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Supporting information

Interfacial Contact Barrier and Charge Carrier Transport of MoS_2/Metal(001) Heterostructure

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Fig. S1

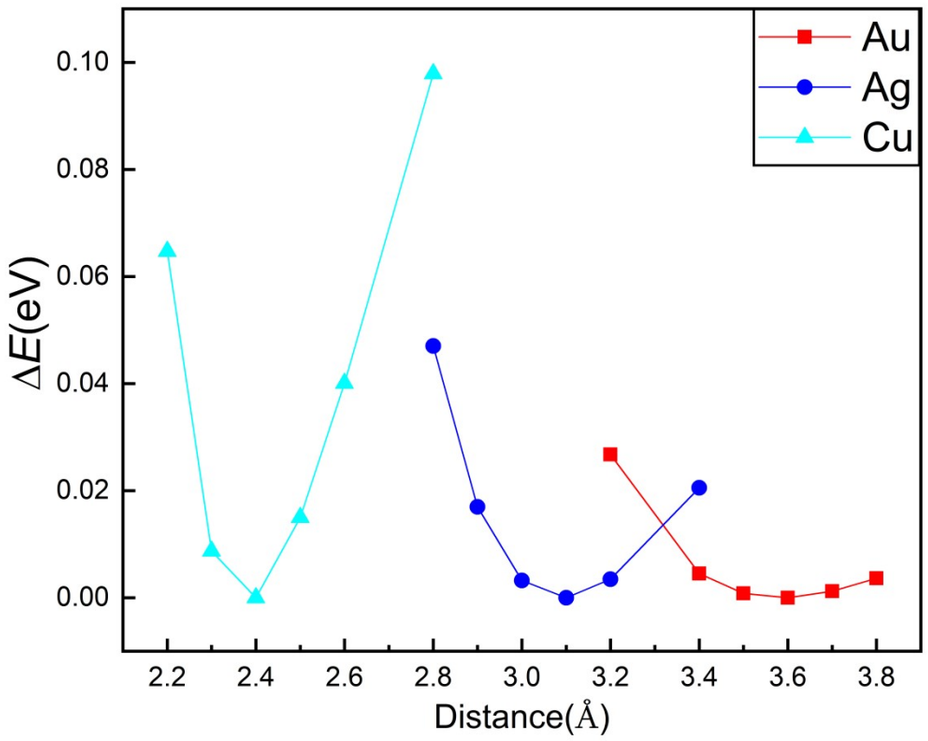

Fig S1. The function of interlayer distance d and energy difference △E between interlayer distance and equilibrium distance. Red, blue and cyan lines represent MoS_2/Au, MoS_2/Ag and MoS_2/Cu heterostructures, respectively.

Table S1

Au	Distance (Å)	Energy (eV)	Ag	Distance (Å)	Energy (eV)	Cu	Distance (Å)	Energy (eV)
	3.2	-101.835		2.8	-95.048		2.2	-105.714
	3.4	-101.857		2.9	-95.078		2.3	-105.770
	3.5	-101.861		3.0	-95.092		2.4	-105.778
	3.6	-101.862		3.1	-95.095		2.5	-105.763
	3.7	-101.860		3.2	-95.092		2.6	-105.738
	3.8	-101.858		3.4	-95.075		2.8	-105.680

Table S1. Calculated total energies of MoS_2/Metals (metals = Au, Ag and Cu) as the function of interlayer distance d.

Fig. S2

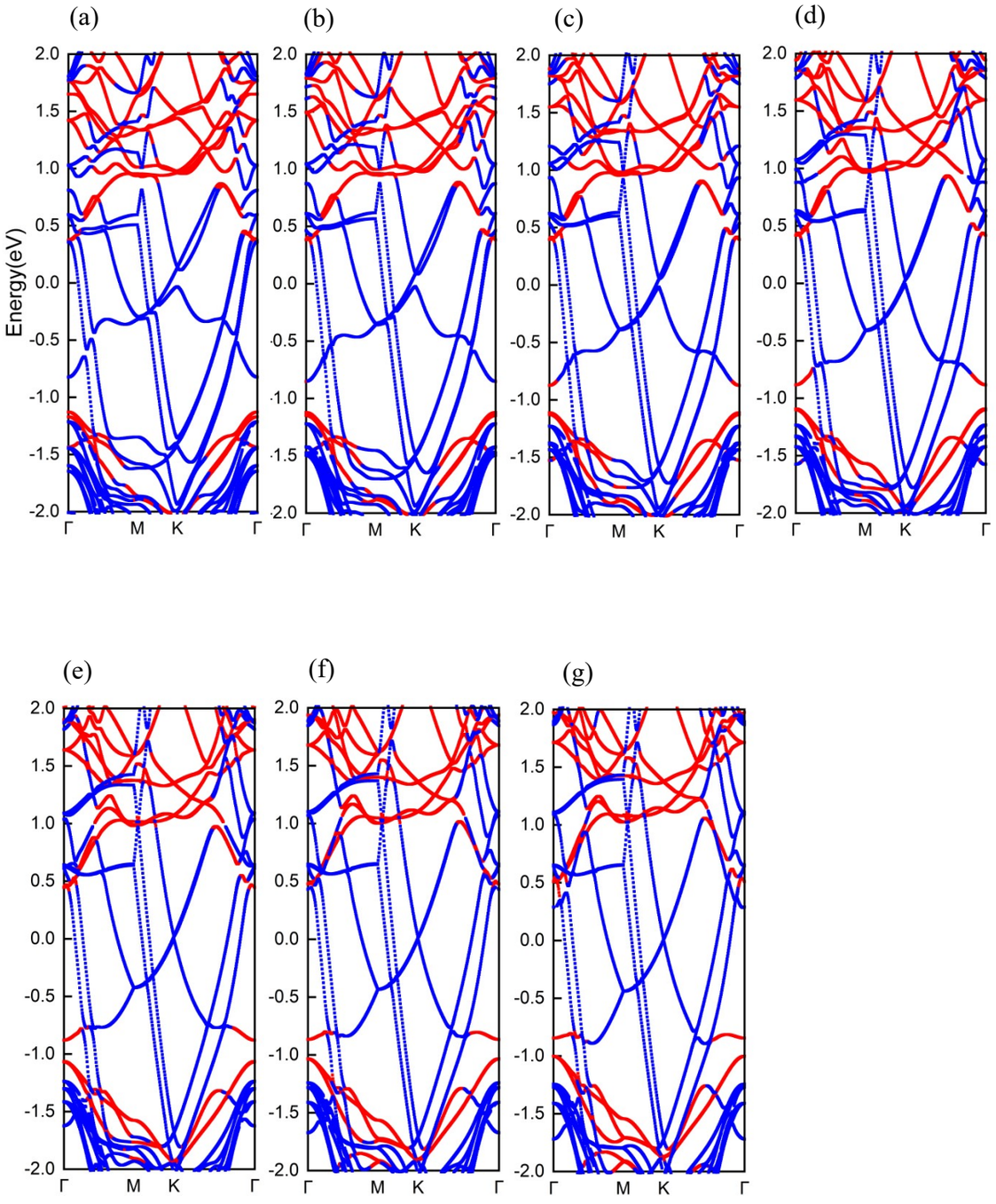

Fig S2. Projected band structure of MoS_2/Au heterostructure with tunable distance (a) 2.4Å, (b)2.6Å, (c)2.8Å, (d)3.0, (e)3.2Å, (f)3.4, (g)3.6Å. The blue, and red lines represent the electronic orbital contributions of Au, MoS_2, respectively.

Fig. S3

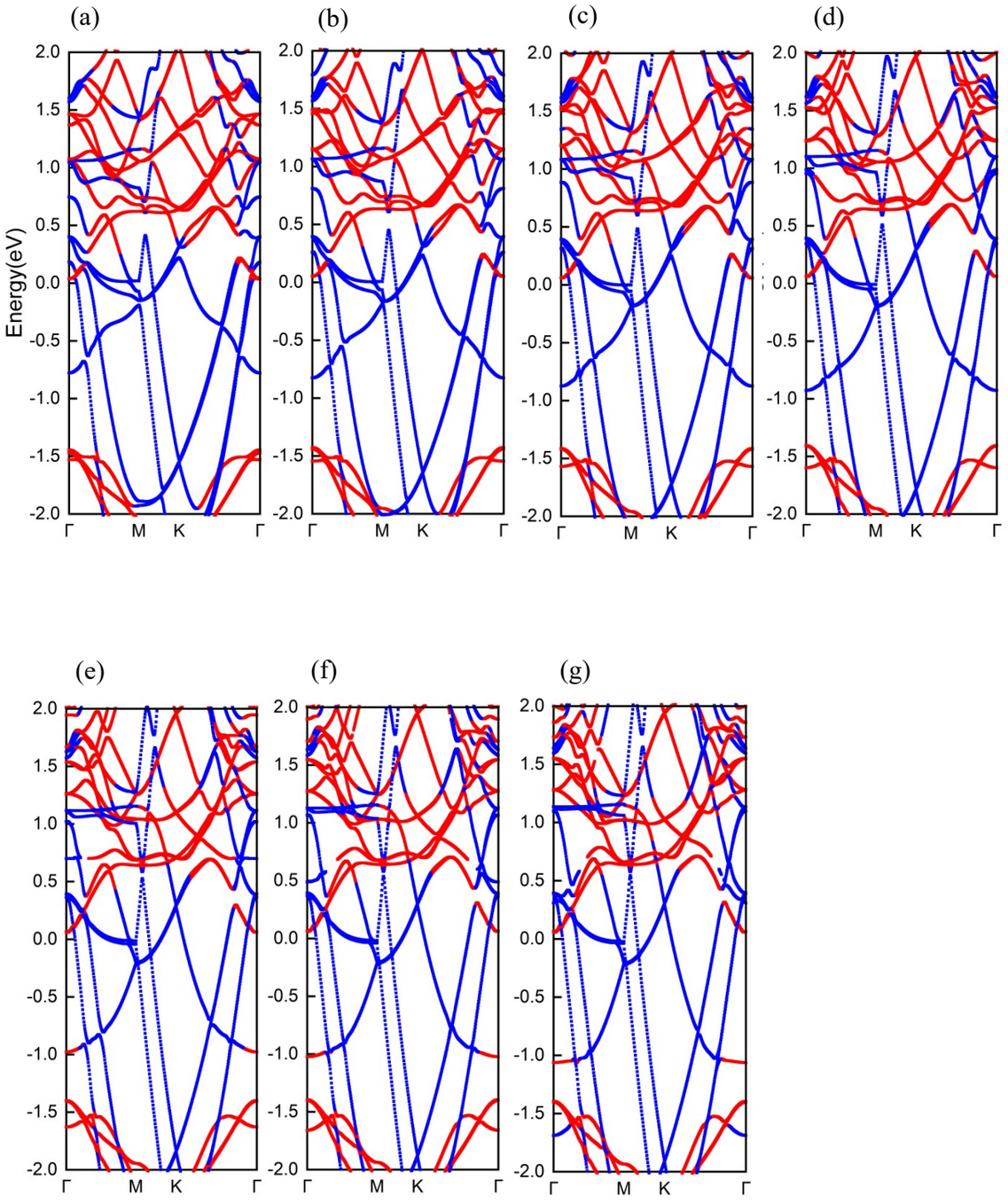

Fig. S3. Projected band structure of MoS_2/Ag heterostructure with tunable distance (a) 2.4Å, (b)2.6Å, (c)2.8Å, (d)3.0, (e)3.2Å, (f)3.4, (g)3.6Å. The blue, and red lines represent the electronic orbital contributions of Ag, MoS_2, respectively.

Fig. S4

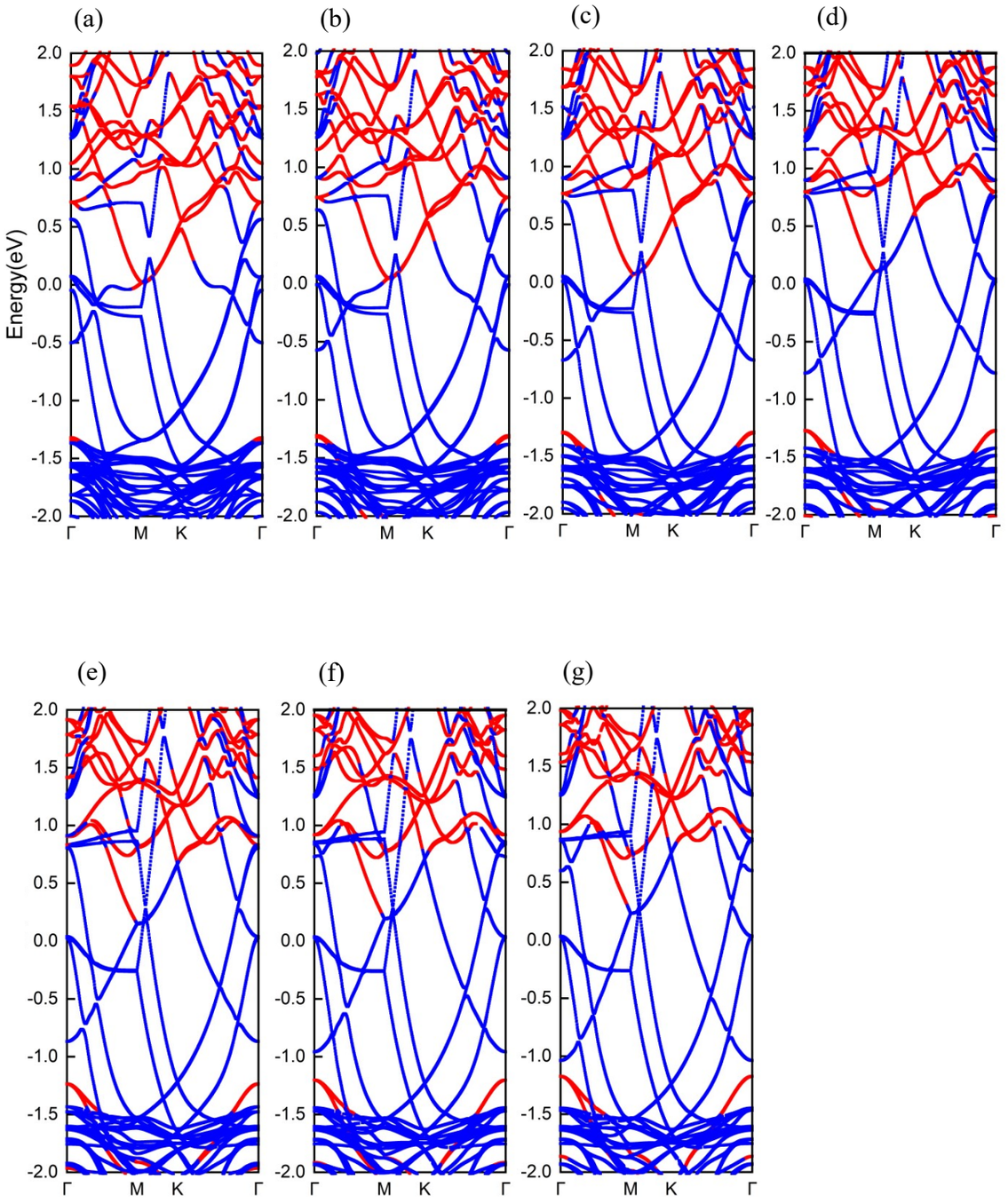

Fig. S4. Projected band structure of MoS_2/Cu heterostructure with tunable distance (a)2.4Å, (b)2.6Å, (c)2.8Å, (d)3.0Å, (e)3.2Å, (f)3.4Å, (g)3.6Å. The blue, and red lines represent the electronic orbital contributions of Cu, MoS_2, respectively.

Fig. S5

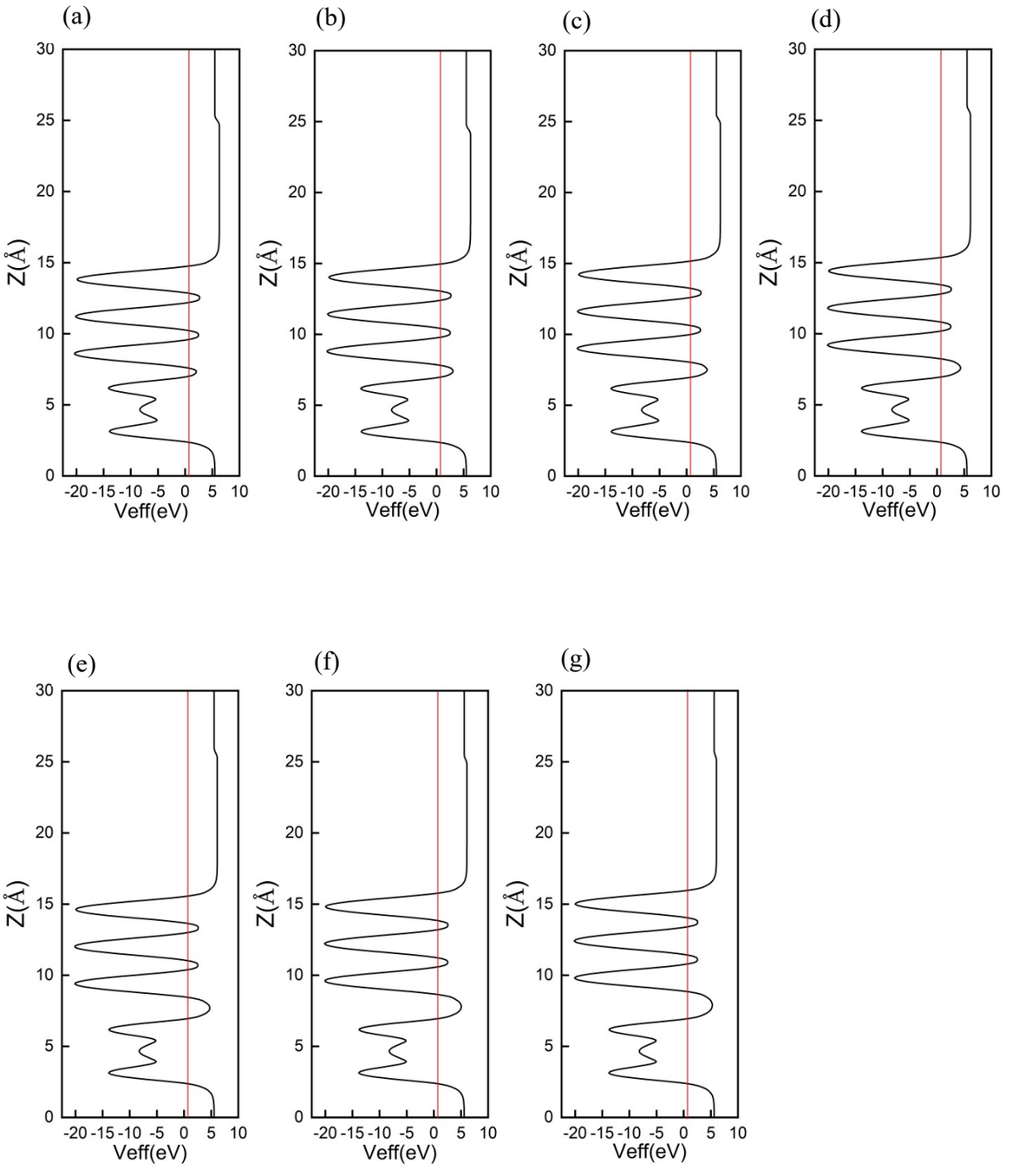

Fig S5. Effective potential profile of MoS_2/Au heterostructure with tunable distance (a) 2.4Å, (b)2.6Å, (c)2.8Å, (d)3.0, (e)3.2Å, (f)3.4, (g)3.6Å. The red line represent the Fermi level.

Fig. S6

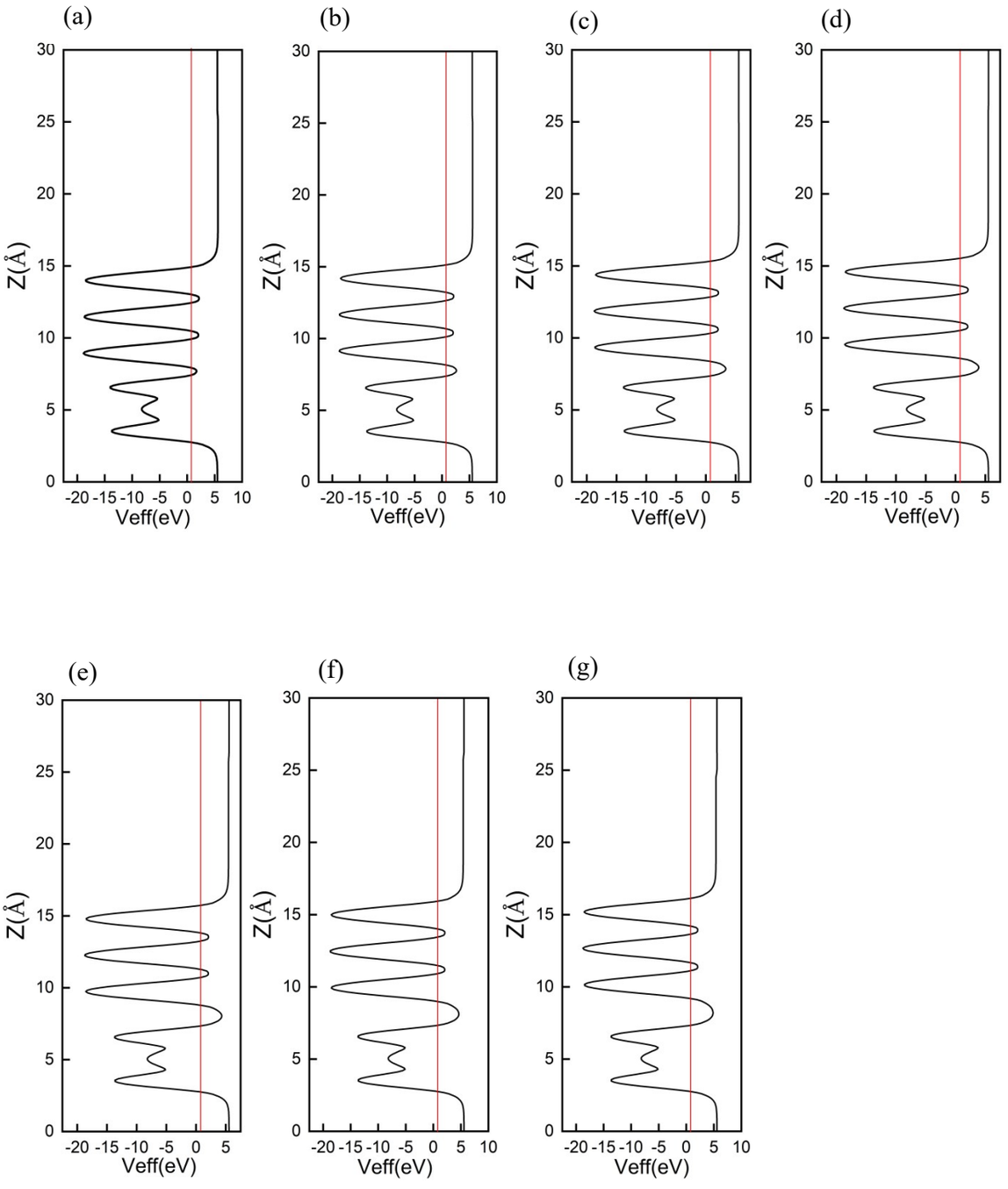

Fig S6. Effective potential profile of MoS_2/Ag heterostructure with tunable distance (a) 2.4Å, (b)2.6Å, (c)2.8Å, (d)3.0, (e)3.2Å, (f)3.4, (g)3.6Å. The red line represent the Fermi level.

Fig. S7

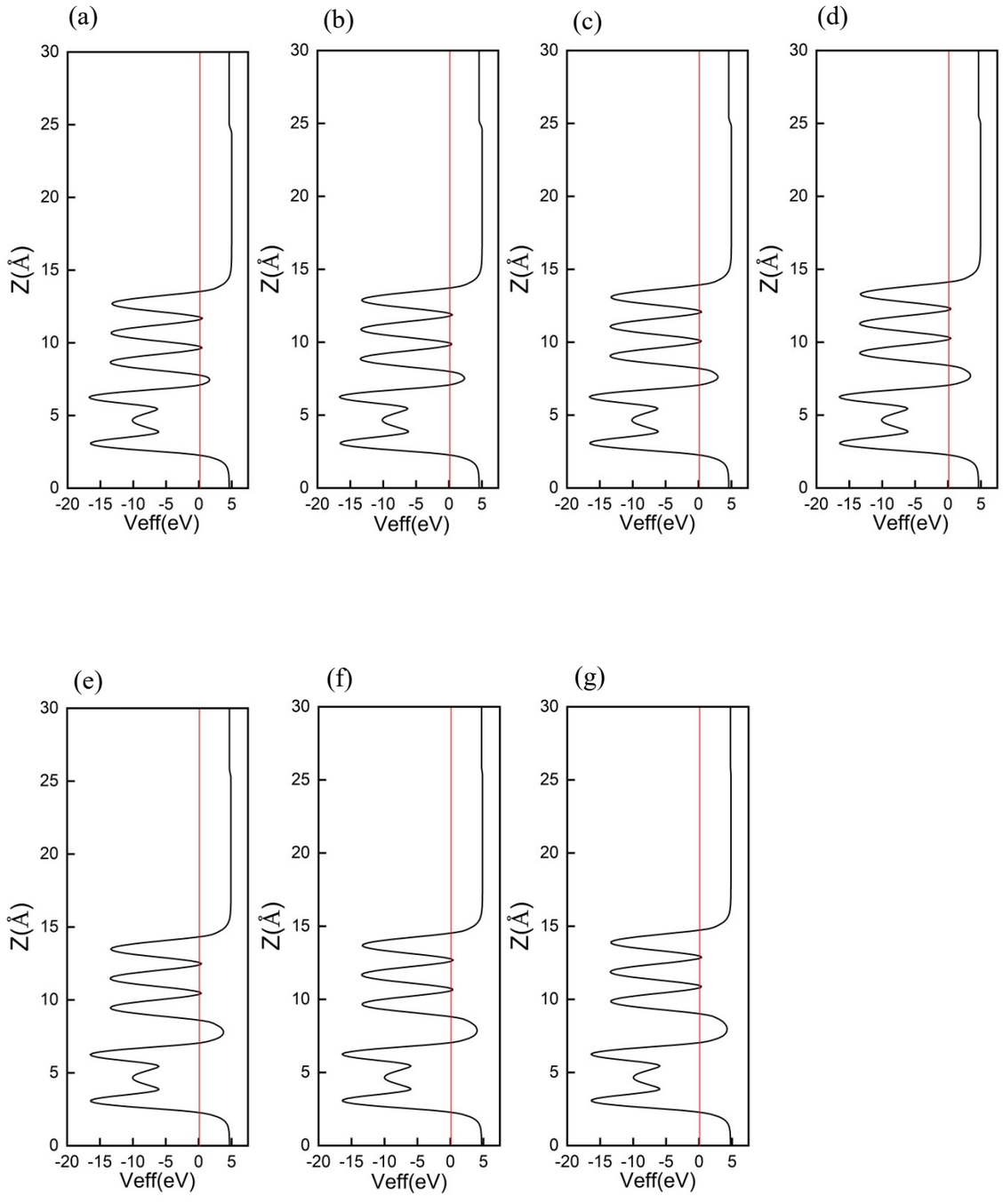

Fig S7. Effective potential profile of MoS_2/Cu heterostructure with tunable distance (a) 2.4Å, (b)2.6Å, (c)2.8Å, (d)3.0, (e)3.2Å, (f)3.4, (g)3.6Å. The red line represent the Fermi level.

Fig. S8

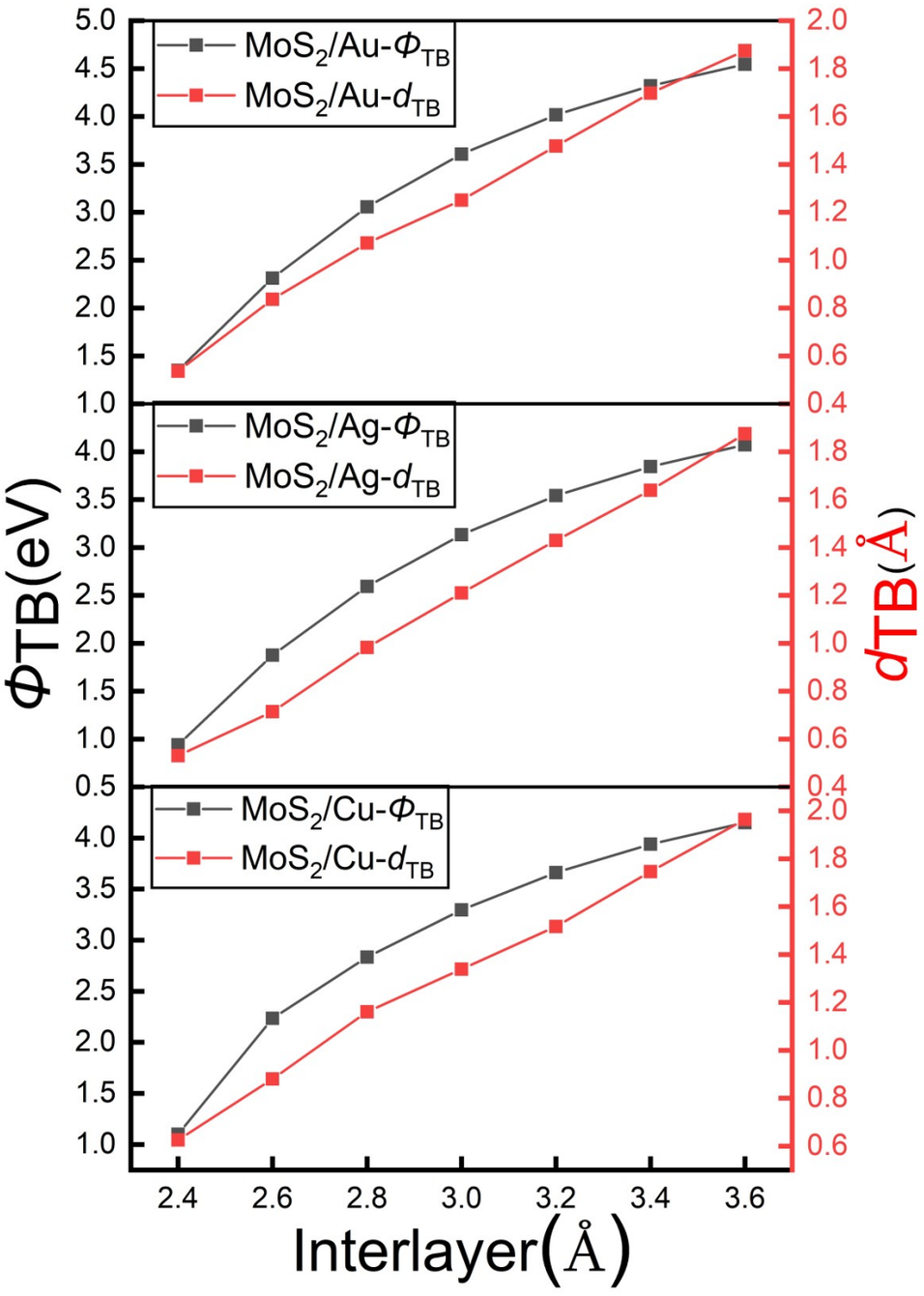

Fig S8. Barrier height(Φ_{TB}) and width(d_{TB}) at different interlayer distance. Black and red represent the value of Φ_{TB} and d_{TB}.

Table S2

MoS_2/Au	Distance (Å)	Φ_{TB} (eV)	d_{TB} (Å)	Probability (%)
	2.4	1.348	0.536	53.87
	2.6	2.311	0.836	28.74
	2.8	3.056	1.071	15.93
	3.0	3.606	1.250	9.74
	3.2	4.016	1.476	5.49
	3.4	4.319	1.697	3.14
	3.6	4.545	1.875	1.98
MoS_2/Ag	Distance (Å)	Φ_{TB} (eV)	d_{TB} (Å)	Probability (%)
	2.4	0.940	0.530	60.40
	2.6	1.876	0.714	38.31
	2.8	2.592	0.982	21.20
	3.0	3.133	1.210	12.23
	3.2	3.541	1.429	7.15
	3.4	3.844	1.639	4.27
	3.6	4.072	1.875	2.44
MoS_2/Cu	Distance (Å)	Φ_{TB} (eV)	d_{TB} (Å)	Probability (%)
	2.4	1.099	0.625	52.58
	2.6	2.234	0.880	27.51
	2.8	2.833	1.161	14.70
	3.0	3.296	1.339	9.21
	3.2	3.662	1.517	5.79
	3.4	3.940	1.746	3.34
	3.6	4.150	1.964	1.97

Table S2. Barrier height(Φ_{TB}), width(d_{TB}) and the electron tunneling probability at different interlayer distance.