Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Does P-type Ohmic Contact Exist in WSe_2-metal Interfaces?

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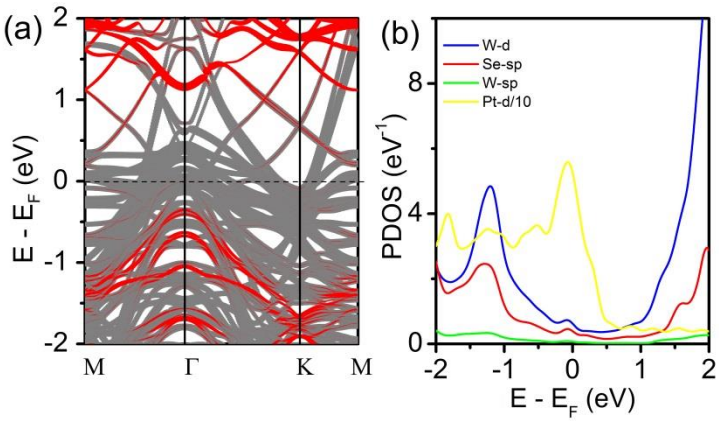

Figure S1. (a) d-orbital projected band structure of the ML WSe_2-Pt contact. Gray and red lines represent the *d*-orbitals of metal surface and W atoms, respectively. The line width is proportional to the weight. (b) Partial density of states (PDOS) of W-*d*, Se-*sp*, W-*sp*, Pt-*d* electron orbitals in the ML WSe_2-Pt contact, respectively. The PDOS of Pt-*d* is given as the one-tenth of the origin values.

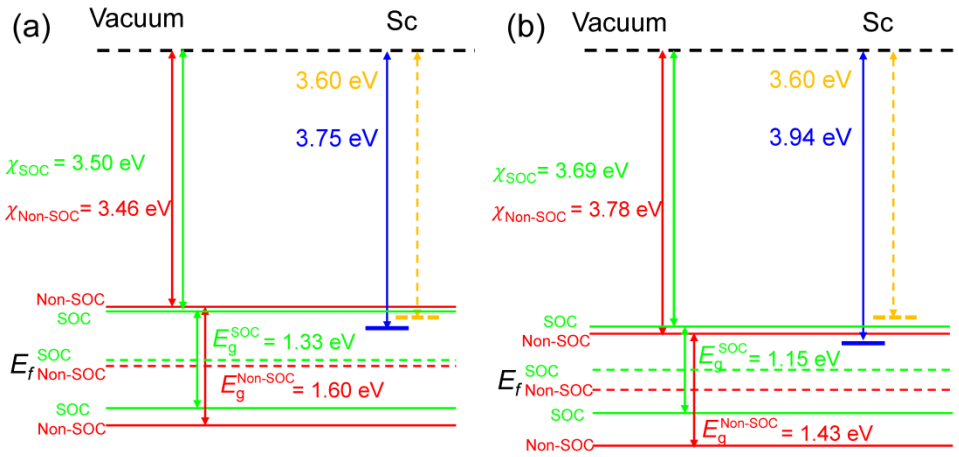

Figure S2. Line-up of the Fermi level of metal Sc with electronic bands of free-standing (a) ML and (b) BL WSe_2 in terms of the calculated work function at the DFT level with (green lines) and without (red lines) inclusion of the SOC effects. The blue lines represent the Fermi level of absorbed system, and the yellow dashed lines represent the Fermi level of pure metal. Note that the work functions of the combined systems are insensitive to the SOC effects, for example, *W* of ML WSe_2-Sc complex is only increased by 0.05 eV after considering the SOC effects.

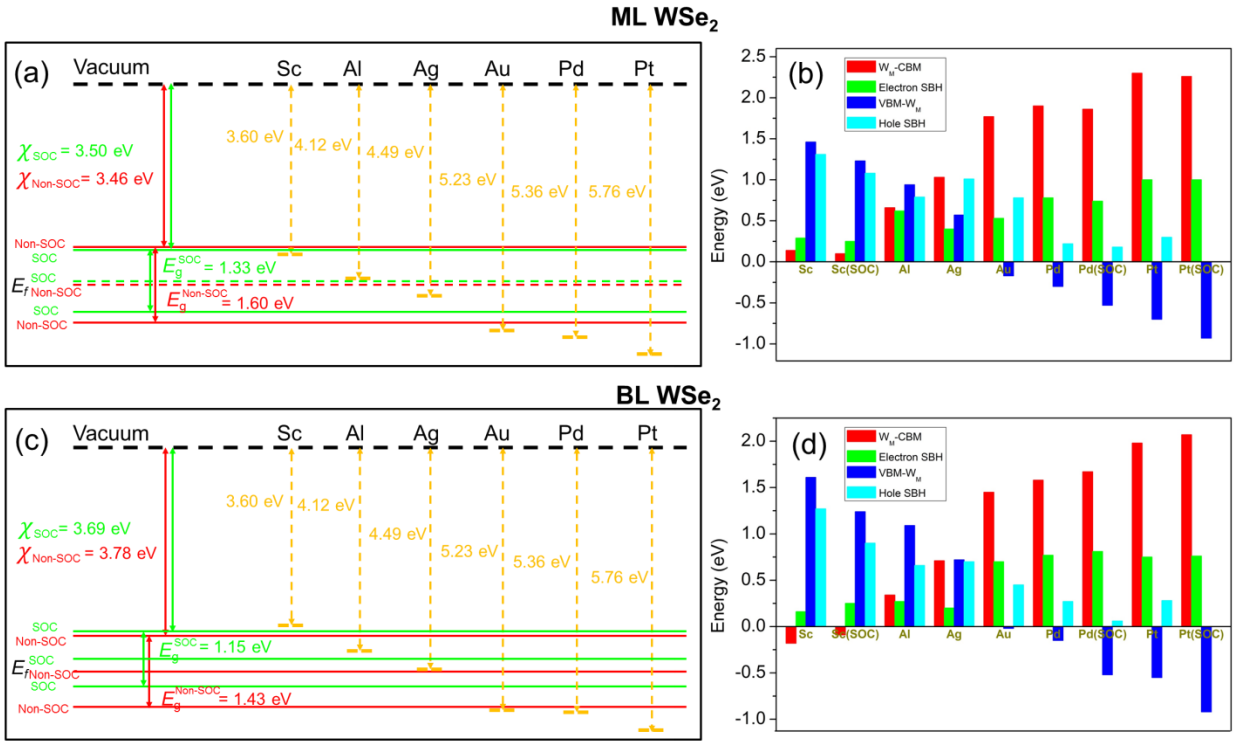

Figure S3. (a) Band alignments between ML WSe_2 and various metals. The yellow dashed lines represent the Fermi levels of different pure metals. (b) The differences between metal work function and CBM (VBM) of ML WSe_2 are compared with the electron (hole) SBHs obtained by our energy band calculations. (c) same as (a), and (d) same as (b) just for BL WSe2 cases.

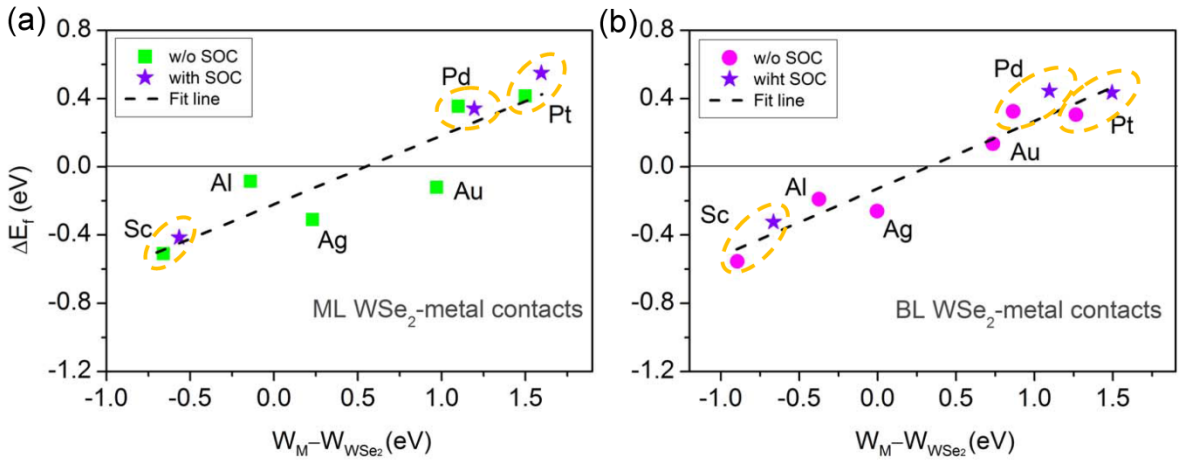

Figure S4. Calculated Fermi level shift ΔE_f in the (a) ML and (b) BL WSe_2-metal contacts as a function of $W_M - W_{WSe2}$, the difference between the work functions of clean metal and ML or BL WSe_2 at the DFT level. The dashed lines are the fit curves to all the data in the plot.

Note that the bands bend in the opposite sense in 2D WSe_2-metal and the corresponding *n*-type or *p*-type conventional bulk semiconductor-metal blocking contacts. This difference arises from the opposite charge flowing directions in these two cases. Take *n*-type SBH as an example, donor states are absent in the 2D WSe_2, and electrons flow from metal to 2D WSe_2 leaving WSe_2 *n*-type doped because $\chi_{WSe2} < W_M < W_{WSe2}$ (Figure S3a), while the electrons flow from *n*-type conventional semiconductor to metal leaving the semiconductor positively charged within a depletion region (the positive charge residing on the ionized donor atoms) because $W_M > W_{SemiS}$ (Figure S3b). The opposite band bending is a response to the opposite internal electrical field that results from the charge separation at the junction. This different bending behavior is not limited in WSe_2-metal contacts, but a general phenomenon in 2D material-metal contacts. Another difference between 2D material-metal and conventional bulk semiconductor-metal contacts should also be noticed. In 2D material-metal contacts, the band bending of the same doping type Ohmic and Schottky contacts are the same; by contrast, in conventional bulk semiconductor-metal contacts, the band bending of the same doping type Ohmic and Schottky contacts are opposite. The reason lies in the same (opposite) charge flowing directions in the same doping type Ohmic and Schottky 2D material (conventional bulk semiconductor)-metal contacts.

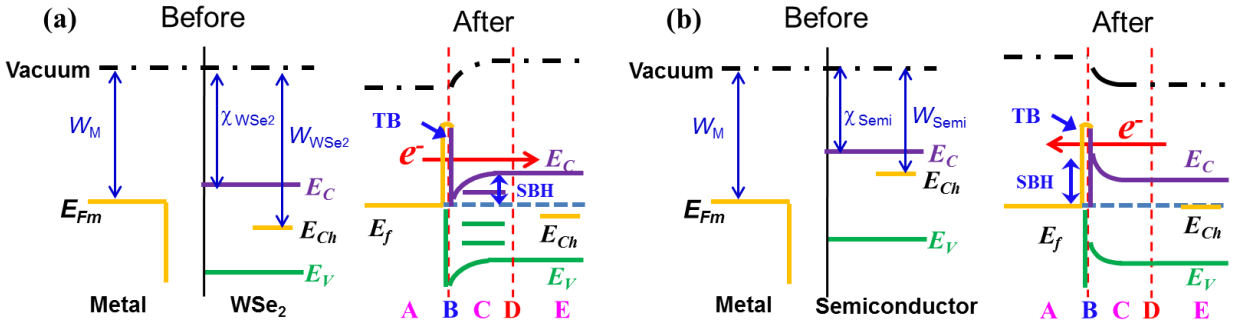

Figure S5. Illustrations of the band bending of *n*-type SBHs that occur at (a) WSe_2-metal and (b) *n*-type conventional semiconductor-metal contacts. E_{Fm}, E_{Ch} and E_f denote the Fermi levels of the clean metal, uncontacted channel and absorbed system, respectively. Red arrows indicate the direction of electron flow. W_M, W_{WSe2}, and W_{Semi} are the work functions for clean metal surface, 2D WSe_2, and conventional bulk semiconductor, respectively.