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Physisorption-Mediated Exfoliation of Centimeter-Sized Monolayer MoS_2 on Gold

The conflict between the material quality and production scalability is one of the major challenges for future applications of two-dimensional materials. The typical lateral size of monolayer transition metal dichalcogenides (TMDCs), such as MoS_2, achieved by mechanical exfoliation is currently limited to ca. 100 µm on insulating substrates [1]. Recently, direct exfoliation of TMDCs on metallic substrates of larger dimensions has been reported, with the focus on potential applications in optoelectronics and catalysis [2].

Herein, we report mechanical exfoliation of centimeter-sized monolayer MoS_2 on gold substrates (Figure 1), which is facilitated by strong physisorption between the two materials and also extends to other TMDCs [3]. The surface contamination and roughness of the Au substrates are found to be the key parameters for successful high-yield exfoliation. Microscopic and spectroscopic characterization, and first-principles density functional theory calculations of the MoS_2/Au heterostructures confirm the existence of a strong van der Waals interaction (physisorption) between MoS_2 and Au, resulting in a significant charge transfer between the two materials without compromising the structural integrity of the monolayer MoS_2. Furthermore, electrochemical characterization reveals that the monolayer MoS_2 passivates the chemical properties of the underlying Au, and that the Au significantly modulates the electronic band structure of the MoS_2.

This simple and reproducible exfoliation technique facilitates the production of large-area TMDCs, enabling studies previously limited by their small lateral size. It is likely that these findings will be applied in research areas such as electrode modification, photovoltaics, and photocatalysis.

References

[1] Velický, M. et al., Nano Letters, 16 (2016), 2023
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[3] Velický, M. et al., ACS Nano, 12 (2018), 10463

Figures

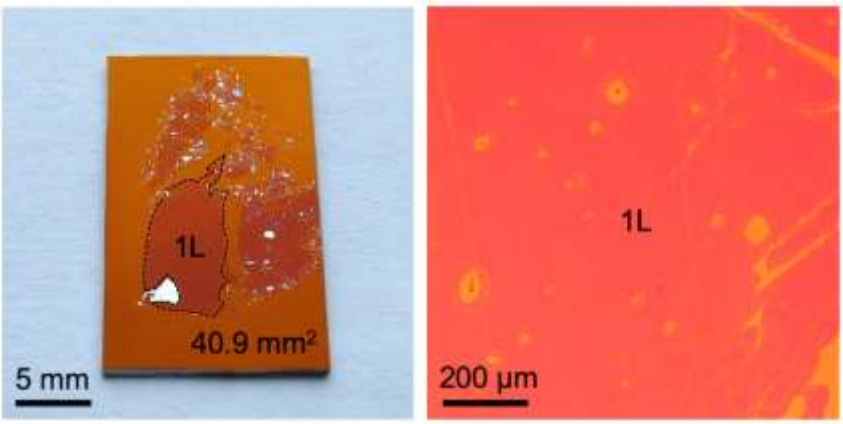

Figure 1: Macroscopic (a) and microscopic (b) optical images of monolayer MoS_2 on an Au substrate