**Supporting information for**

# Contact effect of $ReS_2$/metal interface

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## S-1. Fabrication method

FET devices with $ReS_2$ channels and several different metal contacts were prepared to estimate the current rectifying performance. First, the $ReS_2$ flakes were exfoliated and transferred to a $SiO_2$/Si substrate. The $SiO_2$/Si substrate consists of a p-type Si wafer with thermally-grown $SiO_2$ surfaces. The thickness of $ReS_2$ was estimated via AFM profile and the optical color in the optical microscope image. Patterned Al and Pt electrodes with a thickness of 50 nm were fabricated by electron beam lithography (EBL), electron-beam evaporation, and the lift-off process. The transfer method was used to attach graphene to $ReS_2$ with a PDMS stamp. The device performance was measured by modulating the source/drain and source/gate voltage at room temperature using a Keithley 2400 source meter.

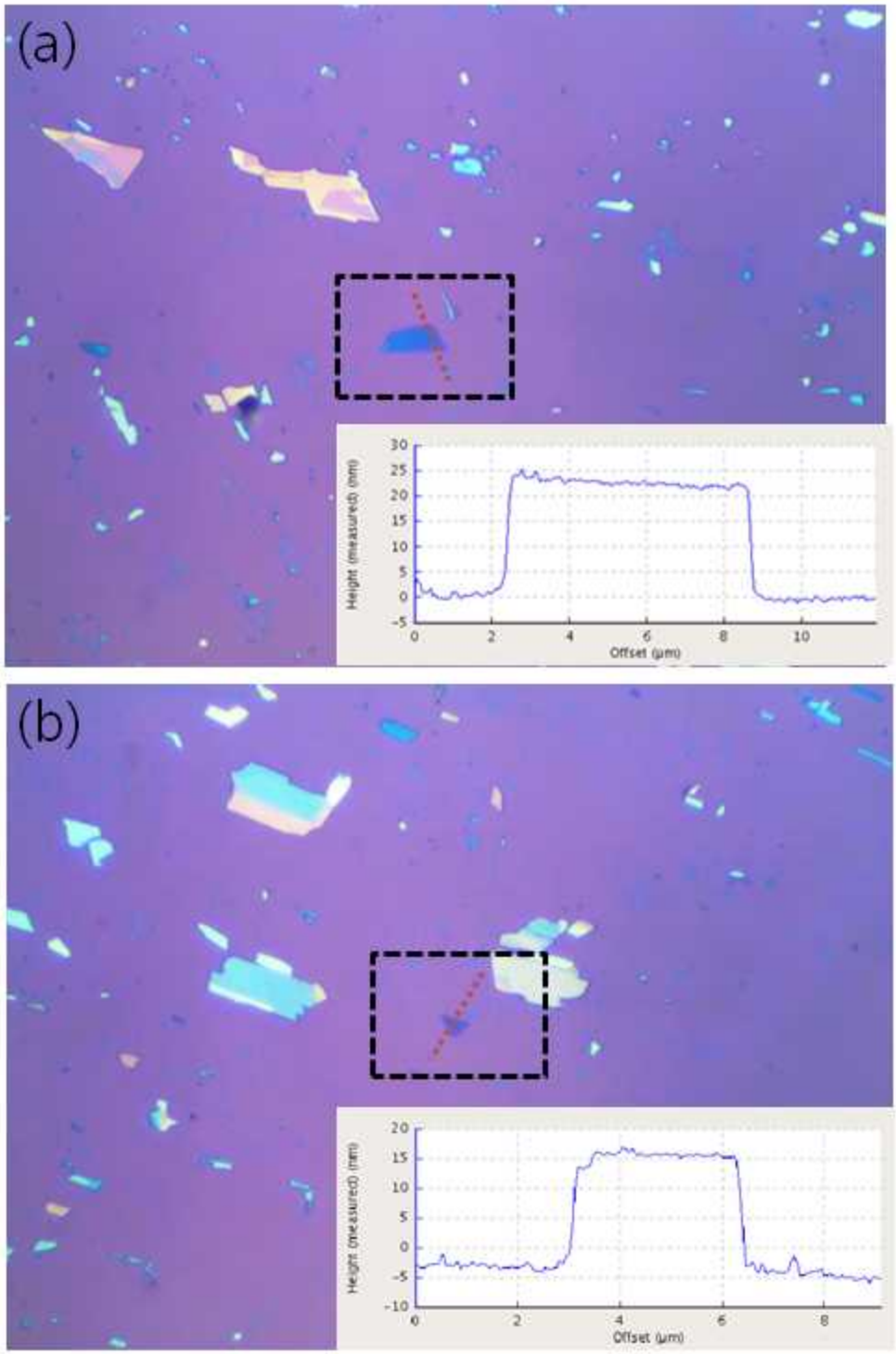



Figure. S1 Thickness of two $ReS_2$ flakes measured from AFM. (a) 20~25nm thickness (b) 15nm thickness.

## S-2. DFT calculation

### Methods

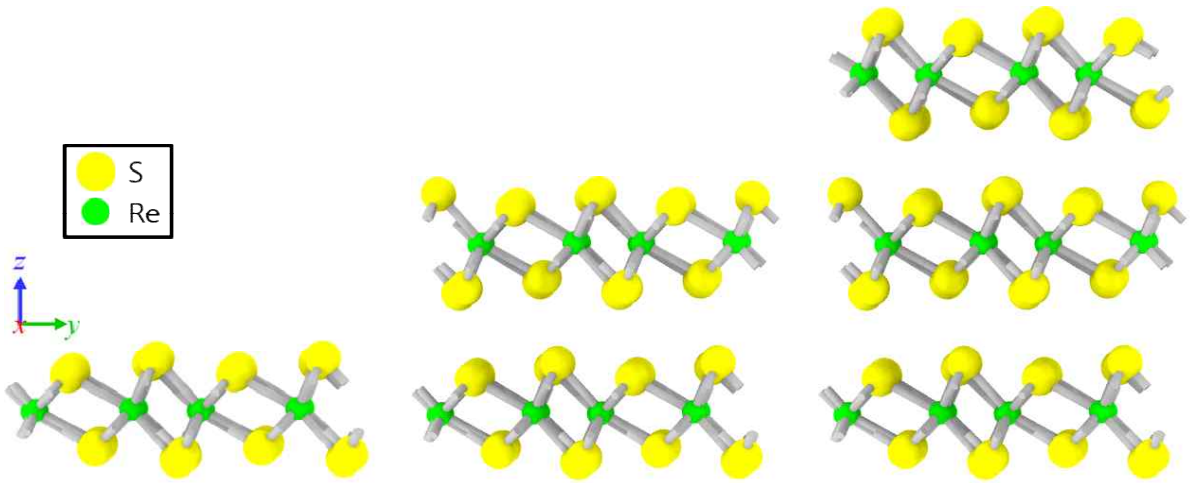
Ab initio calculations of electron affinity $\chi$ in $ReS_2$ are conducted using VASP (*Vienna ab initio simulation package*) [1-4]. Structural and electronic properties are calculated using GGA-PBE (Perdew-Burke-Ernzerhof) functional with PAW (Projector Augmented-Wave) potentials [5-8]. A cutoff energy for the basis set is extend to 500 eV for throughout all calculations, and convergence criteria of $10^{-5}$ eV is used for self-consistency. The atomic force criteria of 0.01 eV/Å is used during geometry optimizations by the conjugate gradient method. A 2×2 supercell of monolayer $ReS_2$ (1L) is constructed with 4 rhenium (Re) atoms and 8 sulfur (S) atoms. K-points for the Brillouin-zone sampling is 8×8×1 with Gamma (Γ) point centered. In Figure S, two-layer (2L) and three-layer (3L) structures are ordered in rhombohedral (ABC) staking [9]. A vacuum spacing of 16 Å perpendicular to the layer is fixed irrespective of the number of layers.

### Results

Direct bandgap $E_{gap}$ and electron affinity $\chi$ of 1L is obtained as 1.42 eV and 4.32 eV, respectively. Similar value of bandgap was reported in other papers [10-12] and experiment value is 1.55 eV from absorption spectroscopy [10]. In Table S1, as the number of layers increases, the bandgap $E_{gap}$ is monotonically decreased, while electron affinity $\chi$ is nearly constant.

Table S1. Electronic properties of $ReS_2$: Bandgap $E_{gap}$ and Electron affinity $\chi$

| | 1L | 2L | 3L |
|---|---|---|---|
| $E_{gap}$ (eV) | 1.42 | 1.31 | 1.26 |
| $\chi$ (eV) | 4.32 | 4.30 | 4.32 |




(a) (b) (c)

Figure S2. $ReS_2$ stacked structures: (a) 1L, (b) 2L, (c) 3L

## S-3. Surface potential

The specimen composed of $ReS_2$ flakes on a gold substrate was prepared to evaluate the surface potential difference between gold and $ReS_2$. A 200 nm thick gold coating was deposited on a $Si/SiO_2$ wafer by using an evaporator, and the $ReS_2$ flakes were then transferred onto the gold-coated wafer by using a PDMS stamp. The $ReS_2$ flakes were purchased from 2D-Semiconductors. Kelvin probe force microscopy (XE-7, Park Systems Corp.) was used to measure the surface potential with applied 1V, 17kHz of AC bias voltage and frequency in ambient condition. The work function of Au/Cr tip was calibrated from the work function of HOPG (4.6 eV) which is electrically stable materials.

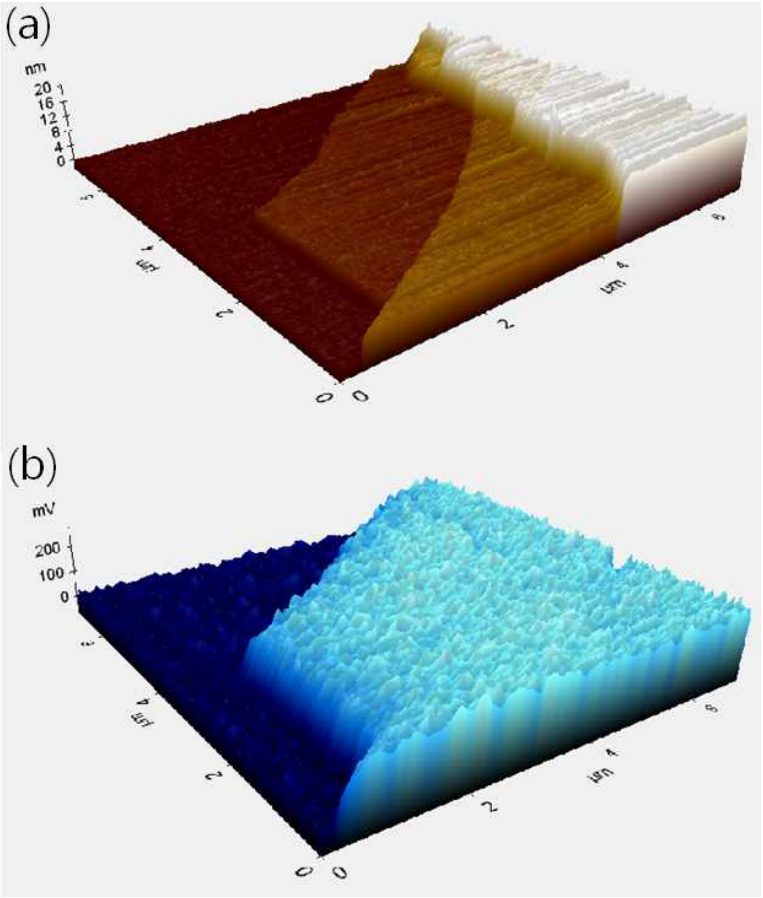



Figure S3. (a) 3D mapping image of AFM (b) 3D mapping image of KPFM

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