New phase change mechanism could lead to new class of chemical vapor sensors

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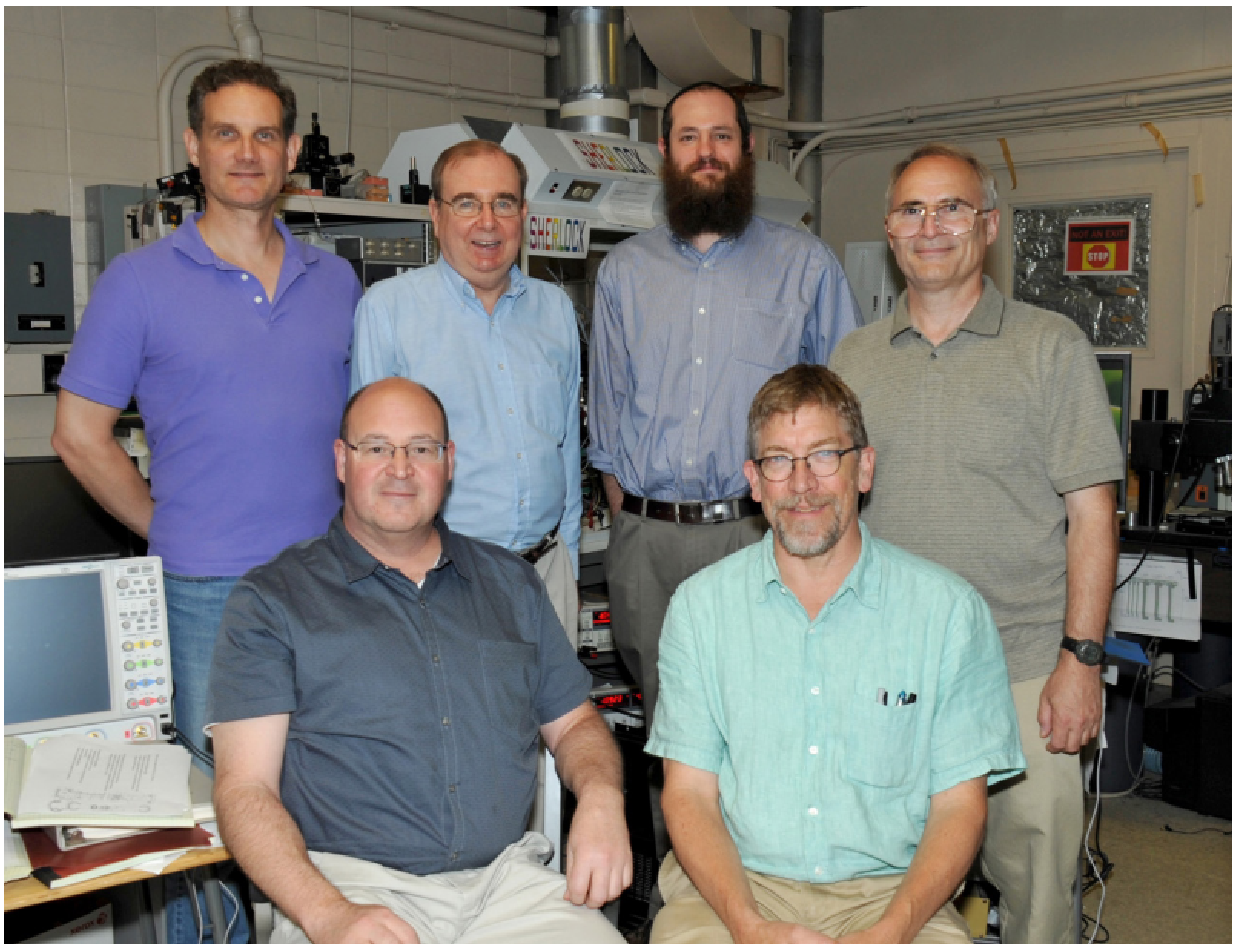

An interdisciplinary team of scientists at the U.S. Naval Research Laboratory (NRL) has demonstrated optical and electronic evidence of semiconductor-to-metallic phase transition when exposed to airborne chemical vapors, and how the behavior can be used to create an entirely new class of chemical vapor sensors. Back row from left to right: Research physicists Drs. Aubrey Hanbicki, Paul Campbell, Adam Friedman, and Jim Culbertson. Seated front: Dr. Glenn

Jernigan, research chemist; and Dr. Keith Perkins, electronics research engineer. Credit: U.S. Naval Research Laboratory/Gayle Fullerton

An interdisciplinary team of scientists at the U.S. Naval Research Laboratory (NRL) demonstrated that monolayer 2-D Transition Metal Dichalcogenides (TMDs)—atomically thin semiconductors—undergo a change from semiconductor-to-metallic phase when exposed to airborne chemical vapors.

The team validated optical and electronic evidence of the phase transition and how the behavior can be used to create an entirely new class of chemical vapor sensors. This new class of instruments are potentially more sensitive than current state-of-the-art models, and selective to specific nerve agents and explosive compounds which are of great concern on today's battlefields.

Since the discovery in 2004-2005 that single monolayer films of TMDs can be isolated from bulk materials due to the weak interlayer bonding of atoms, known as van der Waals bonding, these materials continue to reveal new and remarkable behaviors and properties.

"These materials are extremely promising for chemical vapor sensing applications because the inherent few-atom-thickness of the material greatly enhances their sensitivity to even the smallest surface disturbance," said Dr. Adam L. Friedman, research physicist, Material Science and Technology Division. "Apart from the immediate interest to basic research, as this particular method of creating of phase transition in TMDs has never been observed or explored before, it has great potential application in a new type of phase-based, multifunctional chemical vapor sensor."

Monolayer TMDs offer possible advances in technology over current material models, which pave the way for inexpensive, flexible, high-performance devices that exploit their unique surface-dominated functionality.

Chemically abbreviated as MX2, where M is a transition metal and X is a chalocogen, the monolayer TMDs include insulators, semiconductors, metals and other types of materials, and include a variety of properties not observed in their bulk material equivalents. Certain films respond selectively through a charge transfer process to a class of analytes that includes nerve agents, such as venomous agent X (VX), A microscopic quantity of analyte lying on the surface of the TMD acts as an electron donor and local reducing agent, which measurably affects the conductance of the film.

The NRL team hypothesized that certain strong electron donor chemical analytes, like those relevant for sensing certain nerve agents and explosives, can also provide enough charge transfer to the TMD to achieve a phase change. To test their hypothesis, the researchers exposed monolayer TMD films to strong electron donor chemical vapor analytes and monitored them for their conductance and optical response. They found that the conductance response of their devices ceased after moderate exposure and the overall magnitude of the conductance abruptly increased significantly that moment, which signaled a phase change. The optical response also corroborated a phase change.

Friedman said, "We assembled an exceptionally large data set that included multiple methods of measuring these types of films and concluded that the behavior that we observed is not due to doping and is most likely due to partial, localized phase changes in the areas of the TMD film where weakly adsorbed analyte transfers charge to the lattice."

This newly discovered behavior opens up an entirely new possibility for low-power, flexible, versatile chemical vapor sensor devices. If the phase transition can be harnessed to directly sense strong electron donor analytes it will create an entirely new chemical vapor-sensing model. It will allow passive-type optical measurements to be combined with, or used separately from, active conductance measurements to identify analyte vapors all with the same device and be used as the operating mechanism for a new method to identify chemical compounds and the presence of dangerous vapor.

Previous studies of similar diffusionless phase changes have shown speeds in the nanosecond range, and the envisioned devices will also be fast, which will exceed the state-of-the art in detection speed. Because the amount of charge necessary to induce a phase change in each TMD material is different, a suite of concurrently sensing TMD materials will allow various strength electron donors/acceptors to be detected and even identified with the necessary redundancy to minimize error. Due to their low space requirements and expense, these sensors can also easily be combined with current sensors to create an even more versatile instrument for current Department of Defense (DoD) platforms.

The results are reported in the June 2017 issue of *Nature* Publishing Group's *Scientific Reports*.

More information: Adam L. Friedman et al. Evidence for Chemical Vapor Induced 2H to 1T Phase Transition in MoX2 (X = Se, S) Transition Metal Dichalcogenide Films, *Scientific Reports* (2017). DOI: 10.1038/s41598-017-04224-4

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