

Supplementary information

Magnetic proximity effect and electrical field tunable valley degeneracy in MoS₂/EuS van der Waals heterojunctions

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Comparing with other TMDs/EuS heterojunctions

To verify our results that the MPE exists at the MoS₂/EuS interface, we have calculated other TMDs/EuS heterojunctions, such as WS₂/EuS and MoSe₂/EuS. Fig. S1 shows the charge density difference distribution and the spin density distribution at the interface for MoS₂/EuS, WS₂/EuS and MoSe₂/EuS in chemical and vdW adsorption states, respectively. It can be seen, both in chemical and vdW adsorption states, the charge density distribution at these three interfaces are similar, and spin polarizations are observed at Mo(W) atomic layer. Fig. S2 show the band structure for MoS₂/EuS, WS₂/EuS and MoSe₂/EuS in chemical and vdW adsorption states. The calculated adsorption distance “*d*”, binding energy ΔE , induced magnetic moments and valley Zeeman splitting E_z are listed in the table S1 below. We can see the TMDs/EuS have similar adsorption way and distance, and the magnetic proximity effect is generally existed in these systems in different degrees, which is due to the intrinsic SOC of these TMCDs, in addition, the different lattice mismatch and atoms configurations at the interface of these systems can also impact the MPE. The calculated valley Zeeman splitting of WS₂/EuS and MoSe₂/EuS are 33.2 and 15.6 meV in chemical adsorption states, while 4.7 and 2.5 meV in vdW adsorption states.

Considering the measured valley Zeeman splitting rate of $-233 \pm 10 \mu\text{eV}/\text{T}^1$ and $-220 \mu\text{eV}/\text{T}^2$ for single layer WS_2 and MoSe_2 in previous studies, the MPE introduces a MEF of 143 T and 20 T for WS_2/EuS in the chemical and vdW adsorption cases, while 71T and 11T for MoSe_2 in the chemical and vdW adsorption cases.

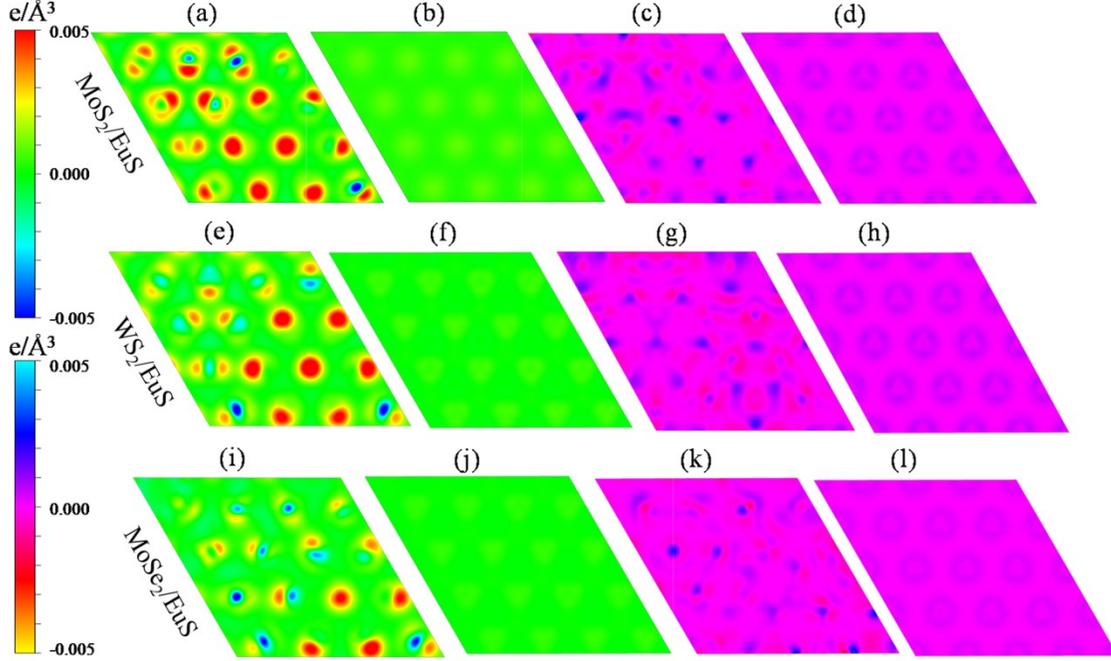


Figure S1. The charge density difference distribution at the interface of MoS_2/EuS (a, b), WS_2/EuS (e, f) and MoSe_2/EuS (i, j), in which the left column (a, e, i) indicate the chemical adsorption, and the right column (b, f, j) indicate the vdW adsorption. Also shown are the spin density distribution at the Mo (W) atomic layer of MoS_2/EuS (c, d), WS_2/EuS (g, h) and MoSe_2/EuS (k, l), in which the left column (c, g, k) indicate the chemical adsorption, and the right column (d, h, l) indicate the vdW adsorption.

Table S1. The adsorption distance “ d ”, binding energy ΔE , averaged induced magnetic moments in Mo (W) and valley Zeeman splitting E_z calculated for MoS_2/EuS , WS_2/EuS and MoSe_2/EuS heterojunctions in chemical and vdW adsorption states.

System	MoSe_2/EuS		WS_2/EuS		MoS_2/EuS	
	Chemical	vdW	Chemical	vdW	Chemical	vdW
d (Å)	2.624	6.820	2.586	6.511	2.554	6.456
ΔE (meV)	166	32	185	47	192	44
Mo\W (μ_B/atom)	0.076	0.013	0.118	0.023	0.124	0.024
E_z (meV)	15.6	2.5	33.2	4.7	37.3	5.1

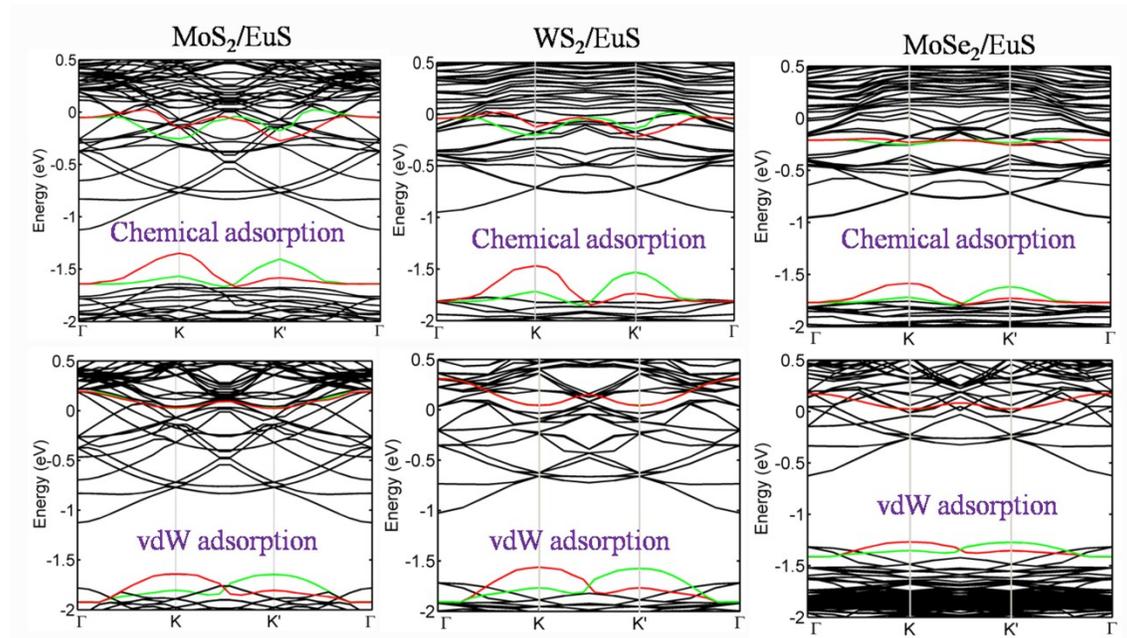


Figure S2. The band structure calculated for MoS₂/EuS, WS₂/EuS and MoSe₂/EuS heterojunctions in chemical and vdW adsorption states.

Comparing several vdW correction methods

To check the vdW correction method used in our study, we also using other vdW correction method to check our results on MoS₂/EuS system, such as optB88-vdW³ and optB86b-vdW⁴, which are also appropriate for layered systems⁵. Table S2 shows the adsorption distance “*d*”, binding energy ΔE , averaged induced magnetic moments calculated for MoS₂/EuS using different vdW correction methods. We can see these three methods give out similar adsorption distance and binding energy, in particular, the magnetic moments induced in Mo atoms are agree well with each other, which indicated the degrees of our estimated MPE at this interface is reasonable. Fig. S3 shows the projected density of states (PDOS) of Mo, S, Eu atoms at the MoS₂/EuS interface using different vdW correction methods. From the calculated PDOS, we can see the three different vdW correction has little effect on the electron structure, in particular, the band gap of MoS₂.

Table S2. The adsorption distance “ d ”, binding energy ΔE , averaged induced magnetic moments calculated for MoS₂/EuS using different vdW correction methods.

vdW correction	optB86b-vdW		optB88-vdW		revB86b-vdW-DF2	
Adsorption type	Chemical	vdW	Chemical	vdW	Chemical	vdW
d (Å)	2.538	6.423	2.634	6.611	2.554	6.456
ΔE (meV)	198	50	185	48	192	44
Mo (μ_B /atom)	0.121	0.026	0.112	0.019	0.124	0.024
S (μ_B /atom)	0.003	0.000	0.000	0.000	-0.005	0.000
Eu (μ_B /atom)	6.932	6.947	6.910	6.922	6.951	6.982

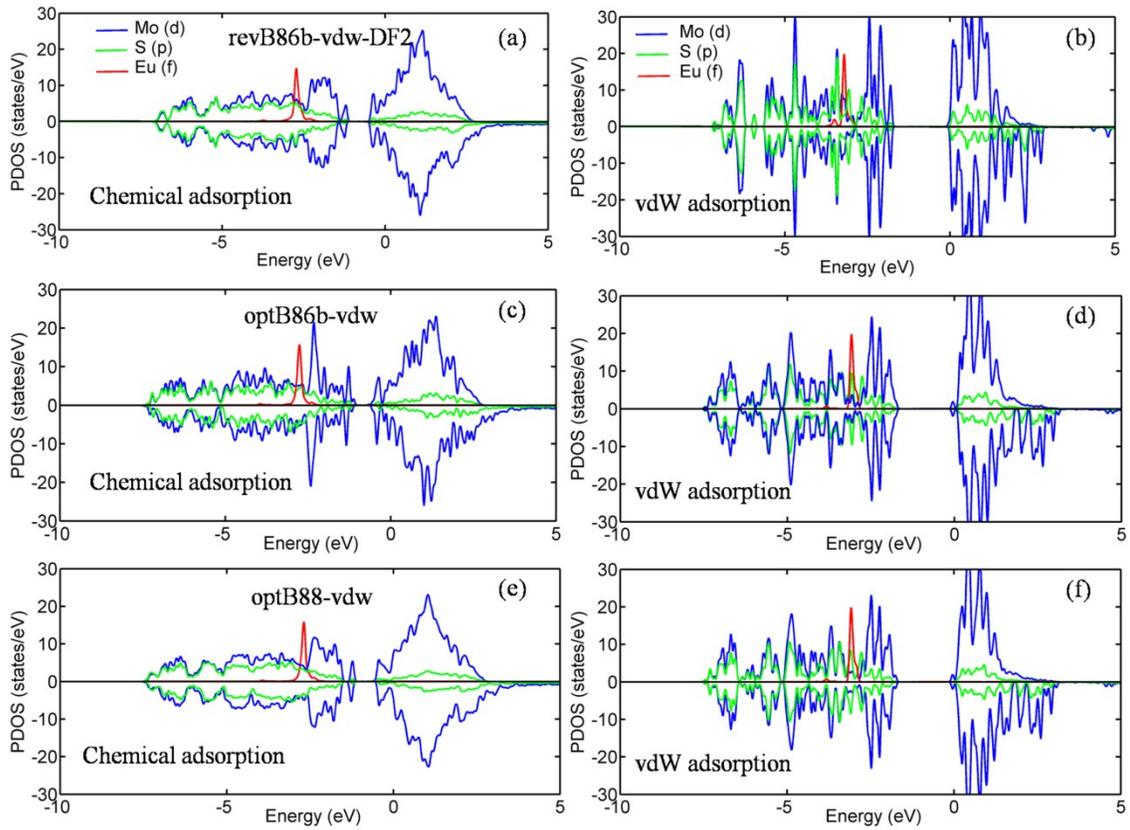


Figure S3. The calculated projected density of states (PDOS) of Mo, S, Eu atoms at the MoS₂/EuS interface using different vdW correction methods.

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