(Supplementary Information)

Sub-10 nm Monolayer ReS_2 Transistor for Low Power Applications

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1. Basis sets

The differences of transmission spectra at L_g = 4 nm and V_g = -1.3 V in zigzag direction between Double-Zeta-Polarized (DZP) and Single-Zeta-Polarized (SZP) are shown in Fig. S1. Our tests shown that the calculated results using SZP and DZP basis set are consistent.

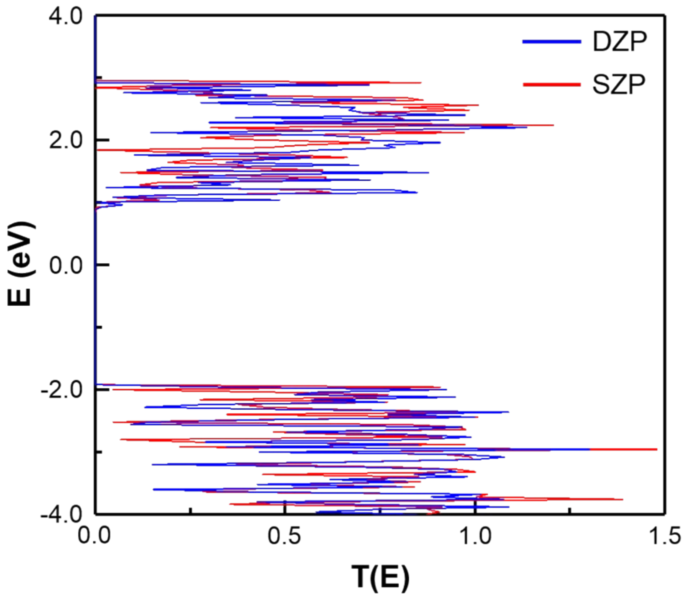

Fig. S1. Transmission spectra of zigzag-directed ReS_2 transistor (at L_g = 4 nm and V_g = -1.3 V) using SZP and DZP basis sets, respectively.

2. Influences induce by the applied gate in ReS_2

The applied gate in ReS_2 may induce structure distortion in ReS_2 monolayer. We considered this situation and done some experiments to analyze the possible effects. We have compared the results with and without the applied gate on the unit cell level and the device level, respectively.

At the unit cell level, we chosen a high gate voltage of V_g = -1.1 V to compare with the case of V_g = 0 V. Several important parameters were compared and the results were listed in the Table S1. It is found that the optimized ReS_2 layer with and without gates show quite similar lattice constants (the difference is less than 0.15%). Their type and value of the band gaps are the same.

Table S1. Material parameters of ReS_2 unit cell with and without a gate.

	Without applied gate	With applied gate (V_g = -1.1 V)
Lattice constant *a* (Å)	6.46	6.47
Lattice constant *b* (Å)	6.56	6.57
Band gap (eV)	1.47	1.47
Type of band gap	direct band gap	direct band gap

At the device level, we have compared the performance of the 8 nm gate-length zigzag-directed ReS_2 transistor with and without the consideration of the structural distortion induced by the gate. Their transmission spectra of the same order of magnitude and have transmission gaps of the same size (Fig. S2).

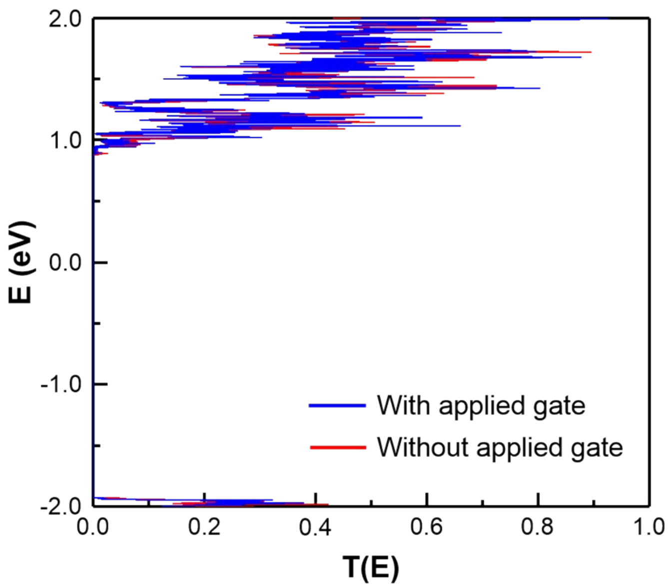

Fig. S2. Transmission spectra of the zigzag-directed ReS_2 transistor (at L_g = 8 nm and at V_g = -1.1 V) with and without consideration of the structural distortion induced by a gate.

In summary, we prove that the structure distortion of ReS_2 induced by the applied gate is negligible, and the device performance with and without the consideration of this structural distortion are expected to be similar.

3. van der Waals correction

Van der Waals (vdW) force plays an important role in layered materials. To check the effects of the vdW force, we adopted Grimme DFT-D2 vdW correction method at both the unit cell level and the device level.

At the unit cell level, we compared the key geometric and electronic parameters of ReS_2 with and without considering the vdW correction as shown in Table S2. No apparent difference is found.

Table S2. Material parameters of ReS_2 cell with and without van der Waals correction.

	Without vdW correction	With vdW correction
Lattice constant *a* (Å)	6.46	6.46
Lattice constant *b* (Å)	6.56	6.56
Band gap (eV)	1.47	1.47
Type of band gap	direct band gap	direct band gap

At the device level, the comparison of transmission spectra of the zigzag-directed ReS_2 transistor (at L_g = 8 nm and at V_g = -1.1 V) with and without vdW correction as shown in Figure S3. The transmission spectra are nearly the same with similar magnitudes and transmission gaps.

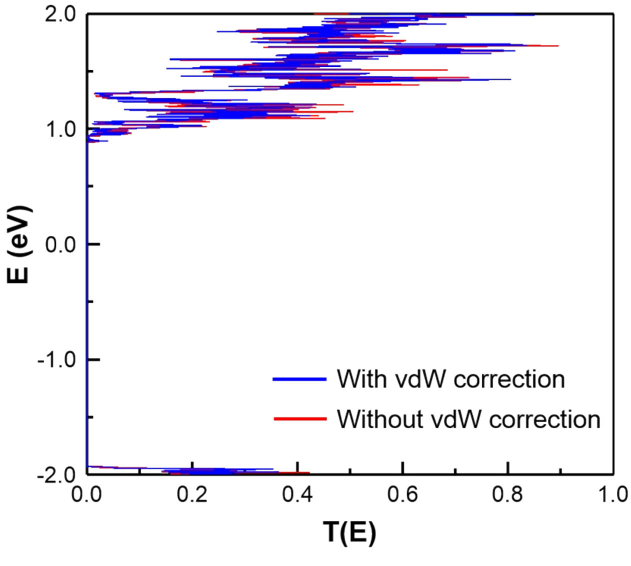

Fig. S3. Transmission spectra of zigzag-directed ReS_2 transistor (at L_g = 8 nm and V_g = -1.1 V) with and without vdW correction.

In summary, we proved that the differences taking van der Waals correction into account in ReS_2 are negligible.