Study shows temperature can dramatically affect behavior of 2-D materials

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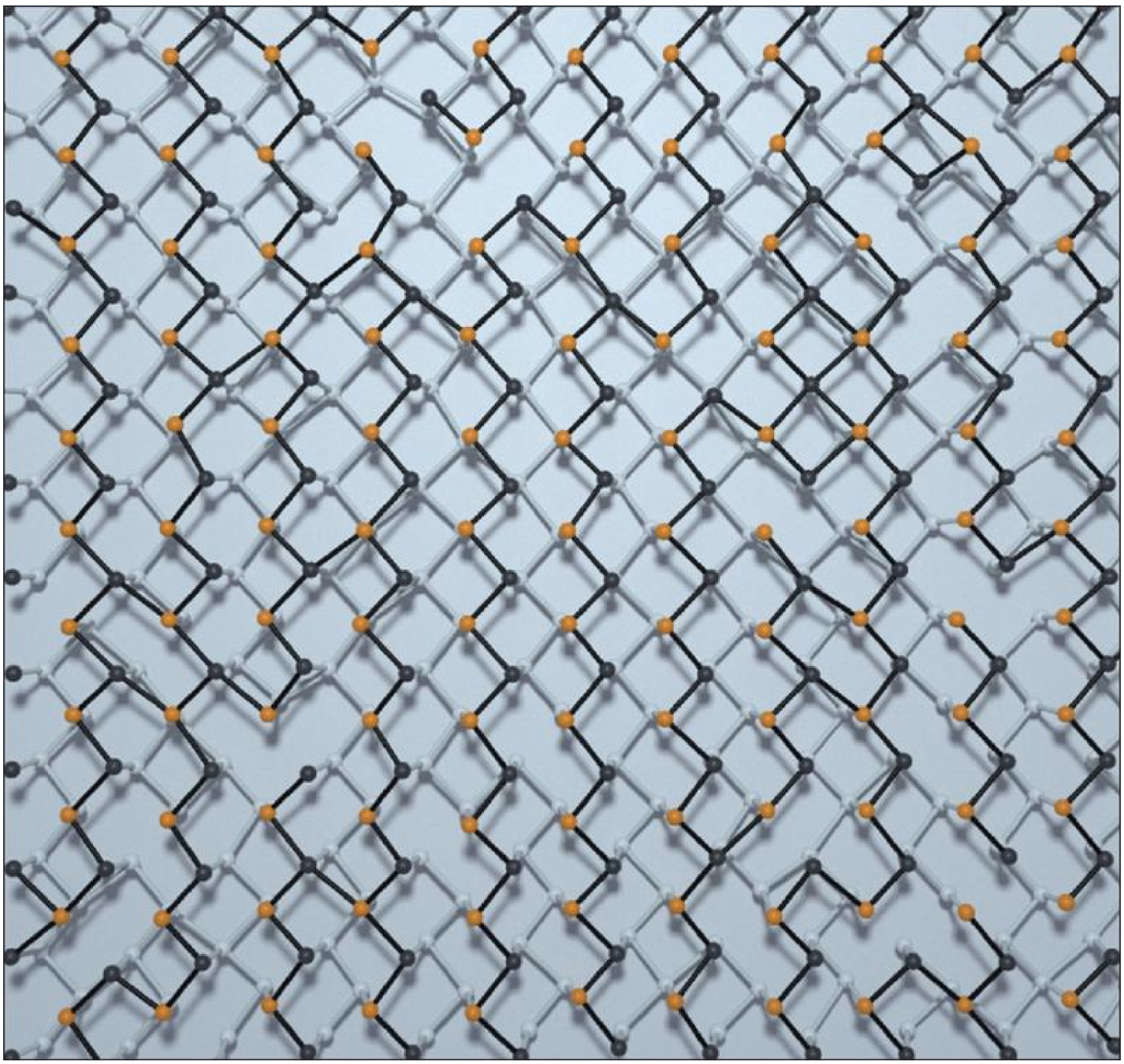

A tin selenide monochalcogenide monolayer at room temperature. Credit:

Edmund O. Harriss

New research at the University of Arkansas shows that temperature can be used to dramatically alter the behavior of two-dimensional materials that are being investigated as candidates to power the next generation of electronic devices.

The research revealed black phosphorous and monochalcogenide monolayers act differently than any other known 2-D materials at any given temperature because there are four ways to create their atomistic arrangement, and these four arrangements compete and lead to disorder, said Salvador Barraza-Lopez, an assistant professor of physics at the University of Arkansas.

"Remarkably, nobody had found that some of these two-dimensional materials become disordered at a room temperature and well before they melt," Barraza-Lopez said. "At the transition temperature the unit cell transforms from a rectangle onto a square and all material properties change."

An international research team led by Barraza-Lopez and Pradeep Kumar, assistant professor of physics at the U of A, published its findings in *Nano Letters*, a journal of the American Chemical Society.

The black phosphorous and monochalcogenide monolayers become disordered at a finite temperature, Barraza-Lopez said.

"At that moment, the structure transforms from a rectangle to a square and its behavior also changes," he said.

Having access to the Trestles supercomputer at the Arkansas High

Performance Computing Center was crucial to the study, Barraza-Lopez said.

Barraza-Lopez and Mehrshad Mehboudi ran multiple calculations on Trestles for about three weeks each and without interruption. Mehboudi is a doctoral student in the university's interdisciplinary microelectronics-photonics graduate program.

"There is no way we could have achieved these results in the timeframe we did without Trestles," Barraza-Lopez said.

More information: Mehrshad Mehboudi et al. Two-Dimensional Disorder in Black Phosphorus and Monochalcogenide Monolayers, *Nano Letters* (2016). DOI: 10.1021/acs.nanolett.5b04613

Provided by University of Arkansas

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