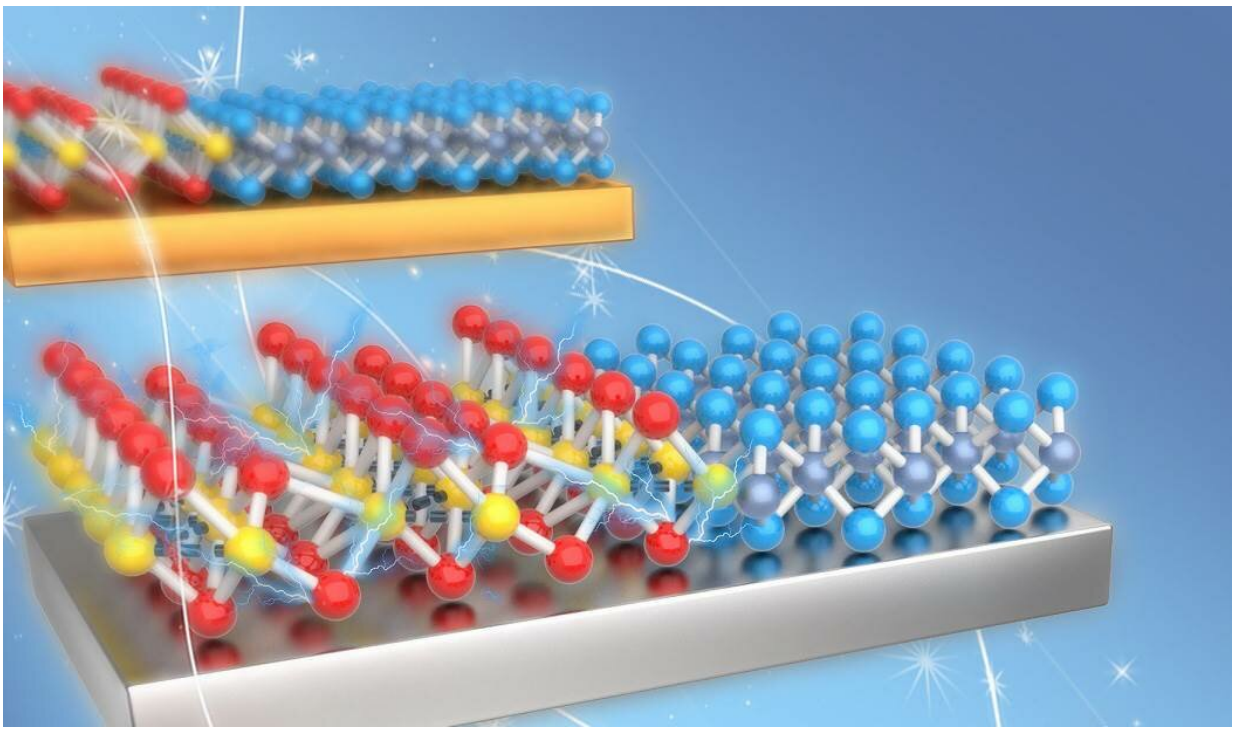
Phase transition dynamics in two-dimensional materials

February 12 2019



Molecules of monolayer molybdenum disulphide (MoS2) and tungsten diselenide (WSe2) on top of a metal substrate. Credit: National University of Singapore

Scientists from National University of Singapore have discovered the mechanism involved when transition metal dichalcogenides on metallic substrates transform from the semiconducting 1H-phase to the quasi-metallic 1T'-phase.

Two-dimensional transition metal dichalcogenides (2-D-TMDs) such as monolayer molybdenum disulphide (MoS_2) are atomically thin semiconductors in which a layer of transition metal atom is sandwiched between two layers of chalcogen atoms, in the form MX2. They can exist in both a semiconducting 1H-phase and a quasi-metallic 1T'-phase, with each having a different crystal structure. The 1T'-phase is particularly interesting as theoretical predictions show that it has potential to be used in less conventional applications, such as super capacitor electrodes and hydrogen evolution reaction catalysts. However, the quantity of 1T'-phase 2-D-TMDs that can be obtained by converting them from the 1H-phase through a phase transition process is low. This potentially limits the use of such novel materials for a wide range of applications.

A research team led by Professor Andrew Wee from the Department of Physics at the National University of Singapore's (NUS) Faculty of Science has discovered that while different 2-D-TMD materials have their own intrinsic energy barriers when transiting from the 1H to the 1T' structural phase, the use of a metallic substrate with higher chemical reactivity can significantly increase the 1H- to 1T'- phase transition yield. This is a convenient and high-yielding method to obtain 2-D-TMD materials in their 1T' metallic phase. When the 2-D-TMD material is placed in contact with the metal substrate, such as gold, silver and copper, electric charges are transferred from the metal substrate to the 2-D-TMD material. Furthermore, it weakens the bond strength of the 2-D-TMD structure significantly, and increases the magnitude of the interfacial binding energy. This in turn increases the susceptibility of the 1H-1T' structural phase transition. As a result, this enhanced interfacial hybridisation at the interface of the two materials makes the 1H-1T' structural phase transition much easier to achieve.

The NUS research team combined multiple experimental techniques and first-principles calculations in their research work. These includes

optical spectroscopies, high resolution transmission electron microscopy and density functional theory based first-principles calculations to identify the phase changes—both 1H- and 1T'-phases—of the 2-D-TMDs in the samples.

This study provides new insights on the influence of interfacial hybridisation affecting the phase transition dynamics of 2-D-TMDs. The findings can potentially be used in a model system for the controlled growth of 2-D-TMDs on metallic substrates, creating possibilities for new 2-D-TMDs-based device applications.

Prof Wee said, "The controllability of the semiconductor to metal phase transition at the 2-D-TMD and metal interfaces can enable new device applications such as low contact resistance electrodes."

More information: Xinmao Yin et al. Unraveling High-Yield Phase-Transition Dynamics in Transition Metal Dichalcogenides on Metallic Substrates, *Advanced Science* (2019). DOI: 10.1002/advs.201802093

Provided by National University of Singapore

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