**ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)**

# Mixed-dimensional 2D/3D heterojunctions between $MoS_2$ and Si(100)

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## 1. Electronic charge densities of $MoS_2$/Si heterostructures

To identify the electronic charge densities of $MoS_2$/Si heterostructures depending on the interaction between two contact materials, we obtain electronic charge densities of (a) $MoS_2$/clean Si(100) and (b) $MoS_2$/H-covered Si(100) heterostructures in Fig. S1; especially, we obtain cross sectional electronic charge densities at $x$ = 3.79 and 7.21 Å (See inset of Fig. S1 for details.). Our calculations show that for the case of $MoS_2$/clean Si(100) heterostructure, $MoS_2$ is hybridized with clean Si(100) due to the strong covalent bonds between S and Si atoms, as shown in Fig. S1(a). On the other hand, S atoms of $MoS_2$ and H atoms of H-covered Si(100) are not hybridized each other, as shown in Fig. S1(b), indicating the weak van der

Waals (vdW) interaction between them. As a result, we identify that electronic charge densities can be different depending on the binding behaviors between two contact materials.

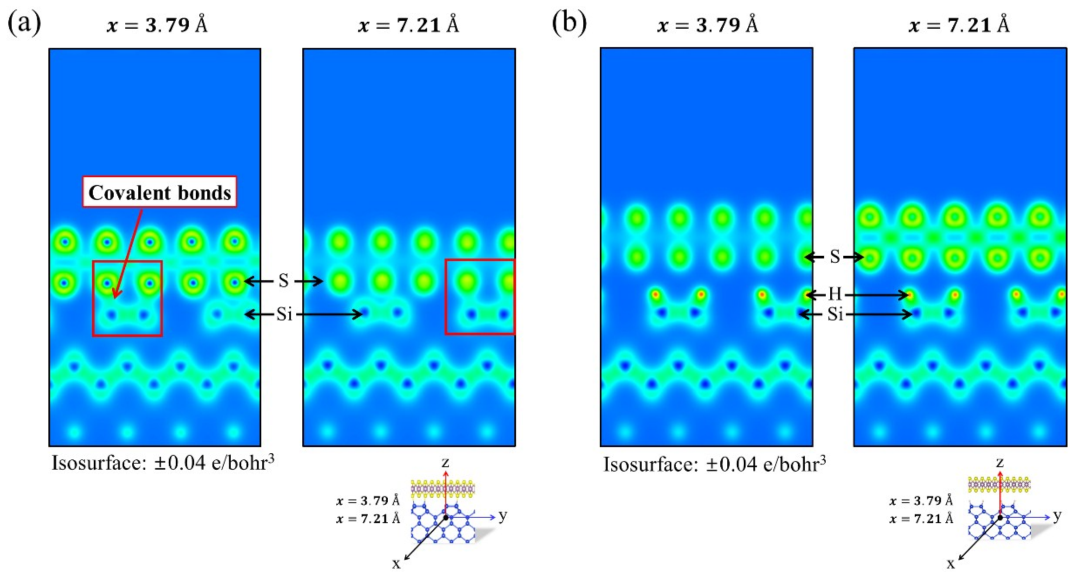


**Fig. S1** Cross sectional electronic charge densities of (a) $MoS_2$/clean Si(100) and (b) $MoS_2$/H-covered Si(100) at x = 3.79 and 7.21 Å. Here, the isosurface level is ±0.04 e/bohr$^3$.

## 2. Tunneling probability of $MoS_2$/clean Si(100) heterojunction

For the $MoS_2$/clean Si(100) heterostructure which have possibility of metallic contact, we obtain the tunneling probability ($T_B$) to give the another criterion to the contact characteristics except for the Schottky barrier height (SBH). To estimate the value of $T_B$, we calculate the electrostatic potential in Fig. S2. By using the height (~1.90 eV) and width (~0.84 Å) of potential barrier between $MoS_2$ and clean Si(100) in Fig. S2, we obtain $T_B$ of about 30 % using Wentzel-Kramers-Brillouin (WKB) approximation:

$$T_B = exp\left( - 2 \times \frac{\sqrt{2m\Delta V}}{\hbar} \times w_B \right) \times 100\ (\%)$$

where $m$, $\Delta V$, and $w_B$ are the electron mass, height and width of tunnel barrier, respectively. It means that electrons can pass through $MoS_2$/clean Si(100) heterojunctions with the tunneling probability of about 30 %.

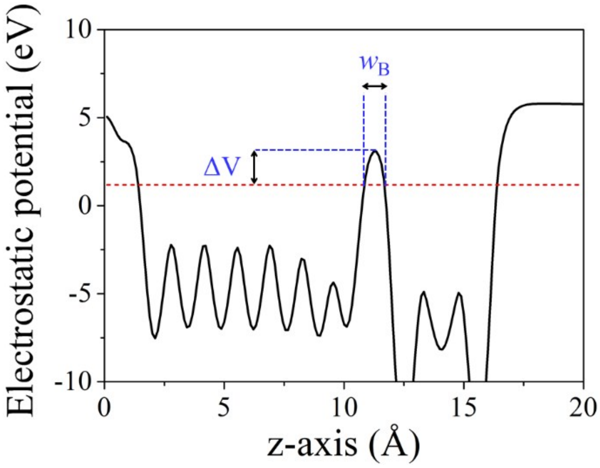


**Fig. S2** Electrostatic potential of $MoS_2$/clean Si(100) heterostructure. Fermi level is represented by red dashed line.