

# Atomic scale STM/STS analysis on transition metal dichalcogenide heterostructures

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Transition-metal dichalcogenide layered materials, consisting of a transition-metal atomic layer sandwiched by two chalcogen atomic layers, have been attracting considerable attention because of their desirable physical properties for semiconductor devices, and a wide variety of pn junctions, which are essential building blocks for electronic and optoelectronic devices, have been realized using these atomically thin structures. Engineering the electronic/optical properties of semiconductors by using such heterojunctions has been a central concept in semiconductor science and technology. Here, we report the first scanning tunneling microscopy/spectroscopy (STM/STS) study on the electronic structures of a monolayer  $WS_2/Mo_{1-x}W_xS_2$  heterojunction that provides a tunable band alignment<sup>1</sup>. Fig.1 shows a typical STM image of  $Mo_{1-x}W_xS_2$  monolayer alloy with a triangular shape. Smaller bright triangular area inside monolayer is corresponds to  $Mo_{1-x}W_xS_2$  which is surrounded by outer  $WS_2$ . Fig.2 shows the empty state STM image ( $V_s = +1.35V$ ) around  $WS_2/Mo_{1-x}W_xS_2$  heterojunction interface.  $Mo_{1-x}W_xS_2$  side appears brighter due to lower energy of conduction band minimum ( $E_{CBM}$ ) of  $MoS_2$  compared to that of  $WS_2$ . Fig. 3 shows a map of  $dI/dV$  calculated from the spatially resolved STS measured across the interface. The upper and lower edges of the band gap region, corresponding respectively to  $E_{CBM}$  and  $E_{VBM}$ , continuously shifted as a function of the distance across the interface, whose position was determined from the STM image and is indicated by the dashed line. The result clearly demonstrates that a type-II staggered gap heterojunction with a nanoscale built-in potential distribution was formed at the interface

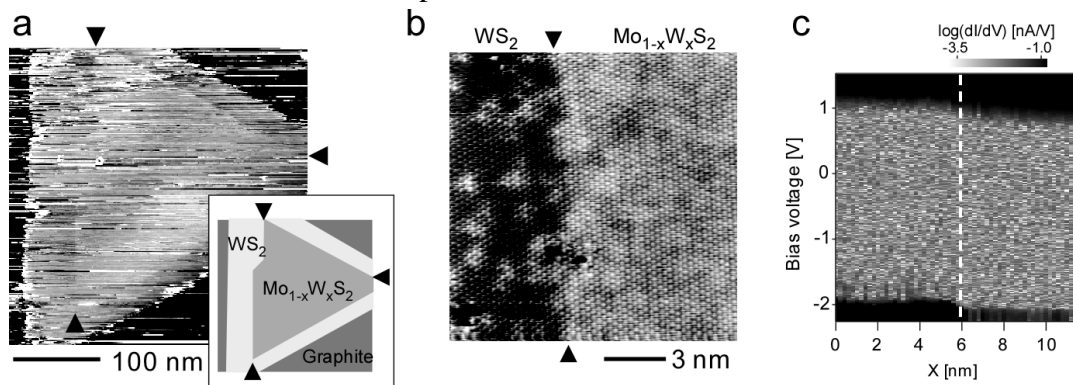


Fig a. STM image of a  $WS_2/Mo_{1-x}W_xS_2$  monolayer on graphite b. Magnification of the part of the heterojunction interface c.  $dI/dV$  profile across the heterojunction interface

<sup>1</sup>. S.Yoshida, et al., Sci. Rep. 5, 14808 (2015)