Supporting Information for

Junction-Configuration-Dependent Interfacial Electronic States of Monolayer MoS_2/Metal Contact

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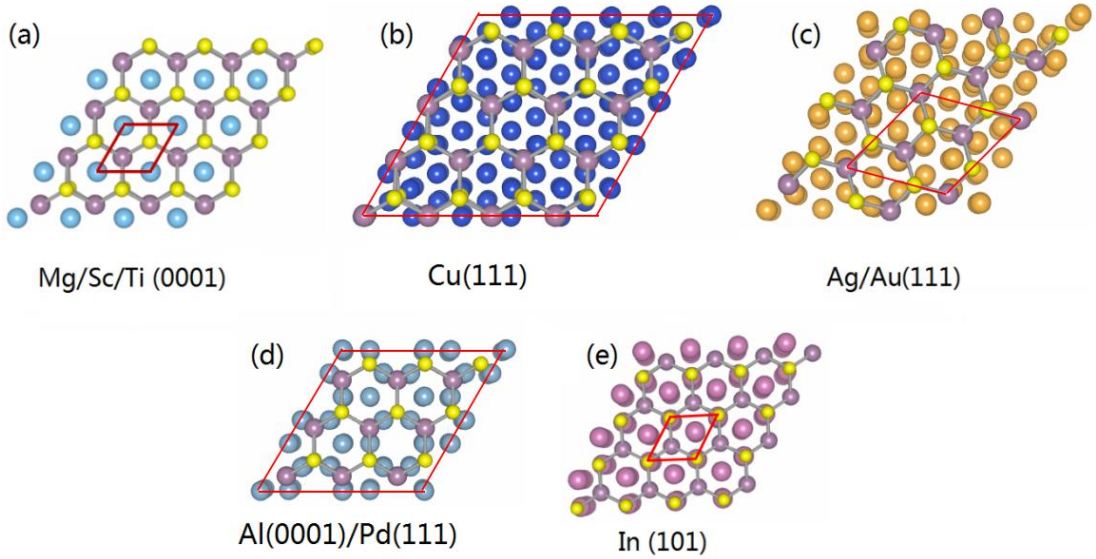

Fig. S1 Top view of interfacial structures for monolayer MoS_2 contacted with metals in the top contact configuration: (a) Mg, Sc, and Ti(0001), (b) Cu(111), (c) Ag and Au, (d) Al(0001) and Pd(111), and (e) In(101) faces. The rhombi plotted in red line shows the unit cell for each structure.

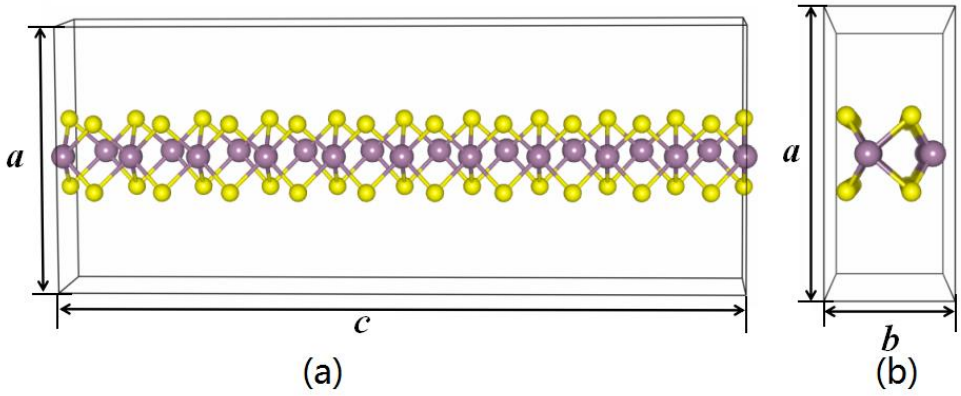

Fig. S2 Side views of the atomic structure for monolayer MoS_2 nanoribbon.

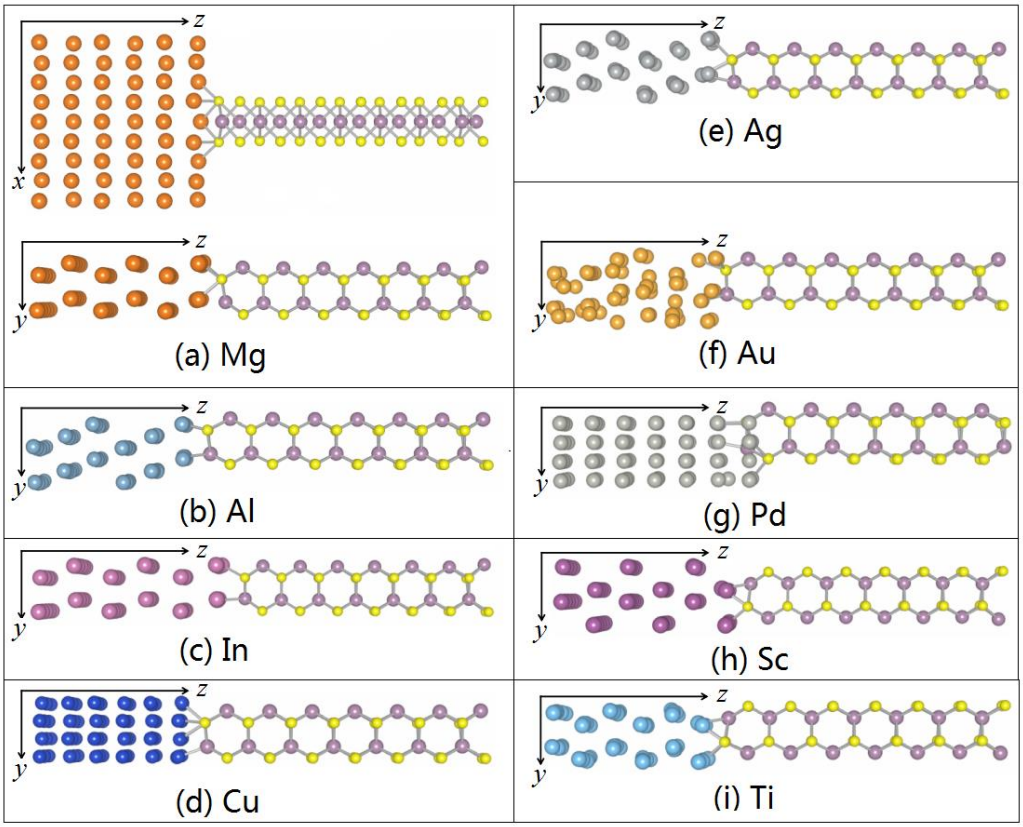

Fig. S3 Side view of interfacial structures for monolayer MoS_2 contacted with metals in the edge contact configuration through Mo and S atoms at armchair termination: (a) Mg, (b) Al, (c) In, (d) Cu, (e) Ag, (f) Au, (g) Pd, (h) Sc, and (i) Ti.

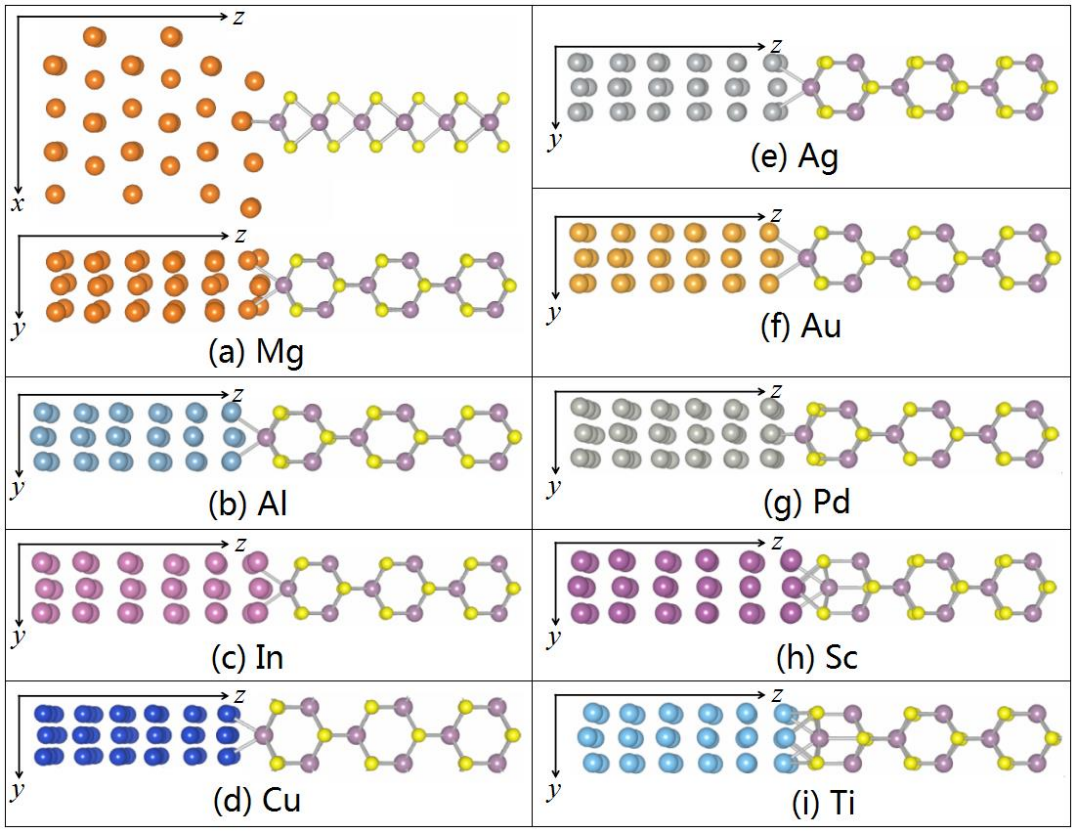

Fig. S4 Side view of interfacial structures of monolayer MoS_2 contacted with metals in the edge contact configuration through Mo atoms at zigzag termination: (a) Mg, (b) Al, (c) In, (d) Cu, (e) Ag, (f) Au, (g) Pd, (h) Sc, and (i) Ti.

Table S1 Bond lengths of metal-Mo ($L_{metal-Mo}$), metal-S ($L_{metal-S}$), and Mo-S (L_{Mo-S}) in the interfaces of monolayer MoS_2 contacted with metals in the edge contact configuration through Mo and S atoms at armchair termination .

	$L_{Metal-Mo}$ (Å)	$L_{Metal-S}$ (Å)	L_{Mo-S} (Å)
Mg	2.805	2.565	2.461
Al	2.667	2.363	2.442
In	2.869	2.744	2.406
Cu	2.433	2.312	2.433
Ag	2.825	2.610	2.380
Au	2.783	2.658	2.341
Pd	2.460	2.303	2.443
Sc	2.822	2.577	2.531
Ti	2.708	2.485	2.505

Table S2 Bond lengths of metal-Mo ($L_{metal-Mo}$) and Mo-S (L_{Mo-S}) in the interfaces of monolayer MoS_2 contacted with metals in the edge contact configuration through Mo atoms at zigzag termination .

	$L_{Metal-Mo}$ (Å)	L_{Mo-S} (Å)
Mg	2.813	2.404
Al	2.655	2.358
In	2.879	2.414
Cu	2.549	2.419
Ag	2.828	2.355
Au	2.756	2.364
Pd	2.776	2.353
Sc	2.905	2.424
Ti	2.612	2.551

Table S3 Bond lengths of metal-S ($L_{metal-S}$) and Mo-S (L_{Mo-S}) in the interfaces of monolayer MoS_2 contacted with metals in the edge contact configuration through S atoms at zigzag termination .

	$L_{Metal-S}$ (Å)	L_{Mo-S} (Å)
Mg	2.480	2.461
Al	2.425	2.442
In	2.775	2.406
Cu	2.163	2.433
Ag	2.630	2.380
Au	2.480	2.341
Pd	2.342	2.443
Sc	2.543	2.531
Ti	2.361	2.505

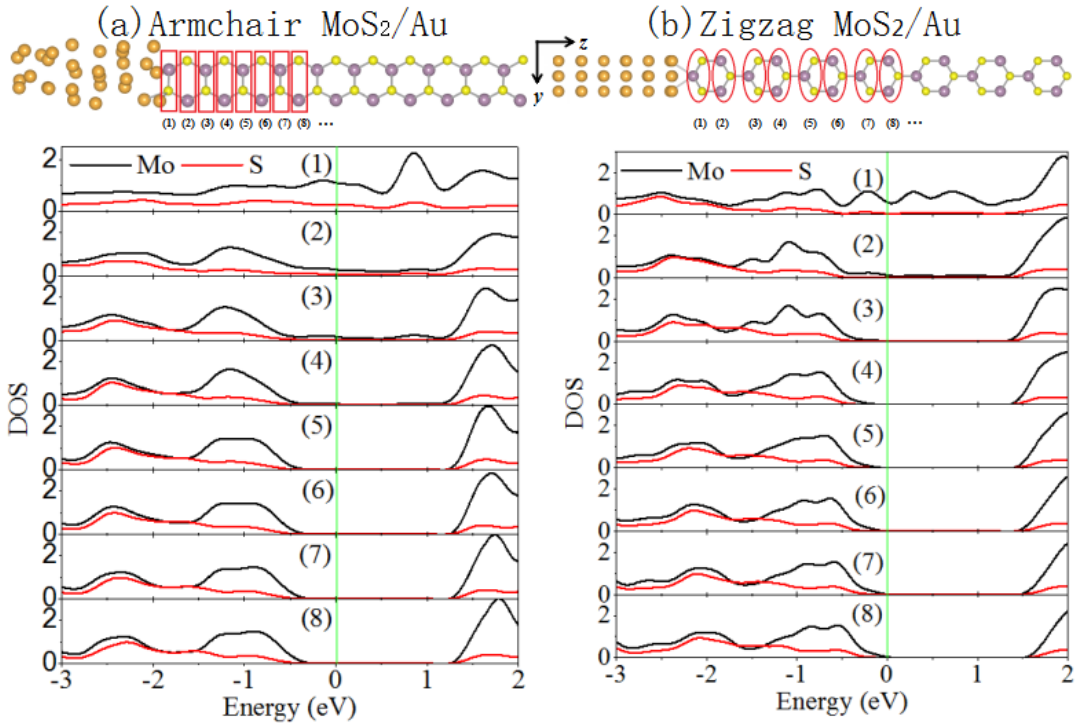

Fig. S5 Atomic structure and PDOSs projected on each Mo and S atoms of MoS_2 nanoribbon contacted with Au electrodes in the edge contact configurations: (a) armchair MoS_2 nanoribbon and (b) zigzag MoS_2 nanoribbon with Mo atom termination.

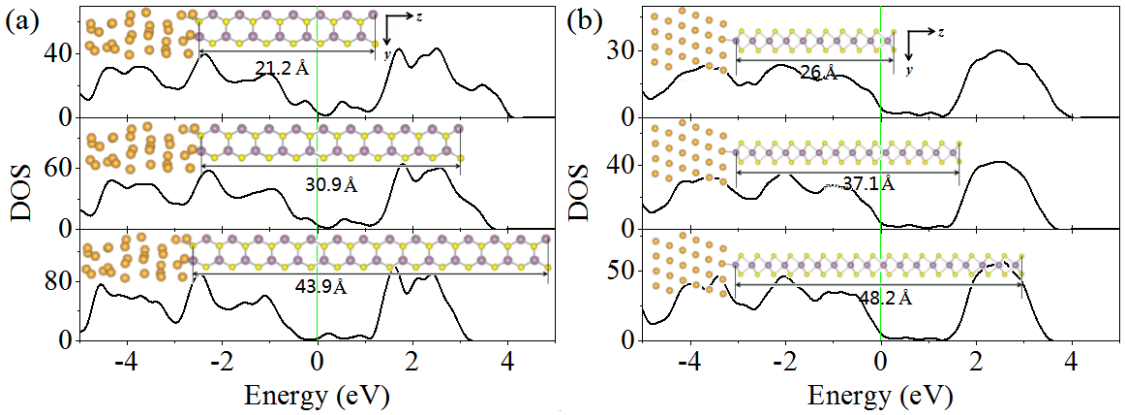

Fig. S6 Density of states (DOS) of MoS_2 nanoribbon contacted with Au electrodes in the edge contact configurations: (a) armchair MoS_2 nanoribbon and (b) zigzag MoS_2 nanoribbon with Mo atom termination.

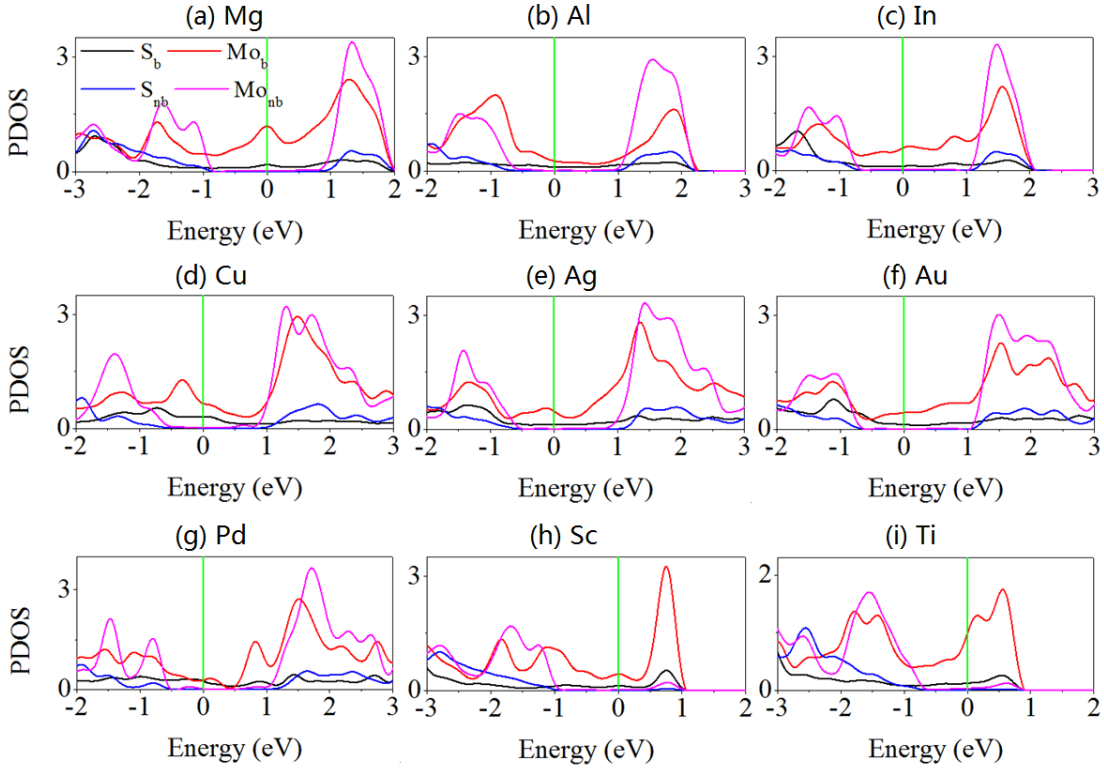

Fig. S7 Electronic density of states (DOS) of monolayer MoS_2 contacted with metals in the edge contact configuration through Mo atoms at zigzag termination : (a) Mg, (b) Al, (c) In, (d) Cu, (e) Ag, (f) Au, (g) Pd, (h) Sc, and (i) Ti. S_b (black line) and S_{nb} (blue line) indicate the sulphur atoms at the interface and far away from interface, respectively. Similarly, Mo_b (red line) and Mo_{nb} (magenta line) are the molybdenum atoms at the interface and far away from interface, respectively.

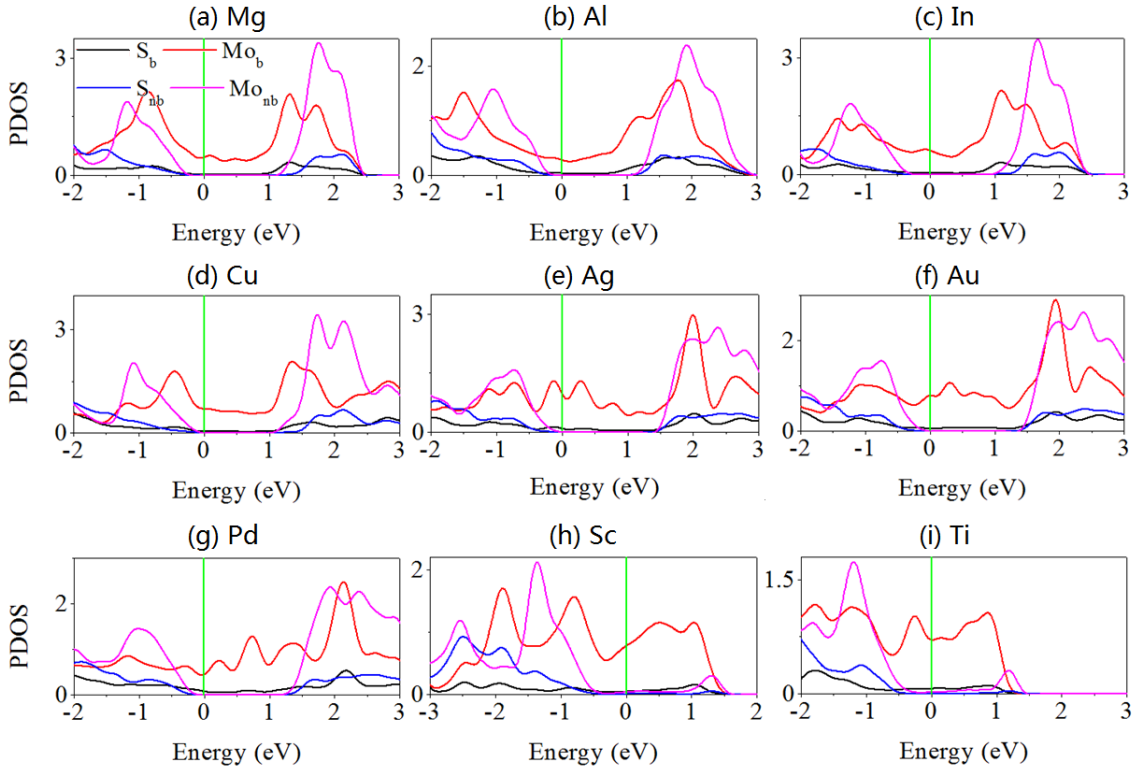

Fig. S8 Electronic density of states (DOS) of monolayer MoS_2 contacted with metals in the edge contact configuration through S atoms at zigzag termination: (a) Mg, (b) Al, (c) In, (d) Cu, (e) Ag, (f) Au, (g) Pd, (h) Sc, and (i) Ti. S_b (black line) and S_{nb} (blue line) indicate the sulphur atoms at the interface and far away from interface, respectively. Similarly, Mo_b (red line) and Mo_{nb} (magenta line) are the molybdenum atoms at the interface and far away from interface, respectively.

Table S4 Experimentally and theoretically obtained SBH and pinning factor (*S*) of MoS_2 contacted with metals in the top contact configuration.

Metal	Work function	Thinness	SBH (eV)	Pinning factor	Ref
Ag	4.3	7~30	0.04	0.09	Y. Liu et al., Nature 2018, 557, 696-700
Cu	4.6		0.1		
Au	5.1		0.06		
Pd	5.3		0.12		
Ti	4.3	bulk	0.23	0.11	C. Kim et al., ACS Nano 2017, 11, 1588-1596
Au	5.2		0.32		
Pd	5.6		0.30		
Ti	4.3	mono	0.35	0.34	J. Kang et al., Phys. Rev. X 2014, 4, 031005
In	4.1		0.47		
Au	5.3		0.62		
Pd	5.6		0.9		
Sc	3.5	mono	-0.1	0.28	Y. Guo etal., ACS Appl. Mater. Interfaces 2015, 7, 25709-25715
Mg	3.7		0.12		
Al	4.27		0.23		
Ti	4.33		0.41		
Pd	5.13		0.66		
Al	4.24	mono	0.51	0.27	C. Gong et al., Nano Lett 2014, 14, 1714-1720
Ag	5.14		0.54		
Au	5.76		0.88		
Pd	5.83		0.85		
Sc	3.593	mono	0	0.33	H.X. Zhong et al., Sci Rep 2016, 6, 21786
Ti	4.427		0.216		
Ag	4.489		0.212		
Au	5.226		0.763		
Sc	3.593	bi	0	0.27	
Ti	4.427		0.161		
Ag	4.489		0.138		
Au	5.226		0.667		