Defect passivation of two-dimensional semiconductors by fixating chemisorbed oxygen molecules via *h*-BN encapsulation

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Hexagonal boron nitride (*h*-BN) is a key ingredient for various two-dimensional (2D) van der Waals heterostructure devices, but the exact role of *h*-BN encapsulation in relation to the internal defects of 2D semiconductors remains unclear. Here, we report that *h*-BN encapsulation greatly removes the defect-related gap states by stabilizing the chemisorbed oxygen molecules onto the defects of monolayer WS_2 crystals. Electron energy loss spectroscopy (EELS) combined with theoretical analysis clearly confirms that the oxygen molecules are chemisorbed onto the defects of WS_2 crystals and are fixated by *h*-BN encapsulation, with excluding a possibility of oxygen molecules trapped in bubbles or wrinkles formed at the interface between WS_2 and *h*-BN. Optical spectroscopic studies show that *h*-BN encapsulation prevents the desorption of oxygen molecules over various excitation and ambient conditions, resulting in a greatly lowered and stabilized free electron density in monolayer WS_2 crystals. This suppresses the exciton annihilation processes by two orders of magnitude compared to that of bare WS_2. Furthermore, the valley polarization becomes robust against the various excitation and ambient conditions in the *h*-BN encapsulated WS_2 crystals.

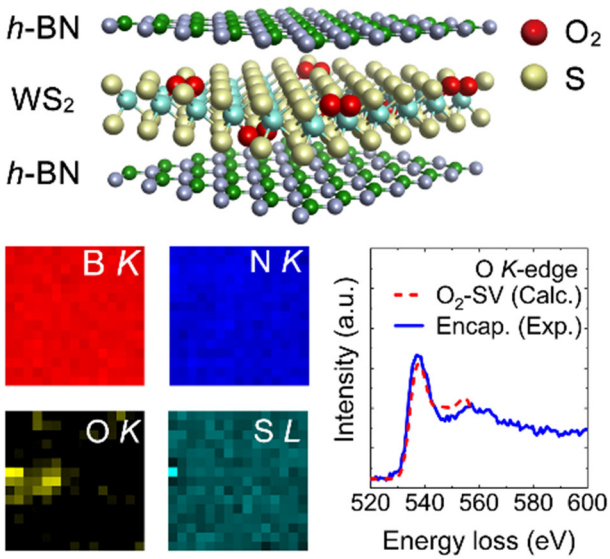

Fig.1. Schematic illustration showing the chemisorbed oxygen molecules on sulfur vacancies in WS_2 crystal, which are anchored by the *h*-BN encapsulation, resulting in the defect passivation in WS_2 crystals, as confirmed by EELS spectroscopy [1].

References

[1] J. W. Jung et al, *Advanced Science* **11**, 2310197 (2024).

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