First-principles calculation of the non-equilibrium quasi-Fermi level in WSe_2 *p-n* junctions

Tae Hyung Kim, Juho Lee, Jun Seong 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

While the two-dimensional (2D) *p-n* junctions have been extensively studied for electronic and optoelectronic devices, the semiclassical approaches without considering atomistic details are still insufficient to describe its electronic structures, such as long depletion width and band edge profiles. To overcome such limitations, we combine the multi-space constrained-search density functional theory (MS-DFT) formalism [1] together with the simulated doping method [2] for describing the doped *p-n* junction under finite-bias conditions. Then, by calculating the lateral WSe_2 *p-n* junctions, we find that the depletion width calculated within the first-principles approach is several times longer than that of the analytic expressions, which affects the current-voltage characteristics in the 2D *p-n* junctions. Thanks to the MS-DFT that uniquely allows plotting quasi-Fermi levels (QFLs) profiles within the first-principles calculation [1], we also extract the QFLs profiles from the lateral WSe_2 *p-n* junctions under finite-bias conditions and show that the QFLs profiles gradually expand into the depletion region with increasing forward bias voltage. Finally, based on the QFLs profiles and electronic structures, we study the recombination-generation processes of charge carriers inside the depletion layer, including quantum effects. Our findings highlight the importance of the first-principles approaches for 2D *p-n* junction devices in terms of the design of next-generation 2D *p-n* junction devices.

[1] J. Lee, H. S. Kim, and Y.-H. Kim, Adv. Sci. **7**, 2001038 (2020); J. Lee, H. Yeo, Y.-H. Kim, Proc. Natl. Acad. Sci. U.S.A. 19, 10142-10148 (2020).

[2] O. Sinai and L. Kronik, Phys. Rev. B **87**, 235305 (2013).

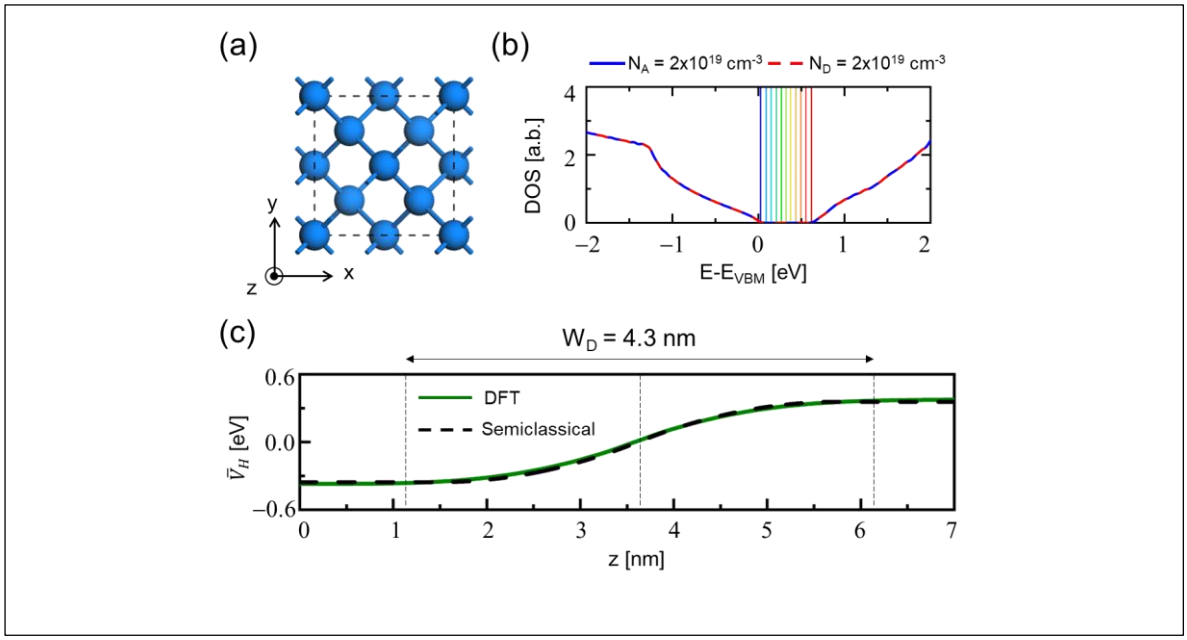

Fig.1: (a) Unit cell structure for bulk silicon crystal. (b) Density of states for *p-doped* (blue solid line) and *n-doped* (red dashed line) bulk silicon, in which doping concentration varies from $N_A = 2 \times 10^{19}\ cm^{-3}$ to $N_D = 2 \times 10^{19}\ cm^{-3}$. (c) The comparison of electrostatic potentials for bulk silicon *p-n* junction within DFT and semiclassical approaches, where the doping concentrations are $N_A = 10^{20}\ cm^{-3}$ and $N_D = 10^{20}\ cm^{-3}$ for *p-* and *n-doped* region, respectively.

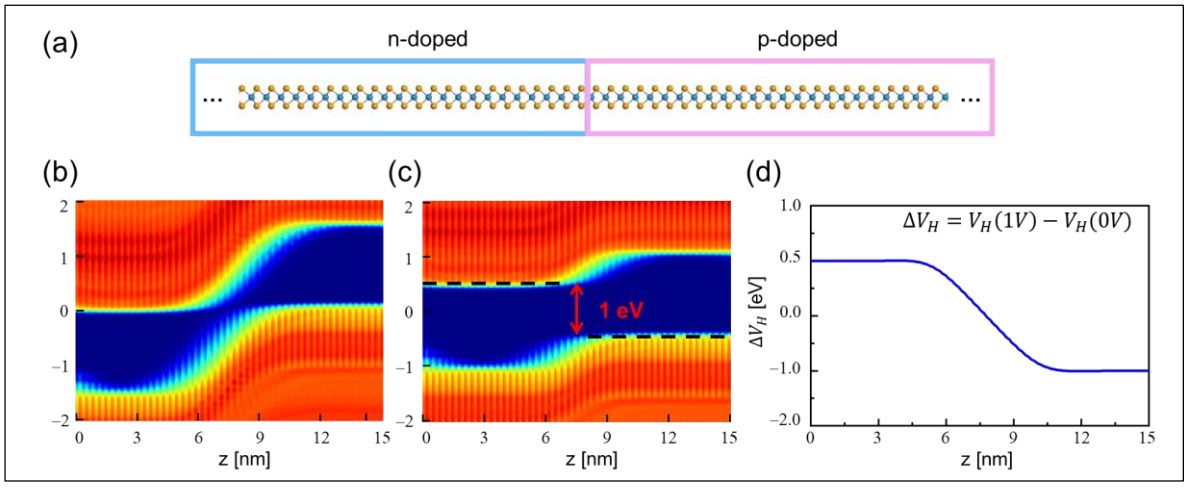

Fig.2: (a) Two-dimensional WSe_2 *p-n* junction structure. Spatially-resolved density of states for monolayer WSe_2 *p-n* junction at (b) 0 V and (c) 1 V forward bias voltage, where the doping concentrations are $N_A = 10^{13}\ cm^{-2}$ and $N_D = 10^{13}\ cm^{-2}$ for *p-* and *n-doped* region, respectively. (d) Electrostatic potential differences calculated from $\Delta V_H = V_H(1V) - V_H(0V)$ for monolayer WSe_2 *p-n* junction.