Mina Maruyama
Susumu Okada
University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Japan

mmaruyama@comas.frsc.tsukuba.ac.jp

Carrier distribution in TMDC thin film transistors under an external electric field

Transition metal dichalcogenides (TMDCs) are one of representative forms of atomic layer materials, which consist of an atomic layer of transition metals forming a triangular lattice sandwiched by atomic layers of chalcogens arranged in prismatic manner, resulting in the hexagonal network of these elements. The most of them are known to be semiconductors with the direct band gap at the K point, which strongly depend on the constituent elements, even thought their thin films or bulks are indirect band gap semiconductors. According to their atomic layer structure, they are regarded as constituent materials for designing van der Waals (vdW) heterostructures by layer-by-layer stacking [1]. In this work, we investigated carrier accumulation in vdW heterosheets of TMDCs under an external electric field for providing a guiding principle to design the field-effect transistor (FET) of TMDC thin films with vdW heterostructures using the density functional theory combined with the effective screening medium methods.

Our calculations showed the asymmetric carrier distribution in MoS_2/WS_2 heterostructures with respect to the electrode arrangement, interlayer stacking arrangement, and carrier spices. Distribution of accumulated carrier in MoS_2/WS_2 is sensitive to mutual arrangements of the constituent TMDC layers with respect to the gate electrode: Electron is primarily injected into MoS_2 layer when it is located at the electrode side. In contrast, electron is spilled out the opposite layer to the electrode exhibiting relatively extended nature when WS_2 layer is situated at the electrode side. For the hole doping, the hole distribution weakly depends on the TMDC arrangement to the electrode. Furthermore, we also found that the the biaxial strain and stacking arrangements modulate the carrier distribution in MoS_2/WS_2 heterostructures, owing to the band alignment around the band edges.

References

[1] A. K. Geim and I. V. Grigorieva, Nature, 499 (2013) 419.

Figures

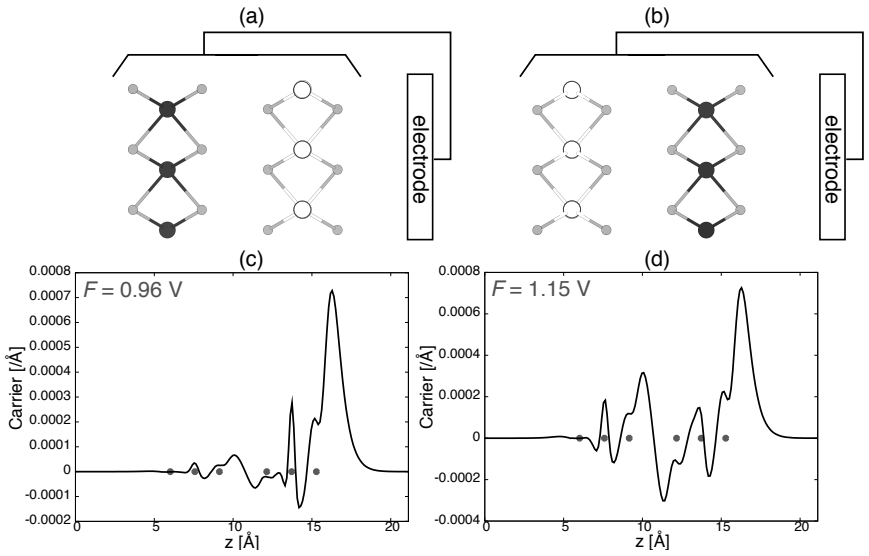

Figure 1: Structural models of (a) WS_2/MoS_2/electrode and (b) MoS_2/WS_2/electrode arrangements. White, gray, and black balls denote Mo, S, and W atoms, respectively. Carrier distribution in heterosheet of MoS_2/WS_2 for (c) WS_2/MoS_2/electrode and (d) MoS_2/WS_2/electrode arrangements.