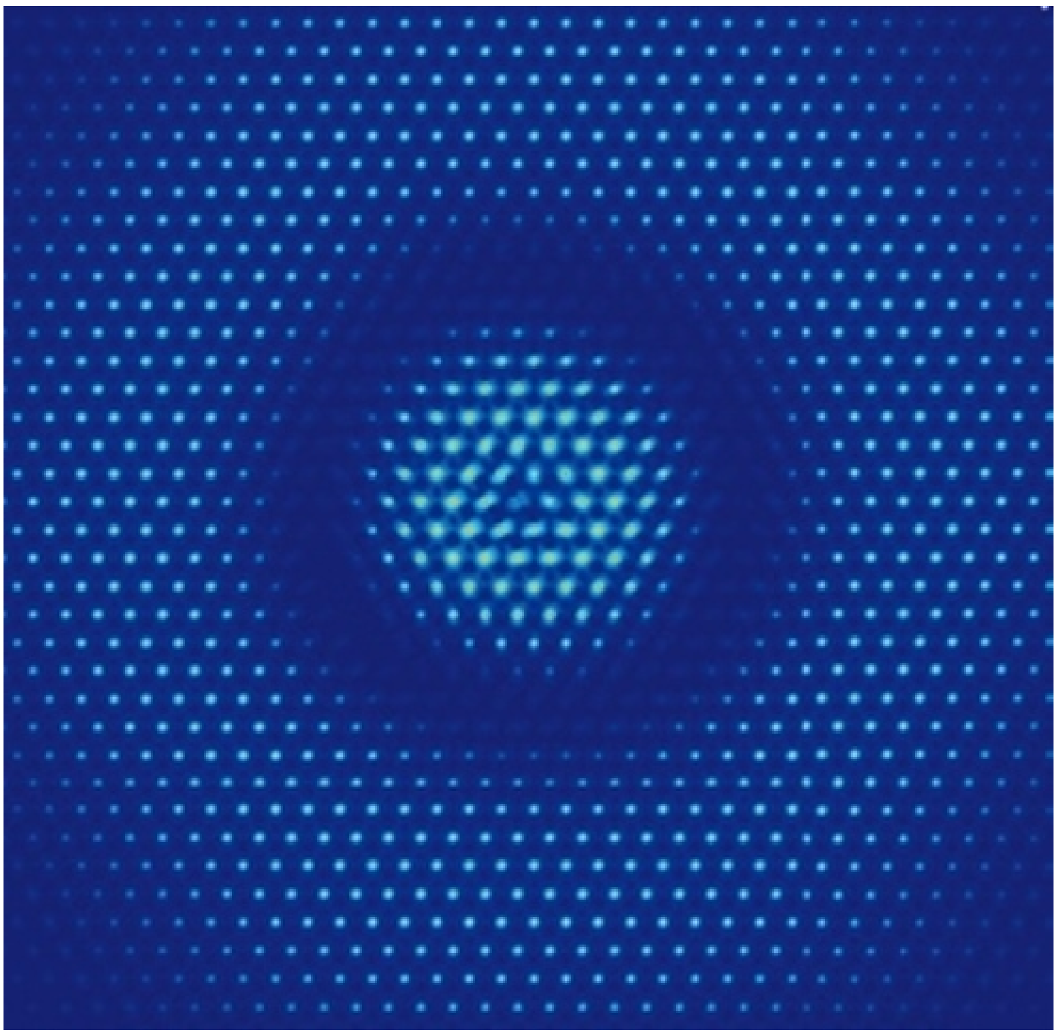

Berkeley Lab researchers have found evidence for excitonic dark states in monolayers of tungsten disulfide that could explain the unusual optoelectronic properties of single atomic layers of transition metal dichalcogenide (TMDC) materials.

(Phys.org) —A team of Berkeley Lab researchers believes it has uncovered the secret behind the unusual optoelectronic properties of single atomic layers of transition metal dichalcogenide (TMDC) materials, the two-dimensional semiconductors that hold great promise for nanoelectronic and photonic applications.

Using two-photon excitation spectroscopy, the researchers probed monolayers of tungsten disulfide, one of the most promising of 2D materials, and found evidence for the existence of excitonic dark states – energy states in which single photons can be neither absorbed nor emitted. These excitons were predicted from ab initio calculations by members of the research team to have an unusual energy sequence, plus excitonic binding energy and bandgaps that are far larger than was previously suspected for 2D TMDC materials.

"Discovery of very large excitonic binding energy and bandgaps and its nonhygrogenic nature in 2D semiconductor materials is important not only for understanding the unprecedented light-matter interaction arising from strong many-body effect, but also for electronic and optoelectronic applications, such as ultra-compact LEDs, sensors and transistors," says Xiang Zhang, director of Berkeley Lab's Materials Sciences Division and the leader of this study. "Such a large binding energy – 0.7eV – could also potentially make room-temperature excitons stable for future quantum computing efforts."

Zhang holds the Ernest S. Kuh Endowed Chair Professor at the University of California (UC) Berkeley, directs the National Science Foundation's Nano-scale Science and Engineering Center, and is a member of the Kavli Energy NanoSciences Institute at Berkeley. He and Berkeley Lab theoretical physicist Steven Louie, also with the Materials Sciences Division and UC Berkeley, are the corresponding authors of a paper in Nature that describes this research. The paper is titled "Probing excitonic dark states in single-layer tungsten disulphide." Co-authors are

Ziliang Ye, Ting Cao, Kevin O'Brien, Hanyu Zhu, Xiaobo Yin, and Yuan Wang.

Excitons are bound pairs of excited electrons and holes that may cause significant deviations between photon absorption or emission energies and the electronic bandgaps that enable semiconductors to function in devices. 2D TMDC materials have generated quite a buzz in the electronics industry because they offer superior energy efficiency and carry much higher current densities than silicon. Furthermore, unlike graphene, the other highly touted 2D semiconductor, TMDCs have finite bandgaps. This makes them more device-ready than graphene, which has no natural bandgaps. However, questions marks hovering over the bandgap size and excitonic effect in 2D TMDCs have hampered their development.

"By experimentally revealing 2D excitonic dark states in a TMDC monolayer, we have demonstrated intense many-electron effects in this class of 2D semiconductors," says Ziliang Ye, a member of Zhang's research group and one of two lead authors of the Naturepaper. "Our discovery provides a basis for exploiting the unusual interactions between light and matter that result from strong excitonic effects, and should also enable better designs of heterostructures that involve TMDC monolayers."

In addition to LEDs and photodetectors, the discovery of strongly bound excitonic dark states could also hold important implications for "valleytronics," a highly promising potential new route to novel electronics and ultrafast data-processing.

"In valleytronics, information is encoded in a wave quantum number that describes which valley of the energy-momentum landscape a carrier belongs to as it moves through a crystal lattice," says Louie. "Our work provides new understanding and information on the photo-excited states, and on the resulting carriers where the valley information is encoded."

Says Ting Cao, a member of Louie's research group and the other lead author of the Nature paper, "2D TMDCs should be also well-suited for the next generation of flexible devices and wearable electronics."

More information: "Probing excitonic dark states in single-layer tungsten disulphide." Ziliang Ye, et al, *Nature* 513, 214–218 (11 September 2014) [DOI: 10.1038/nature13734](https://dx.doi.org/10.1038/nature13734)

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