# First-principles study of gate field effect in vertical van der Waals heterostructures

Juho Lee, Tae Hyung Kim, Ryong Gyu Lee and Yong-Hoon Kim*

*School of Electrical Engineering, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Korea*
*y.h.kim@kaist.ac.kr*

Recent developments in the technology of vertically stacked two-dimensional (2D) van der Waals (vdW) heterostructures have already come up with promising tunneling-based field-effect devices (FED) architectures. Despite the need for a better understanding of quantum tunneling across the vdW heterojunctions for the development of advanced FEDs, most theoretical works currently resort to semi-classical approaches, eliminating the possibility of interpreting and predicting effects that involve atomistic details in an *ab initio* manner. In this presentation, we newly establish the first-principles method of FEDs within the recently developed multi-space constrained-search density functional theory (MS-DFT) formalism (Fig. 1)[1] and report the non-equilibrium electronic structures and quantum transport properties of graphene-based vdW FEDs. Providing the comparable transport properties with the previous experimental report [2], we determine the validity of the vdW FED simulations within MS-DFT. In particular, focusing on the gate field effect in the graphene-based metal-insulator-semiconductor (MIS) tunnel junctions (Fig. 2), we provide not only the mechanism of tunnel diode characteristics in the MIS junction but also design guidelines for the development of advanced graphene-based vdW FEDs.

[1] H.S. Kim and Y.-H. Kim, arXiv:1808.03608[cond-mat.mes-hall] (2018); J. Lee et al, Adv. Sci., **7**, 2001038 (2020); J. Lee et al, Proc. Natl. Adv. Sci. U.S.A., **117**, 10142 (2020)

[2] L. Britnell et al, Nat. Commun. **4**, 1794 (2013)

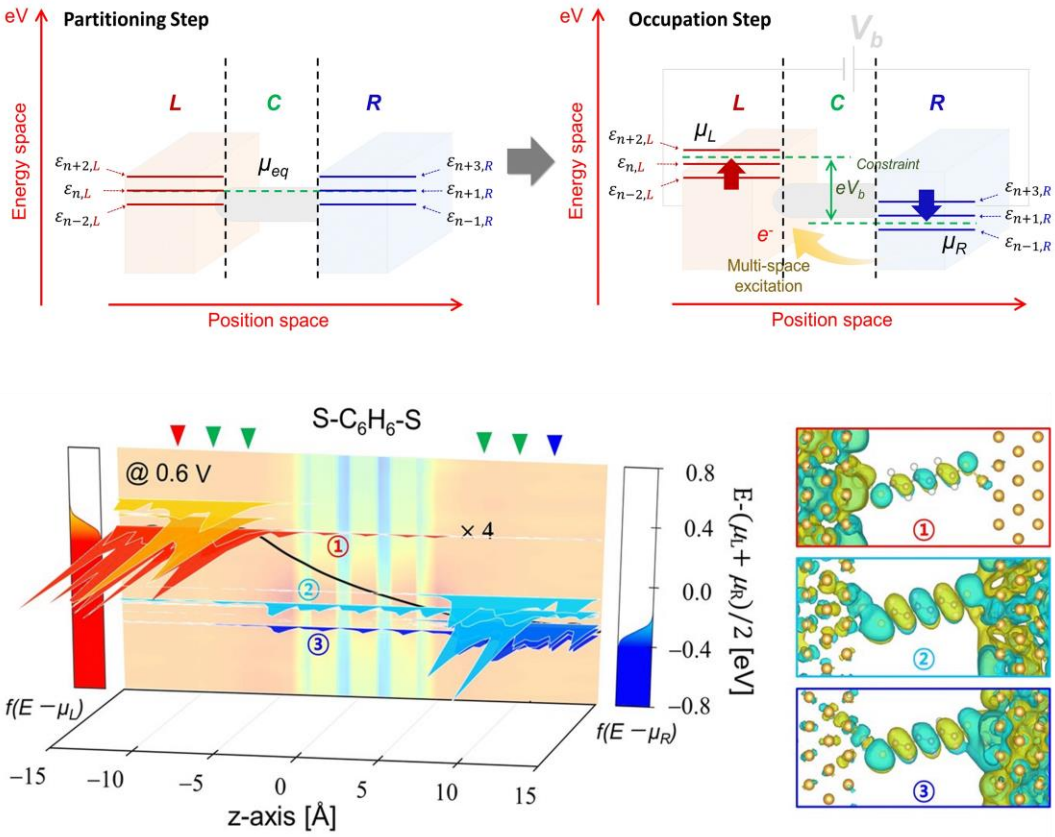


Fig. 1. (top) The newly developed multi-space constrained-search density functional theory (MS-DFT) for the simulation of nanodevice at finite bias voltages. Copyright 2020 Wiley-VCH. (bottom) The quasi-Fermi level splitting within a single molecular junction calculated with MS-DFT (bottom). Copyright 2020 National Academy of Sciences.

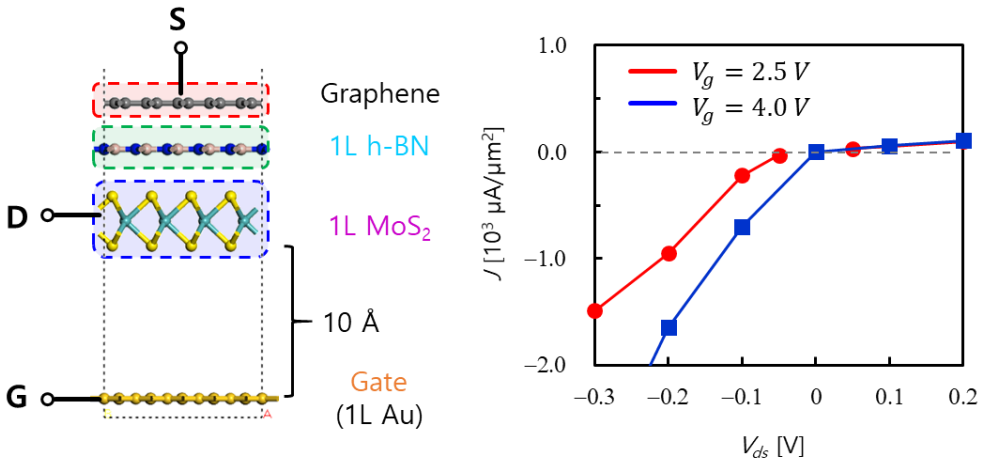


Fig. 2. (left) Atomic structure of graphene/hBN/$MoS_2$ vertical heterojunctions with finite gate electrode. Here, Au monolayer was used for the atomic gate electrode. (right) The gate-field dependent current density – drain bias ($J$ – $V_{SD}$) curves of the graphene/hBN/$MoS_2$ vertical junction at $V_g$ = 2.5 V (red solid line) and 4.0 V (blue solid line).

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