Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supporting Information

Quantum oscillation in carrier transport in two-dimensional junctions

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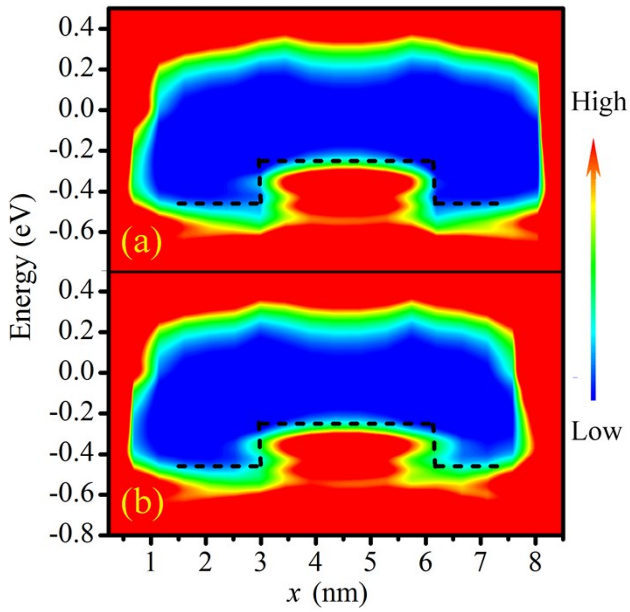

Figure S1. LDOS maps for stacked (a) and staggered (b) homojunction from DFT-NEGF calculations. The dashed line shows bilayer region (~ 3 nm) and the potential well induced by the valence band offset. The density of states increase from the blue to red as labeled in the right side.

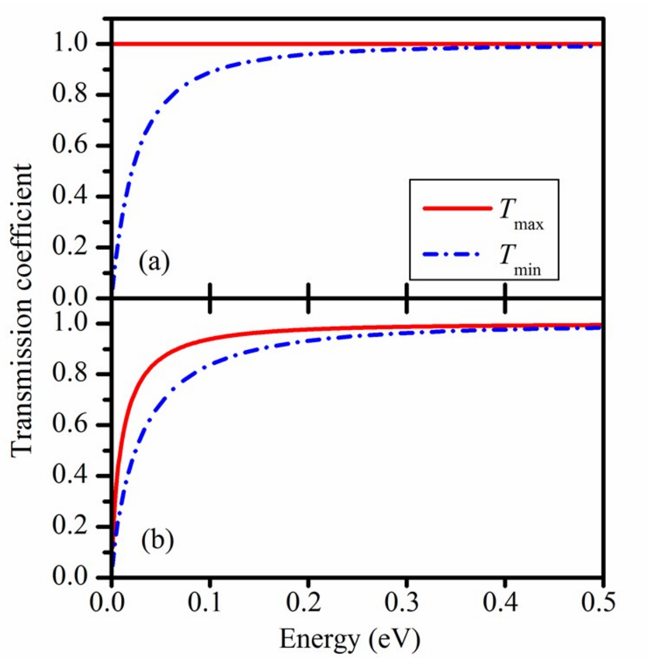

Figure S2. The maximum and minimum transmission coefficients from (a) symmetric and (b) asymmetric QW models, respectively.

Details of the quantum well model.

We first consider the symmetric potential well. For the finite square well as shown in Figure 4a,

$$v(x)=\begin{cases}0,\ \text{for } x<-L_{\mathrm{BL}}/2\\ -V_0,\ \text{for } -L_{BL}/2<x<L_{BL}/2\\ 0,\ \text{for } x>L_{BL}/2\end{cases} \tag{S1}$$

where V_0 is the potential well depth, and L_{BL} is the bilayer region length (potential well length). Here, we only consider the scattering states (with $E>0$). We can write the Schrödinger equation says: $-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2}+v(x)\Psi=E\Psi\rightarrow\frac{d^2\Psi}{dx^2}=k^2\Psi$, where $k=\frac{\sqrt{2m(E-v(x))}}{\hbar}$. The general solution gives:

$$\begin{aligned}&x<-L_{\mathrm{BL}}/2:\psi_1(x)=Ae^{ikx}+Be^{-ikx},\ k=\frac{\sqrt{2mE}}{\hbar}\\ &-L_{\mathrm{BL}}/2<x<L_{\mathrm{BL}}/2:\psi_2(x)=C\sin(lx)+D\cos(lx),\ k_2=\frac{\sqrt{2m(E+V)}}{\hbar}\\ &x>L_{\mathrm{BL}}/2:\psi_3(x)=Fe^{ikx},\ k=\frac{\sqrt{2mE}}{\hbar}\end{aligned} \tag{S2}$$

Then, the transmission coefficient is obtained by considered the boundary conditions:

$$T=|F|^2/|A|^2=[1+\frac{V_0{}^2}{4E(E+V_0)}\cdot\sin^2(\frac{L_{\mathrm{BL}}}{\hbar}\sqrt{2m(E+V_0)})]^{-1} \tag{S3}$$

Next, we consider the asymmetric case as shown in Figure 4b. The potential can be expressed as

$$v(x)=\begin{cases}-V_1,\ \text{for } x<-L_{\mathrm{BL}}\\ -V_2,\ \text{for } -L_{\mathrm{BL}}<x<0\\ 0,\ \text{for } x>0\end{cases} \tag{S4}$$

Similar with that in symmetric one, we can obtain the Schrodinger equations and get the general solutions as follows:

$$
\begin{aligned}
&x < -L_{\mathrm{BL}}: \qquad \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x},\ k_1 = \frac{\sqrt{2m(E+V_1)}}{\hbar} \\
&-L_{\mathrm{BL}} < x < 0: \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x},\ k_2 = \frac{\sqrt{2m(E+V_2)}}{\hbar}\ . \\
&x > 0: \qquad \psi_3(x) = Fe^{ik_3x}, \qquad k_3 = \frac{\sqrt{2mE}}{\hbar}
\end{aligned}
\tag{S5}
$$

The total transmission coefficient can be obtained then:

$$
T = \frac{16k_1k_2^{\,2}k_3}{k^2{}_2(k_1+k_3)^2+(k_2^{\,2}-k_1^{\,2})(k_2^{\,2}-k_3^{\,2})\sin^2 k_2a} \times \frac{k_2k_3}{(k_2+k_3)^2}\ . \tag{S6}
$$