2D TMD Materials with Tunable Electronic Bandgaps

Yu Li Huang*[1,2], Yifeng Chen[2], Su Ying Quek[2], Andrew T. S. Wee[2]
[1]Institute of Materials Research & Engineering (IMRE), A*STAR, 2 Fusionopolis Way, Innovis, 138634, Singapore
[2]Department of Physics, National University of Singapore, 2 Science Drive 3, 117542, Singapore

Introduction

Two-dimensional transition metal dichalcogenides (2D TMDs) have emerged as a new class of semiconductor materials with novel electronic and optical properties of interest to future nanoelectronics technology. Among the most interesting properties of 2D TMD materials is the tunability of their electronic structures. For instance, the bandgaps are tunable with layer thickness and at grain boundaries (GBs) [1]. Whilst a small bandgap (few hundred meV) in graphene can be opened by stress and other methods, the large bandgap tunability of 2D TMDs from a few eV (semiconducting) to 0 (metallic) allow a wide range of applications in a variety of nanoscale and flexible devices.

Results and Discussion

I. Single-layer MoS_2 on graphite

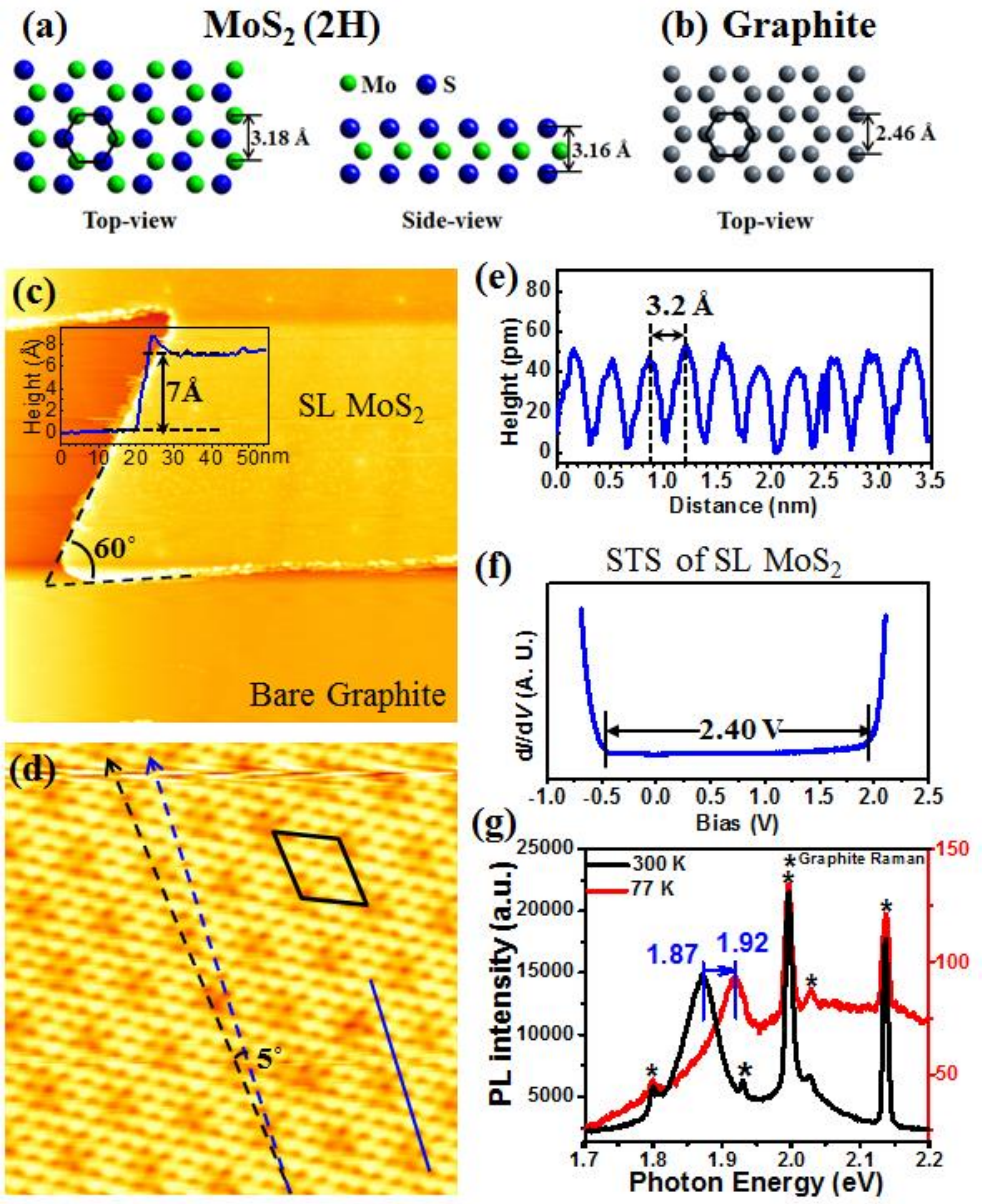

Figure 1. *Atomic structures of (**a**) MoS_2 and (**b**) graphite. (**c**) A large-scale STM of a typical triangular SL MoS_2 island on the graphite (200×200 nm^2; V_{Tip} = 2.2 V). The inserted lateral profile reveals the height of 0.7 Å. (**d**) Moiré superstructure is visible in SL MoS_2 (8×8 nm^2; V_{Tip} = 1.2 V). (**e**) The lateral profile reveals a 3.2 Å lattice constant of MoS_2. (**f**) STS spectrum reveals a 2.40 eV bandgap for SL MoS_2. (**g**) PL spectra acquired at 300 K (black) and 77 K (red). The peak for SL MoS_2 on graphite is located at 1.87 eV at 300 K, and shifts to 1.92 eV at 77K. The other peaks denoted by stars (*) are originating from the graphite substrate.*

II. Bandgap tunable with layer thickness

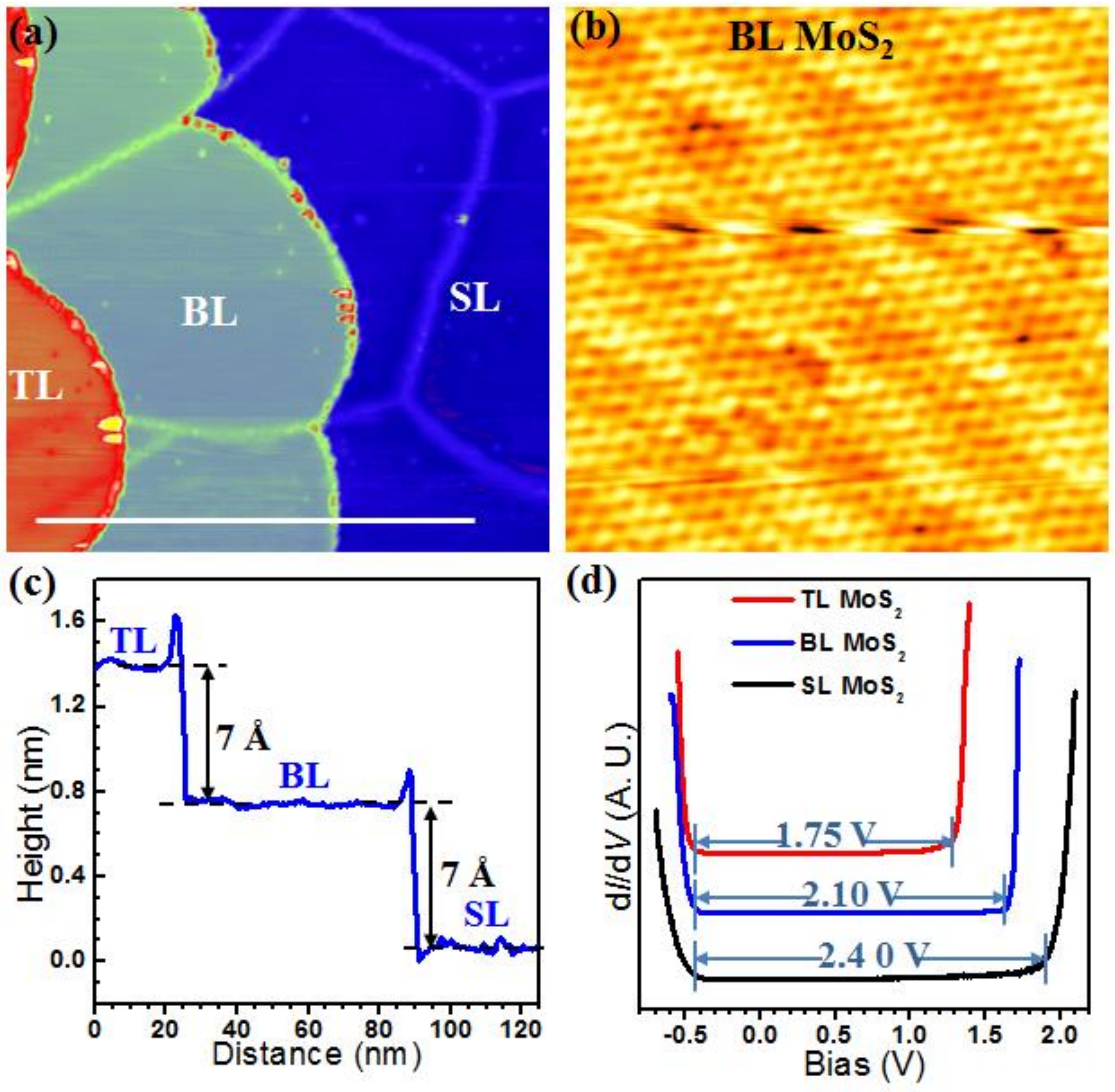

Figure 2 *(**a**) A MoS_2 flake contains single-layer (SL), bilayer (BL) and trilayer (TL) thickness (150×150 nm^2; V_{Tip} = 2.4 V). (**b**) Highly resolved STM image recorded at the BL region, where the honeycomb feature is similar to that observed for SL MoS_2 (8×8 nm^2; V_{Tip} = 1.5 V). (**c**) Lateral profile reveals a 7 Å height for each MoS_2 layer. (**d**) dI/dV spectra taken at the SL, BL and TL MoS_2 respectively, reveals the bandgap decrease with the increasing thickness.*

III. Unexpected bandgap tunability at GB

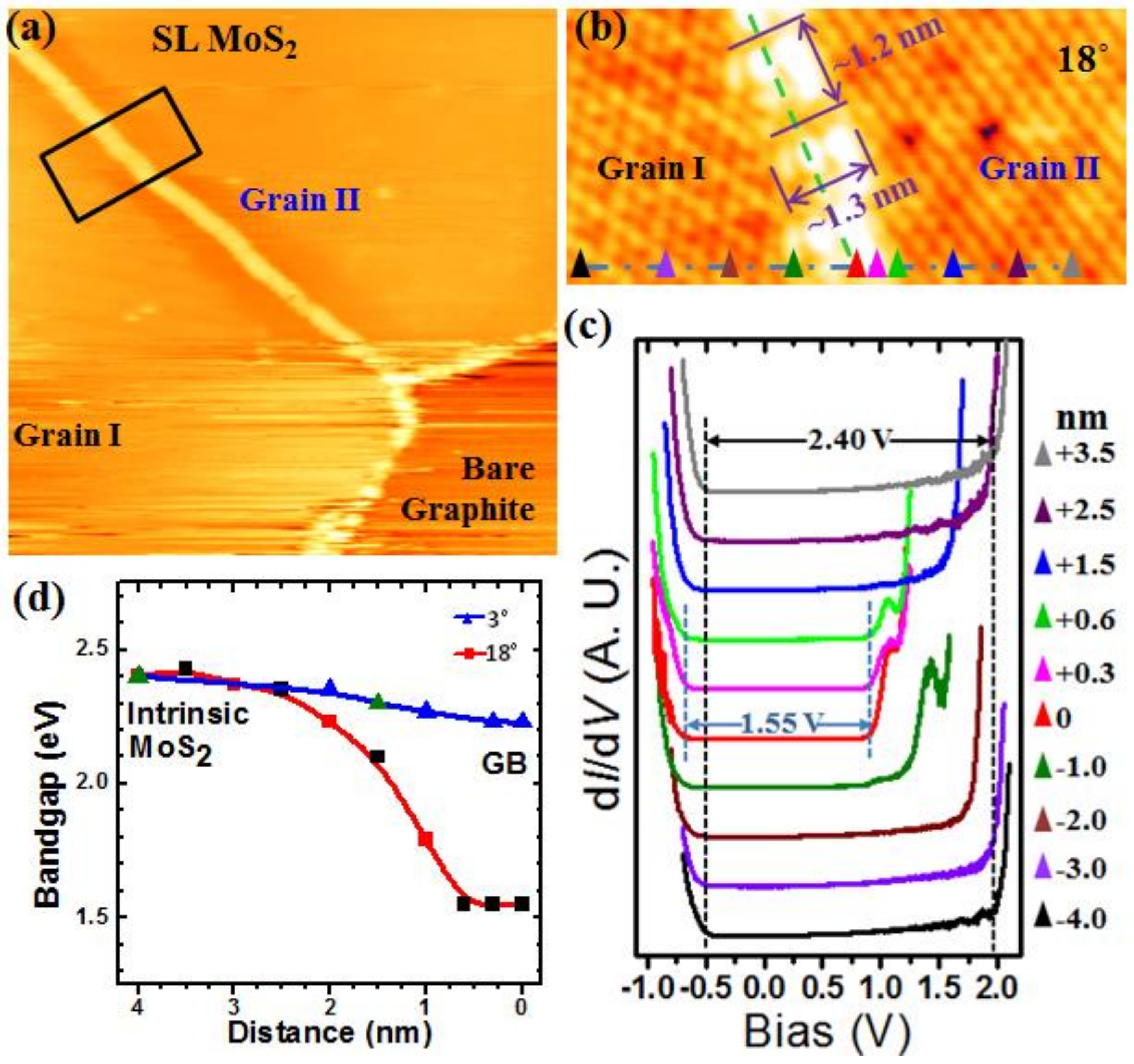

Figure 3 *(**a**) A SL MoS_2 island is composed of two grains, where the GB appears as bright protrusions (75×75 nm^2; V_{Tip} = 1.5 V). (**b**) An atomic-resolved STM image recorded at the boundary region (8 × 4 nm^2; V_{Tip} = 1.2 V). The misorientation between Grain **I** and **II** is 18˚. (**c**) dI/dV spectra recorded at the positions denoted by the triangles in panel (**b**). The variation of the bandgap with distance from the boundary is quite pronounced. (**d**) A schematic diagram of the bandgap (E_g) change with respect to the distance (d) from GBs, with tilt angles of 18˚ and 3˚ respectively.*

Institute of
Materials Research
and Engineering
A*STAR

2 Fusionopolis Way, #08-03 Innovis, Singapore 138634
Email: enquiry@imre.a-star.edu.sg   Website: www.a-star.edu.sg/imre
Tel: (65) 6501 1800   Fax: (65) 6872 0785

References
[1] Y. L. Huang, *et al,* Nat. Comm. 2015, 6, 2298.

November, 2015

huangyl@imre.a-star.edu.sg