Effect of Stacking Order on Band-to-Band Tunneling in van der Waals TMDC Heterojunctions

F. Hashimoto, N. Mori

Graduate School of Engineering, Osaka University,
2-1 Yamada-oka, Suita, Osaka 565-0871, Japan
{hashimoto, mori}@si.eei.eng.osaka-u.ac.jp

Transition metal dichalcogenides (TMDCs) such as MoS_2 and WS_2 have been attracting much attention and van der Waals (vdW) heterostructures of them show the new possibilities and application fields of nanodevices [1]. Recently, tunnel field-effect transistors utilizing band-to-band (BTB) tunneling in vdW heterojunctions were fabricated, showing excellent device characteristics [2]. Here we study effect of stacking order on the BTB tunneling in TMDC heterojunctions by using the non-equilibrium Green function (NEGF) method combined with a tight-bind (TB) approximation.

We consider a MoS_2/WS_2 vdW heterojunction whose schematic diagram is given in Fig. 1. The channel of length L consists of a vdW heterojunction of MoS_2 and WS_2 with inter-layer distance d. We set L = 0.55 nm and d = 4 Å in the present study. The channel width is considered to be infinite with a periodic boundary condition. Semi-infinite electrodes are attached to the both ends of the channel. We assume that electron transfer between MoS_2 and WS_2 occurs only in the channel region. To investigate effect of stacking order, we consider two types of stacking: AA-stacking [Fig. 1(b)] and AB-stacking [Fig. 1(c)], and calculate integrated transmission functions $\tau(E)$ by using the NEGF method.

We use the 11-band TB model [3] to describe TMCD band-structures. Since the conduction and valence band edges are predominantly contributed by the d-orbitals of metal atoms, we consider the nearest neighbor Mo-W hopping with three parameters $v_{dd\sigma}$, $v_{dd\pi}$, and $v_{dd\delta}$ as the inter-layer interaction. In order to determine TB parameters, we fit the TB band-structures to those obtained by the density functional theory (DFT). Figure 2 shows the fitting results for monolayer MoS_2 (green line) and WS_2 (pink line). Figures 3 and 4 show the fitting results for AA-stacked and AB-stacked vdW heterojunction, respectively. The inter-layer TB parameters are extracted as $v_{dd\sigma} = -0.145$ eV, $v_{dd\pi} = 0.120$ eV, and $v_{dd\delta} = 0.877$ eV for AA-stacking, $v_{dd\sigma} = 0.0847$ eV, $v_{dd\pi} = 0.00630$ eV, and $v_{dd\delta} = -0.108$ eV for AB-stacking. Figure 5 shows $\tau(E)$ for AA-stacking and AB-stacking for the energy window ΔE = 0.1 eV, where the WS_2 valence band and the MoS_2 conduction band overlap. We find that BTB tunneling in AA-stacking becomes larger than that of AB-stacking.

[1] A. K. Geim and I. V. Grigorieva, Nature **499**, 419 (2013). [2] T. Roy *et al*., Appl. Phys. Lett. **108**, 083111 (2016). [3] E. Ridolfi *et al*., J. Phys.: Condens. Matter **27**, 365501 (2015).

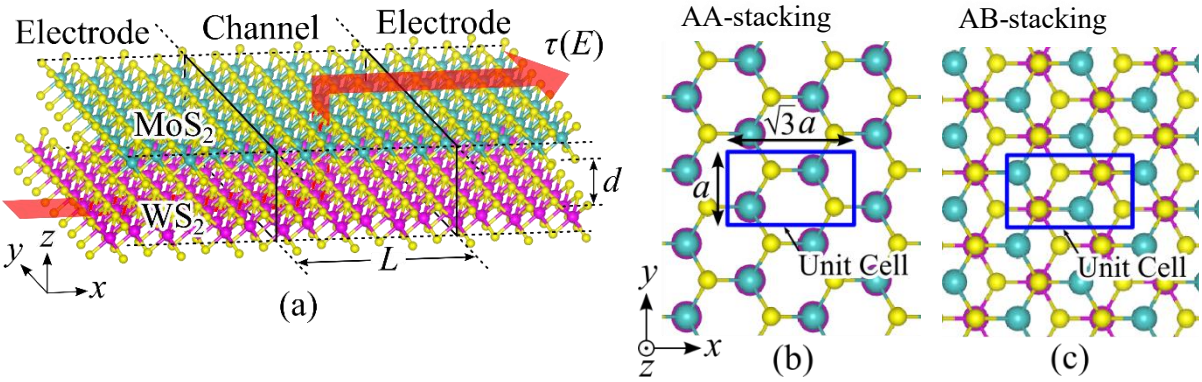


Fig. 1: (a) Device model of MoS_2/WS_2 vdW heterojunction. We set $L = 0.55$ nm and $d = 4$ Å in the present study. Top view of AA-staked (b) and AB-stacked (c) vdW heterojunction.

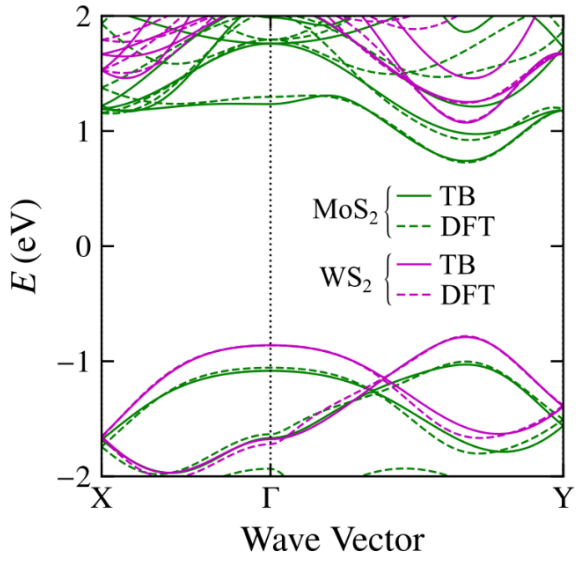


Fig. 2: Band-structure of MoS_2 (green line) and WS_2 (pink line) calculated by DFT (dashed line) compared with the TB band-structure (solid line).

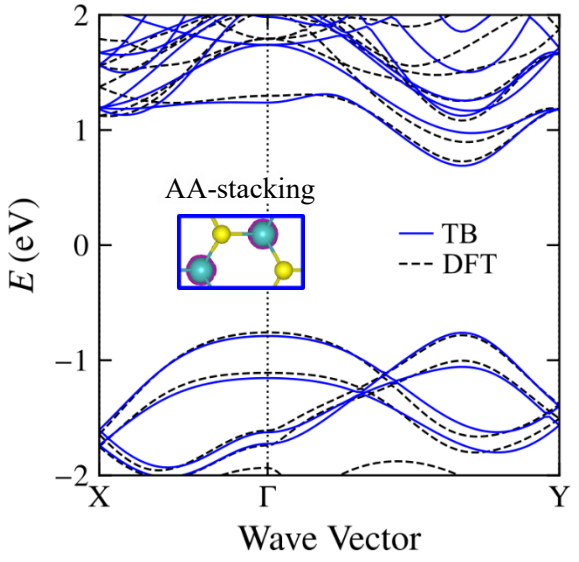
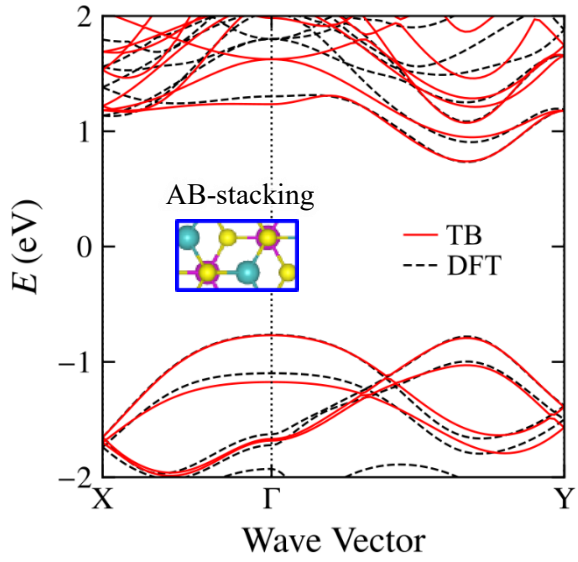


Fig. 3: Band-structure of AA-stacked vdW heterojunction calculated by DFT (dashed line) compared with the TB band-structure (solid line).



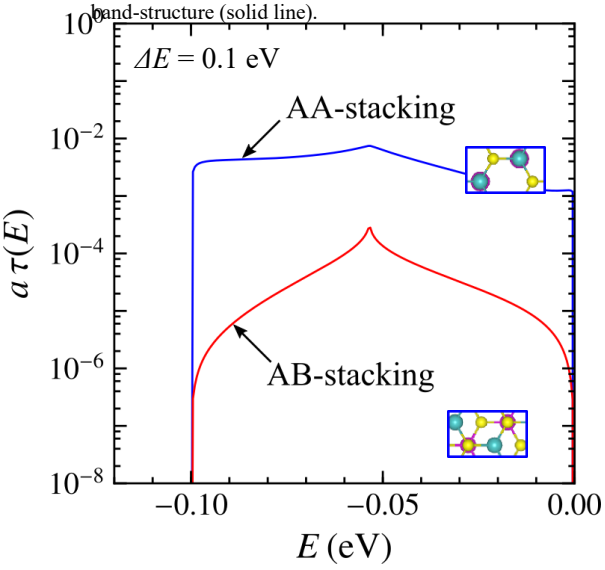


Fig. 5: Integrated transmission function $\tau(E)$ for AA-stacked (blue line) and AB-stacked (red line) vdW heterojunction.