Supporting Information for

Band alignment in multilayered semiconductor homojunctions supported on

metals

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1) For the Methods part

I. Why adopt SCAN+rVV10

All the calculations were carried out using SCAN+rVV10 in our manuscript, the SCAN (nonempirical Strongly Constrained and Appropriately Normed) functional is a meta-GGA which exceeds than LDA and GGA in many aspects, especially in systems with weak interaction, and also give better band gap¹⁻². The rVV10 is the shorthand of revised Vydrov–van Voorhis nonlocal correlation functional which is suitable to describe the van der Waals interaction in atomic layered materials ³⁻⁴.

Table SI Band gap of MoS₂ calculated from SCAN+rVV10 functional, along with those from experiment $E g^{5}$, and calculated by other methods: GGA functional⁶, HSE06 hybrid functional⁶, and GW⁷.

	E_{g}^{Exp} (eV)	$E \frac{GGA}{g} (eV)$	$E \frac{SCAN + rvv10}{g} (eV)$	$E \frac{HSE06}{g}$ (eV)	$E \frac{GW}{g}$ (eV)
monolayer	1.82	1.64	1.74	2.09	2.76
bilayer	1.65	1.17	1.52	1.66	1.89

For the following reasons, we find that the SCAN+rVV10 is the most suitable functional for the systems (multilayer semiconductor supported on 2D metal substrates) we studied. First, we compare the band gap of MoS₂ calculated from SCAN+rVV10 with available GGA, HSE06, GW and experimental values in Table R1. Relative to experiment values, the GGA underestimates band gap obviously, while meta-GGA SCAN+rVV10, makes up this imperfection. Especially for monolayer MoS₂, SCAN+rVV10 fits to experimental band gap value better than HSE06 and GW. Second, the strong Coulombic screening brought by metal with infinite dielectric constant in metal-semiconductor junctions will minimize the many body effect in semiconductor⁸, which will then reduce the underestimation effect of SCAN on band gap in isolated semiconductor. Third, the supercells of some junctions calculated in our work are too large (for example, there are 158 atoms for Mo₂CO₂-2L MoS₂ junctions in $4 \times 4 / \sqrt{13} \times \sqrt{13}$ supercell) to calculate them by HSE06 or GW functional, which is too computational demanding. Therefore, SCAN+rVV10 functional is the best

choice to describe metal-semiconductor junctions with controllable computational cost and accurate description of band gap for our homojunctions on metals.

II. About spin-polarization

The spin-polarization is not considered, since spin-polarized is not that important for our systems studied. We found that all of the semiconductors in the Table 1 in manuscript are not spin-polarized: details can be found on websites <u>https://materialsproject.org/</u> and <u>https://www.materialscloud.org/discover/2dstructures/dashboard/ptable</u>. The three MXenes used as substrates in our manuscript are nonmagnetic which have been reported in literatures⁹⁻¹². Therefore, the spin-polarized calculations are not needed for our systems studied.

III. Details about k-points sampling

Fable SII The lattice	parameters of junctions and th	e corresponding l	k-point samp	ling
	, J	1 0	1 1	<u> </u>

	lattice percentary (Å)	k-point number for	k-point number for
	lattice parameters (A)	structure optimization	electronic properties
hexagonal lattice junction	a=b=3.164	$15 \times 15 \times 1$	$21 \times 21 \times 1$
quadrangular lattice	a=3.27	$1 \times 2 \times 1$	$21 \times 2 \times 1$
junction	b=22.83	21 × 3× 1	21 × 3× 1

We sampled the Brillouin zone (BZ) in the Monkhorst-Pack scheme. The k-points mesh of (a × a× 1), (a × b× 1) was employed for the structure optimization and electronic properties in hexagonal-lattice junction (like MoS₂-Zr₂C(OH)₂. etc.), and in quadrangular-lattice junction (like black phosphorus-Zr₂C(OH)₂. etc.), respectively. The lattice parameters of heterojunctions and the corresponding kpoint number are given in the Table R2. For hexagonal lattice junction using MoS₂-Zr₂C(OH)₂ is an example, and the k-points sampling of the other hexagonal-lattice junctions have similar k-pointdensity.

2) For the Results and Discussion part

I. Geometry structures for bilayer semiconductors



FIG. S1. Five types of bilayer semiconductors as candidates for homojunctions.

II. Supercell, mismatch and formation energy for homojunctions supported on metal

The formation energy (E_b) between 2D metal and semiconductor in the 2D metal-2L semiconductor junction is defined as:

$$E_b = (E_{junction} - E_{metal} - E_{2LSemiconductor})/A$$

where $E_{junction}$, E_{metal} , and $E_{2L\,Semiconductor}$ are the total energies of 2D metal-2L semiconductor junction, isolated 2D metal, and the 2L semiconductor, respectively. A is the interface area. According to the definition, the negative E_b indicates stable interface binding. In the Tables R3 to R5 below, supercell of the metal-semiconductor junction and lattice mismatch ε % are also shown. The lattice mismatch ε % is defined as ε % = (a - a₀)/a, where a₀ and a are the in-plane lattice constants of metal and semiconductor, respectively. A positive number represents tensile strain of metal surface, and vice versa.

The information of MoS_2 and black P is given in separate Tables. E_b of -0.3 J/m² represents a typical physical adsorption. In the above three tables, all binding energies are negative and less than or comparable to -0.3J/m², indicating that all junction structures are stable in energy.

	Mo ₂ CO ₂		Zr ₂ C(OH) ₂			
2D semiconductors	supercell of metal [–] semiconductor junction	3	Binding energy (J/m ²)	supercell of metal - semiconductor junction	3	Binding energy (J/m ²)
BN	$\sqrt{3} \times \sqrt{3}/2 \times 2$	-1.57	-4.34	$\sqrt{3} \times \sqrt{3}/2 \times 2$	11.32	-4.42
BP	$1 \times 1/1 \times 1$	-10.98	-9.36	$1 \times 1/1 \times 1$	0.59	-11.37
BAs	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-2.50	-3.14	$1 \times 1/1 \times 1$	-4.62	-4.59
AlN	$1 \times 1/1 \times 1$	-8.52	-7.34	$1 \times 1/1 \times 1$	3.37	-9.18
AlP	*	*	*	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-5.04	-1.23
GaN	$1 \times 1/1 \times 1$	-10.47	-10.12	$1 \times 1/1 \times 1$	1.16	-11.88
GaP_b	*	*	*	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-3.14	-0.74
GaAs_b	*	*	*	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-6.85	-0.92
InN	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-7.39	-2.28	$2 \times 2/\sqrt{3} \times \sqrt{3}$	4.64	-1.27
InSb_b	$3 \times 3/2 \times 2$	-6.80	-2.03	*	*	*
SiC	$1 \times 1/1 \times 1$	-7.77	-9.66	$1 \times 1/1 \times 1$	4.21	-11.61
GeC	$1 \times 1/1 \times 1$	-11.34	-10.66	$1 \times 1/1 \times 1$	0.19	-12.29
SnC	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-7.79	-2.51	$2 \times 2/\sqrt{3} \times \sqrt{3}$	4.20	-1.14
N_b	$\sqrt{3} \times \sqrt{3}/2 \times 2$	8.42	-7.04	*	*	*
Blue P_b	$2 \times 2/\sqrt{3} \times \sqrt{3}$	1.22	-1.70	$1 \times 1/1 \times 1$	-0.95	-4.11
As_b	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-7.34	-1.65	$2 \times 2/\sqrt{3} \times \sqrt{3}$	4.70	-0.09
2H-MoSe ₂	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-0.07	-0.41	$1 \times 1/1 \times 1$	-2.13	-0.65
2H-MoTe ₂	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-5.82	-0.47	$2 \times 2/\sqrt{3} \times \sqrt{3}$	6.42	-0.63
2H-WS ₂	$1 \times 1/1 \times 1$	-10.19	-0.39	$1 \times 1/1 \times 1$	1.48	-0.63
2H-WSe ₂	$2 \times 2/\sqrt{3} \times \sqrt{3}$	3.71	-0.44	$1 \times 1/1 \times 1$	-2.19	-0.66
2H-WTe ₂	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-5.96	-0.45	$2 \times 2/\sqrt{3} \times \sqrt{3}$	6.26	-0.58
1T-ZrS ₂	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-10.57	-0.23	$2 \times 2/\sqrt{3} \times \sqrt{3}$	1.06	-1.06
1T-ZrSe ₂	*	*	*	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-1.92	-0.99
1T-PtS ₂	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-6.10	-0.28	$2 \times 2/\sqrt{3} \times \sqrt{3}$	6.10	-0.83
1T-HfS ₂	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-8.94	-0.25	$2 \times 2/\sqrt{3} \times \sqrt{3}$	2.89	-0.98
1T-HfSe ₂	*	*	*	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-0.65	-0.97
$1T-SnS_2$	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-9.93	-0.25	$2 \times 2/\sqrt{3} \times \sqrt{3}$	1.77	-1.00
InSe	*	*	*	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-5.34	-0.37

Table SIII. Summary of supercell, mismatch and formation energy of metal-semiconductor junctions.

"*" in the Table means no calculated data due to it is difficult to construct a "relatively small" supercell with small lattice-mismatch.

	supercell of Metal [–] MoS ₂ junction	3	Binding energy (J/m ²)
Zr ₂ C(OH) ₂	$1 \times 1/1 \times 1$	-1.68	-0.41
Ta ₂ C(OH) ₂	$1 \times 1/1 \times 1$	-5.28	-0.58
Mo ₂ CO ₂	$4 \times 4/\sqrt{13} \times \sqrt{13}$	-0.18	-0.24
Pt (111)	$2 \times 2/\sqrt{3} \times \sqrt{3}$	-2.50	-0.52

Table SIV. Supercell, mismatch and formation energy of metal-MoS₂ junctions.

Table SV. Supercell, mismatch and formation energy of Zr₂C(OH)₂-black P junctions.

supercell of $Zr_2C(OH)_2$ -		c at a avia	ε at b axis	Binding energy
	black P junction			(J/m ²)
Black P	$1 \times 4\sqrt{3}/1 \times 5$	-1.62	-2.46	-0.90

III. Projected band structure of the layered semiconductors supported on 2D metals



FIG. S2. The projected band structure of the Group III-V bilayer compounds supported on 2D high work function metals of Mo₂CO₂. The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.



FIG. S3. The projected band structure of the Group IV-IV bilayer compounds supported on 2D high work function metals of Mo_2CO_2 . The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.



FIG. S4. The projected band structure of the Group V bilayer compounds supported on 2D high work function metals of Mo_2CO_2 . The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.



FIG. S5. The projected band structure of the bilayer 2H-TMDC semiconductors supported on 2D high work function metals of Mo₂CO₂. The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.



FIG. S6. The projected band structure of the bilayer 1T-TMDC compounds supported on 2D high work function metals of Mo₂CO₂. The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.



FIG. S7. The projected band structure of the Group III-V bilayer compounds supported on 2D low work function metals of $Zr_2C(OH)_2$. The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.



FIG. S8. The projected band structure of the Group IV-IV bilayer compounds supported on 2D low work function metals of $Zr_2C(OH)_2$. The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.



FIG. S9. The projected band structure of the Group V bilayer compounds supported on 2D low work function metals of $Zr_2C(OH)_2$. The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.



FIG. S10. The projected band structure of the bilayer 2H-TMDC semiconductors supported on 2D low work function metals of $Zr_2C(OH)_2$. The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.



FIG. S11. The projected band structure of the bilayer 1H-TMDC compounds supported on 2D low work function metals of $Zr_2C(OH)_2$. The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.



FIG. S12. The projected band structure of the bilayer InSe supported on 2D low work function metals of $Zr_2C(OH)_2$. The contributions from the first and second layers are marked with red and green dot lines, respectively. Fermi level was set to zero.

IV. 3R stacking bilayer MoS₂ supported on 2D metals

TMDCs are usually found in three polymorphs called 1T, 2H and 3R. Here the numbers stand for the number of layers in the unit cell of 3D bulk materials and the letters indicate symmetry (*T*—trigonal, *H*—hexagonal, and *R*—rhombohedral). Due to the hexagonal chalcogen packing and the compact

interlayer stacking only octahedral and tetrahedral interstitial sites are present in the vdW gap. Therefore, we considered the 2H and 3R polymorph bilayer MoS_2 supported on 2D metals $Zr_2C(OH)_2$, the geometric structures are shown in Figure S13.



FIG. S13. Side view of the 2L MoS₂-Zr₂C(OH)₂ junction with 2H (a) 3R (b) polymorph.



FIG. S14. (a-c) Projected band structure to each layer of 3R stacking 2L MoS₂ supported on 2D metals of $Zr_2C(OH)_2$, $Ta_2C(OH)_2$ and Mo₂CO₂, respectively. (d-f) Plane-averaged electron density difference along the vertical z-direction to the interfaces in Metal-2L MoS₂ junction with 3R stacking MoS₂. Red (blue) regions represent electron accumulation (depletion) regions. The interface between 2D metal and MoS₂ is demonstrated within two black dotted lines, while the interface between the two MoS₂ layers is demonstrated within two red dotted lines. (g-i) Illustration of type II and type II band alignment between MoS₂ layers, where red (green) line indicates energy bands from the first (second) layer.

We have considered 2H polymorph MoS₂ in the manuscript; here we added the projected band structures and plane-averaged electron densities of 3R MoS₂ supported on 2D metals of $Zr_2C(OH)_2$, $Ta_2C(OH)_2$ and Mo₂CO₂ in Figure R2. The values of Δ_{CBM} in 2H and 3R 2L MoS₂ supported on 2D metals are shown in Table R1. The values of Δ_{CBM} in 3R polymorph MoS₂ are 0.55, 1.85, and -0.46 eV supported on $Zr_2C(OH)_2$, $Ta_2C(OH)_2$ and Mo₂CO₂, which numbers are close to those of 2H polymorph MoS₂. As a result, type II band alignment were achieved in 3R polymorph MoS₂ supported on $Zr_2C(OH)_2$ and Mo₂CO₂, while type III were achieved in Ta₂C(OH)₂, which conclusion is exactly the same as the 2H polymorph MoS₂ on metallic MXenes.

	Δ_{CBM} in 2H MoS ₂	Δ_{CBM} in 3R MoS ₂
	(eV)	(eV)
Zr ₂ C(OH) ₂ -2L MoS ₂	0.43	0.55
Ta ₂ C(OH) ₂ -2L MoS ₂	1.78	1.85
Mo ₂ CO ₂ -2L MoS ₂	-0.54	-0.46

Table SVI. Δ_{CBM} in 2L MoS₂-2D metal for 2H and 3R stacking MoS₂.

We also consider the charge redistribution at interfaces for 3R stacking MoS_2 supported on 2D metals of $Zr_2C(OH)_2$, $Ta_2C(OH)_2$ and Mo_2CO_2 , respectively. The charge distribution at two interfaces in a junction is same as that in 2H stacking MoS_2 supported on 2D metals except for a small quantitative difference.

V. Homojunction in Pt-3L MoS₂



FIG. S15. Projected band structure to each layer of $3L MoS_2$ supported on 3D metal Pt. If the second and third layers are used as homojunction, as shown in figure, there is little gap states.

In 3D metal-2L semiconductor, MIGS occurs in the first layer of semiconductor, so type-II band alignment in 2L semiconductor homojunction supported on 3D metal can't form because of the metallization in first layer semiconductor. Therefore, we try to use trilayer (3L) semiconductor supported on 3D metal electrodes to produce type-II band alignment, in which the second and third layers act as homojunction, metal substrates and the first metallized layer act as metal-supports.



VI. Type III homojunctions

FIG. S16. Type III homojunctions, 2L BP-Zr₂C(OH)₂, 2L BAs-Zr₂C(OH)₂, 2L InN-Zr₂C(OH)₂, 2L ZrSe₂-Zr₂C(OH)₂.

VII. Plane-averaged electrostatic potential for MoS₂ homojunctions supported on Zr₂C(OH)₂ and Mo₂CO₂



FIG. S17. Plane-averaged electrostatic potential along the interface normal (z-direction) of 2D metal-2L MoS₂. The metal-semiconductor interface position is indicated by the vertical dashed line, and the potential step ΔV_{M-S} between the vacuum levels of semiconductor and metal sides of metal-2L MoS₂ is shown. The arrows indicate the direction of interface dipoles.

Figure S17 shows the plane averaged electrostatic potential along the interface normal direction. For

MoS₂ homojunctions supported on $Zr_2C(OH)_2$ and Mo₂CO₂, a potential discontinuity, ΔV_{M-S} , of 6.09 eV between the vacuum levels on the MoS₂ and $Zr_2C(OH)_2$ sides , and -3.57 eV between MoS₂ and Mo₂CO₂, are discovered.



VIII. Differences in Δ_{CBM} (or Δ_{VBM}) between Zr₂C(OH)₂-2L MoS₂ and Ta₂C(OH)₂-2L MoS₂.

FIG. S18. Plane-averaged electrostatic potential energy along the interface normal direction in $Zr_2C(OH)_2$ -2L MoS₂ (a) and Ta₂C(OH)₂-2L MoS₂ (b) junction. In (b), the interface potential step Δ_{12} between the 1st- and 2nd- layer MoS₂ is reflected in the potential energy difference between the Mo atomic-layer.

Table SVII. Band edge offsets Δ_{CBM} and interface potential step Δ_{12} between 1st- and 2nd-layer MoS₂ in $Zr_2C(OH)_2/2L$ MoS₂ and Ta₂C(OH)₂/2L MoS₂ junctions.

	$\Delta_{\rm CBM}~({\rm eV})$	$\Delta_{12} (eV)$
Zr ₂ C(OH) ₂ -2L MoS ₂	0.43	1.30
Ta ₂ C(OH) ₂ -2L MoS ₂	1.78	2.98

The interface potential step Δ_{12} is defined in Figure R2b, which shows the plane-averaged electrostatic potential along the interface normal direction. The difference of Δ_{12} in Ta₂C(OH)₂-2L MoS₂ and in Zr₂C(OH)₂-2L MoS₂ is 1.68 eV while the difference of Δ_{CBM} in two junctions is 1.35 eV, which indicates that the electrostatic potential step Δ_{12} caused by charge distribution at S-S interface plays the main role of band offset Δ_{CBM} which is the energy difference between the CBM of first- and second-layer of MoS₂. We also calculated the Bader charge of Ta₂C(OH)₂-2L MoS₂ and

 $Zr_2C(OH)_2$ -2L MoS₂, charge transfer between each layer is shown in the Table R2. The second-layer of MoS₂ in both junctions receive electrons, the amount in Ta₂C(OH)₂-2L MoS₂ is much larger than in $Zr_2C(OH)_2$ -2L MoS₂, which is consistent with the Figure 3d and 3e in the manuscript.

	Metal (e^{-})	$1^{\text{st}} \operatorname{MoS}_2(e^{-})$	$2^{nd} \operatorname{MoS}_2(e^-)$
Zr ₂ C(OH) ₂ -2L MoS ₂	-0.0984	0.0788	0.0196
Ta ₂ C(OH) ₂ -2L MoS ₂	-0.1276	0.0666	0.0609

Table SVIII. Bader charge of each layer in Ta₂C(OH)₂-2L MoS₂ and Zr₂C(OH)₂-2L MoS₂.

As discussed in reply to comment 2, the charge transfer at S-S interfaces is a continuation of the M-S interface in 2D metal-2LMoS₂ junction, the larger charge redistribution at S-S interfaces in $Ta_2C(OH)_2$ -2L MoS₂ should come from the M-S interface. The formation energy and distance at M-S interface is shown in Table R3

Table SIX. Formation energy and distance in Ta₂C(OH)₂-2L MoS₂ and Zr₂C(OH)₂-2L MoS₂. D represents the averaged equilibrium interface distance.

	E _b (J/m ²)	D (Å)
Zr ₂ C(OH) ₂ -2L MoS ₂	-0.41	2.218
Ta ₂ C(OH) ₂ -2L MoS ₂	-0.58	2.119

The larger binding energy and shorter interface vertical separation turns out that the interact of M-S in $Ta_2C(OH)_2$ -2L MoS₂ is more strongly which finally results the more interactive S-S interface in $Ta_2C(OH)_2$ -2L MoS₂.

These differences between $Zr_2C(OH)_2$ and $Ta_2C(OH)_2$ listed above may be related to the different metal cations (Zr, Ta): the Ta 5d electrons have more influence than the Zr 4d electrons since 5d electrons are more delocalized. Furthermore, the shorter interface vertical separation between $Ta_2C(OH)_2$ and MoS_2 provides more convenience for electron transfer.

References

- 1 J. Sun, A. Ruzsinszky, J. P. Perdew, *Phy. Rev. Lett.* 2015, 115,036402.
- J. Sun, R. C. Remsing, Y. Zhang, Z. Sun, A. Ruzsinszky, H. Peng, Z. Yang, A. Paul, U. Waghmare, X. Wu, M. L. Klein, J. P. Perdew, *Nature Chem.* 2016, 8, 831-836.
- 3 H. Peng, J. P. Perdew, *Phys. Rev. B* 2017, 95, 081105.
- 4 H. Peng, Z.-H. Yang, J. P. Perdew, J. Sun, *Phys. Rev. X* 2016, 6, 041005.
- 5 R. Ganatra, Q. Zhang, Acs Nano 2014, 8, 4074-4099.
- 6 J.-Q. Hu, L.-H. Xu, S.-Q. Wu, Z.-Z. Zhu, Current Appl. Phys. 2019, 19, 1222-1232.
- 7 T. Cheiwchanchamnangij, W. R. L. Lambrecht, Phys. Rev. B 2012, 85, 205302.
- 8 C. Gong, L. Colombo, R. M. Wallace, K. Cho, Nano Letters 2014, 14, 1714-1720.
- 9 H. Wang, C. Si, J. Zhou, Z. Sun, J. Phys. Chem. C 2017, 121, 25164-25171.
- 10 M. Khazaei, M. Arai, T. Sasaki, M. Estili, Y. Sakka, *Phys. Chem. Chem. Phys.* 2014, 16, 7841-7849.
- 11 M. Khazaei, M. Arai, T. Sasaki, C.-Y. Chung, N. S. Venkataramanan, M. Estili, Y. Sakka, Y. Kawazoe, *Adv. Fun.Mater.* 2013, 23, 2185-2192.
- H. Weng, A. Ranjbar, Y. Liang, Z. Song, M. Khazaei, S. Yunoki, M. Arai, Y. Kawazoe, Z. Fang, X. Dai, *Phys. Rev. B* 2015, 92, 075436.