

Spatial Mapping of Excitons and Trions in 2D MoS₂

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We report spatially resolved photoluminescence (PL) mapping results of CVD-grown layered MoS₂ in which a monolayer/bilayer (1L/2L) lateral interface is present [1]. Simultaneous analysis of atomic force microscope and Raman mapping results identified a skewed triangular-shaped 1L/2L lateral interface. Interestingly, spatially resolved PL intensity mapping over the 1L and 2L MoS₂ layers revealed that the neutral exciton emission was inhomogeneously enhanced in the 1L region near the 1L/2L boundary, whereas the negative trion emission remained unchanged (figures 1(a) and (b)). We used density functional theory (DFT) to calculate work functions of 1L and 2L MoS₂ surfaces on a SiO₂ substrate. The work function of 1L MoS₂ was smaller than that of 2L MoS₂. Therefore, transfer of electrons from the 1L to 2L MoS₂ should take place across the 1L/2L lateral interface to equilibrate the Fermi energies. Furthermore, DFT calculations showed that the work functions were strongly modulated by the terminal atoms of the MoS₂ edge (figures 2(a) and (b)). Therefore, the oscillatory behavior of the exciton PL intensity enhancement in the 1L MoS₂ region near the 1L/2L boundary was attributed to a non-uniform electrical potential distribution at the 1L/2L lateral interface.

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References

- [1] H. Kim, Y.-G. Kim, H. Ko, S. M. Kim, H. Rho, 2D Materials, 6 (2019) 025004.

Figures

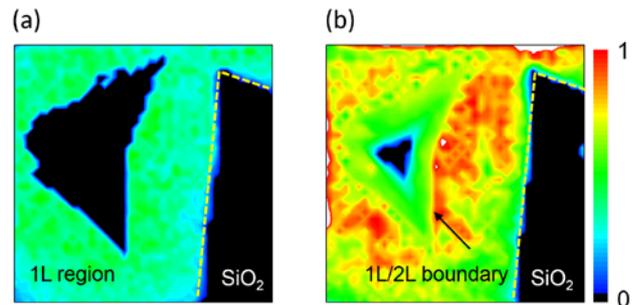
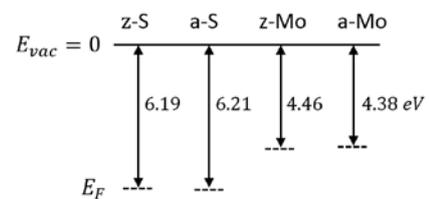


Figure 1: (a) Integrated PL intensity maps of (a) the negative trion and (b) the neutral exciton peaks of CVD-grown layered MoS₂ on the SiO₂ substrate. The thickness of the center region is ~50 nm. The trion emission was only observed in the 1L region. The dashed line denotes the boundary between 1L MoS₂ and SiO₂. The arrow denotes the 1L/2L boundary.

(a) Monolayer MoS₂



(b) Bilayer MoS₂

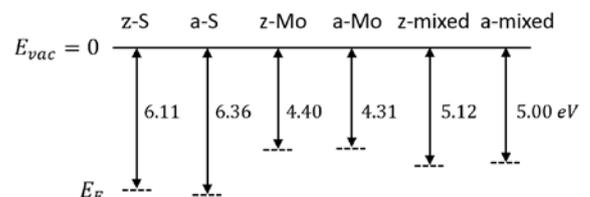


Figure 2: Calculated work functions of the zigzag and antenna edges with the S- and Mo-terminations for (a) 1L and (b) 2L MoS₂. Mixed terminations, whose outer edge atoms are both S and Mo, are additionally considered in the case of 2L MoS₂.