Supporting Information

Influence of interlayer stacking on gate-induced carrier accumulation in bilayer MoS_2

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Electronic structures of bilayer MoS_2 with twisted arrangement

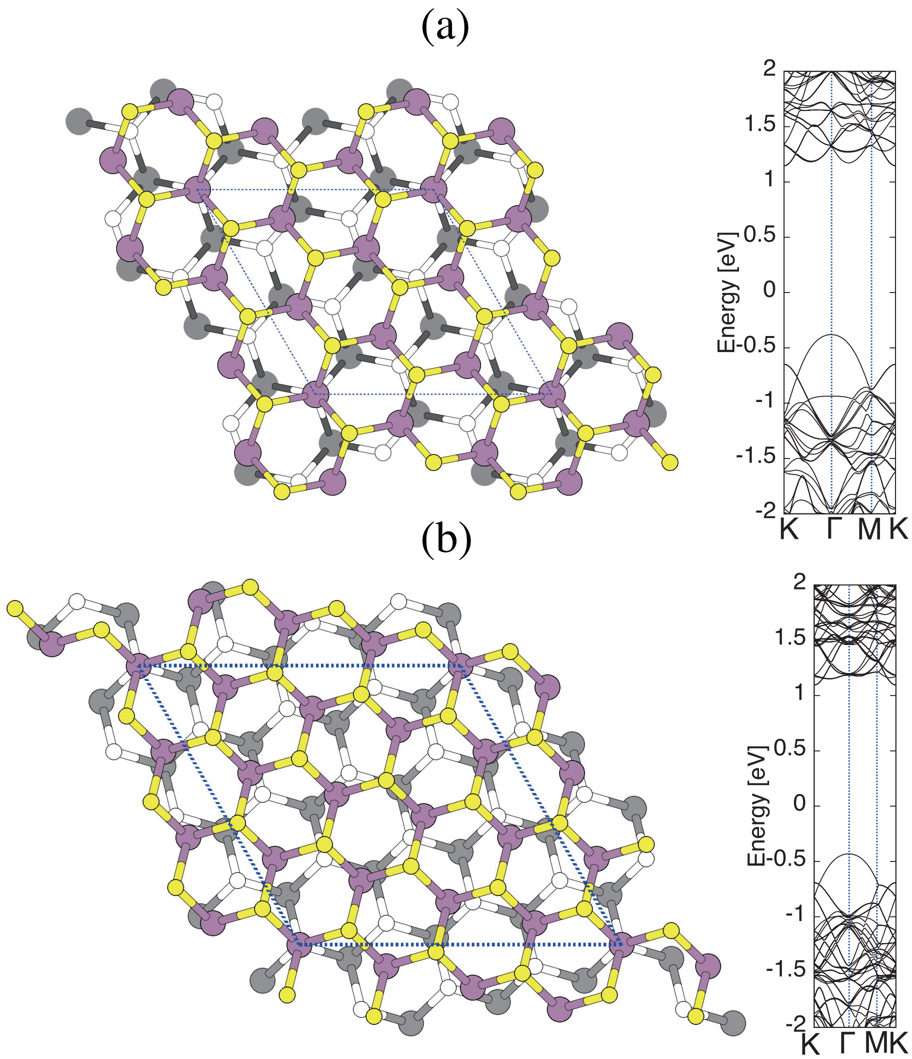

Figure S1: Electronic and geometric structures of twisted bilayer MoS_2 with twisted angles of (a) 38 and (b) 27°. Purple and gray large balls indicate Mo atoms belonging to the top and bottom layers, respectively. Yellow and white small balls indicate S atoms belonging to the top and bottom layers, respectively. The energy is measured from that of the vacuum level. The valence band top is indicated by the arrow.

Effective Screening Medium Method

In ordinary density functional theory (DFT) calculations, the electronic structure of matters is solved under the periodic boundary condition along x, y, and z directions. Thus, as for the electrostatic potential, we have a Poisson equation

$$\nabla \cdot [\epsilon(\mathbf{r})\nabla]V(\mathbf{r}) = -4\pi\rho_{tot}(\mathbf{r}), \tag{1}$$

where $\epsilon(\mathbf{r})$ is the permittivity possessing the spatial dependence. By using the Green's function, the Poisson equation is expressed

$$\nabla \cdot [\epsilon(\mathbf{r})\nabla]G(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r} - \mathbf{r}'). \tag{2}$$

Then, electrostatic potential $V(\mathbf{r})$ is obtained by using the Green's function as

$$V(\mathbf{r}) = \int d\mathbf{r}' G(\mathbf{r}, \mathbf{r}')\rho_{tot}(\mathbf{r}'). \tag{3}$$

In the present work, to apply the electric field along z direction together with the excess carriers, we assume that the relative permittivity only depends along z direction (Figure S2). The choice of the permittivity leads to the anisotropic Poisson equation

$$\partial_z[\epsilon(z)\partial_z] - \epsilon(z)g_{\parallel}^2 G(\mathbf{g}_{\parallel}, z, z') = -4\pi\delta(z - z'), \tag{4}$$

where $\mathbf{g}_{\parallel}$ and $g_{\parallel}$ denote the wave vector parallel to the layer and absolute value of $\mathbf{g}_{\parallel}$. Then, the Green's function is determined by the conditions,

$$V(\mathbf{g}_{\parallel}, \frac{c}{2}) = \phi_T \tag{5}$$

$$V(\mathbf{g}_{\parallel}, -\frac{c}{2}) = \phi_B \tag{6}$$

$$\tag{7}$$

with the z dependent permittivity

$$\epsilon(z) = \begin{cases} 1 \; if \; |z| \leq \frac{c}{2} \\ \infty \; if \; |z| \geq \frac{c}{2}. \end{cases} \tag{8}$$

Accordingly, we can calculate the slab under electric field corresponding to the potential difference $V_T + V_B (= \phi_T - \phi_B)$ between cell boundaries along z direction and the excess carrier Q with counter carriers $q_T + q_B (= Q)$.

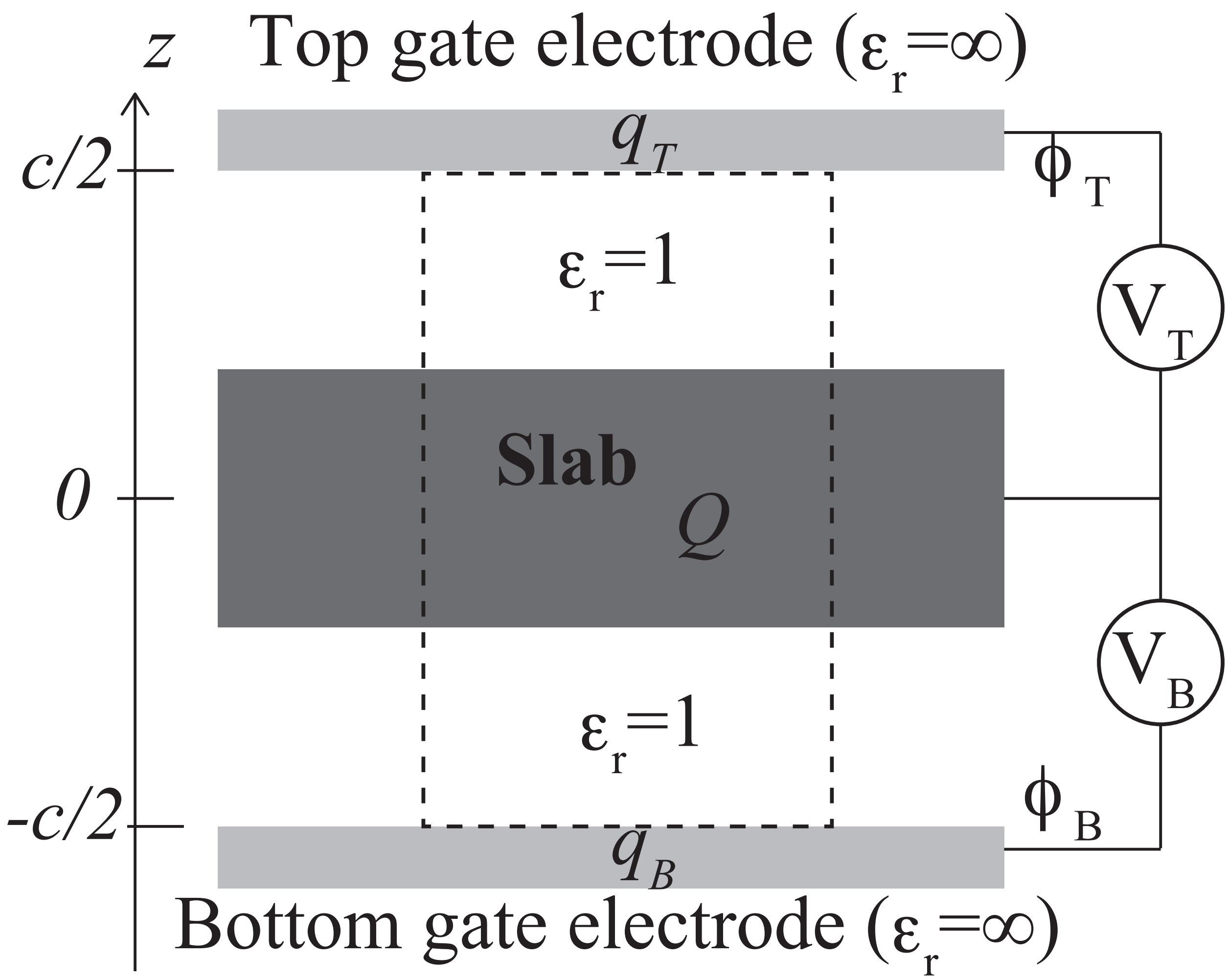

Figure S2: Calculation model using the DFT combined with the ESM method.