

Supplementary Materials for

Van der Waals metal-semiconductor junction: Weak Fermi level pinning enables effective tuning of Schottky barrier

Yuanyue Liu, Paul Stradins, Su-Huai Wei

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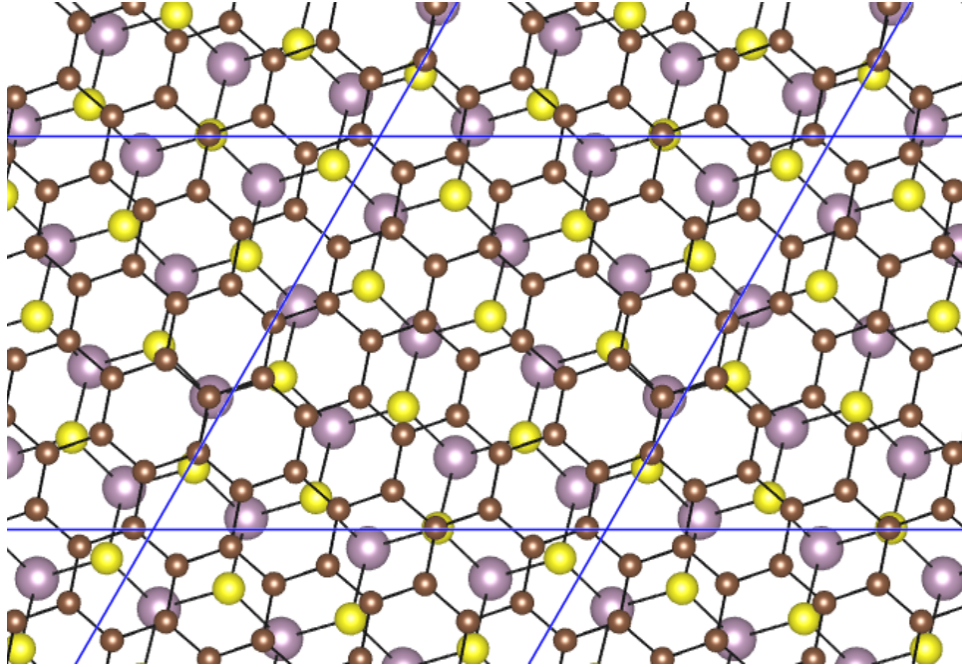


fig. S1. Supercell used for modeling graphene-*H*-MoS₂ junction. The blue lines indicate the cell boundaries. Brown: C; Yellow: S; Purple: Mo.

Comparison of pinning factor between vdW and chemically-bonded junctions:

In order to compare the strength of FLP between the vdW MSJ and the 3D metal—2D *H*-MoS₂ junction, we take the calculated Φ from literature for the latter case, and recalculate the Φ in the former case by using the same method with literature (i.e. LDA functional). As shown in fig. S2, compared with 3D metals, 2D metals show a more prominent linear correlation between Φ and W , indicating a weaker FLP. We have also used PBE-D3 method to double check the conclusion, and find that it gives a similar level of correlation.

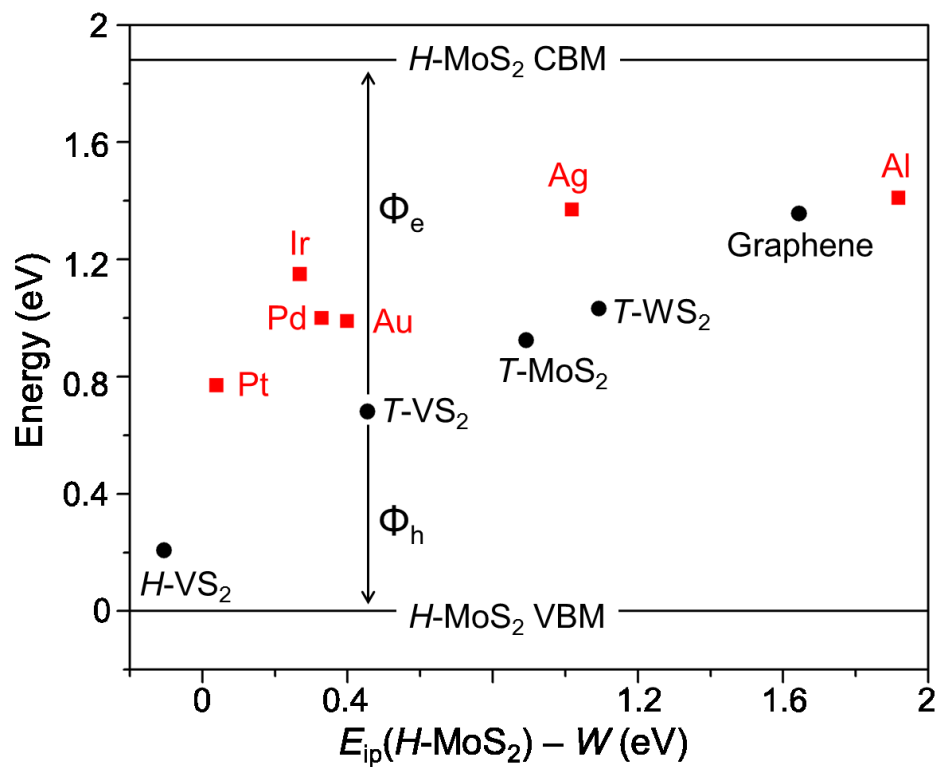


fig. S2. Red squares: Φ between 2D $H-MoS_2$ and various 3D metals. The values are taken from Nano Lett. 14, 1714-1720 (2014). Black dots: Φ between 2D $H-MoS_2$ and various 2D metals, calculated by using same methods (i.e. LDA functional).

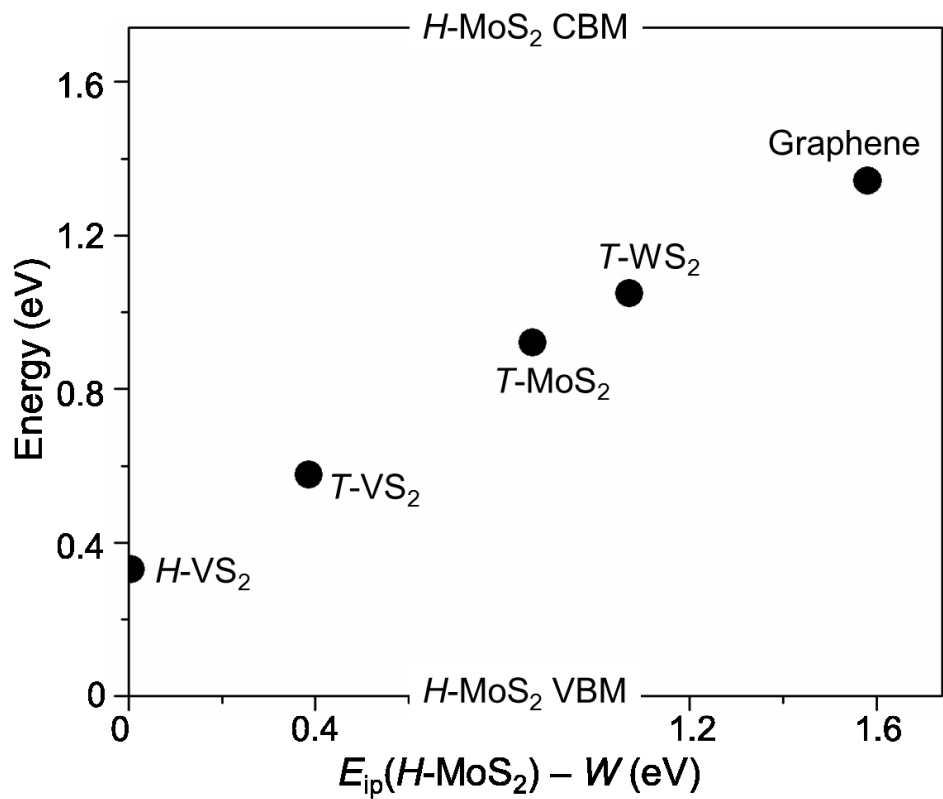


fig. S3. Φ between 2D *H*-MoS₂ and various 2D metals calculated by using PBE-D3 method.

Schottky barrier heights for 2D NbS₂ and C₂₀N with various 2D semiconductors:

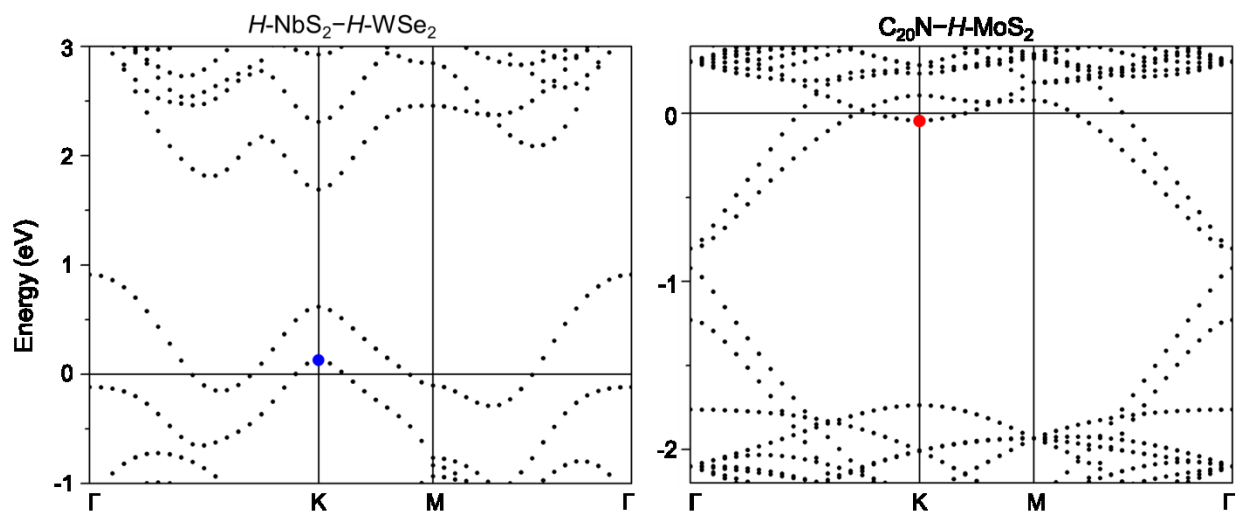


fig. S4. Band structure of $H\text{-NbS}_2\text{-}H\text{-WSe}_2$ (left) and $\text{C}_{20}\text{N-}H\text{-MoS}_2$ (right) junctions (calculated by using PBE functional). Blue and red dots mark the valence band maximum (VBM) and the conduction band minimum (CBM) of the semiconductors. Fermi level is set to zero. Note that the Fermi level of the junction is lower than the VBM (left), or higher than the CBM (right), indicating a strong charge transfer.

$\text{NbS}_2\text{-}$	WTe_2	MoTe_2	WSe_2	MoSe_2	WS_2	MoS_2
PBE	-0.12	-0.09	-0.12	-0.07	-0.03	0.06
PBE+D3	-0.14	-0.13	-0.13	-0.07	0.06	0.18
$\text{C}_{20}\text{N-}$	WSe_2	MoSe_2	WS_2	MoS_2		
PBE	0.15	0.00	-0.04	-0.04		
PBE+D3	0.32	0.04	0.01	-0.04		

table S1. Comparison of Φ between PBE and PBE-D3 methods. Φ_h for $H\text{-NbS}_2$ and Φ_e for C_{20}N with various 2D semiconductors are shown in the unit of eV.