Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Highly efficient MoS_2/WS_2 heterojunction for CO_2 reduction reaction: strong electronic transmission

Pengjie Fu,[#,a] Ying Xu,[b] Pingji Ge,[a] Xiaolong Li,[a] Jueming Yang,[a] Guixian Ge,[*,a] Xiaodong Yang,[*,a]

[a] Xinjiang Production & Construction Corps Key Laboratory of Advanced Energy Storage Materials and Technology/College of Science, Shihezi University, Shihezi 832003, Xinjiang, China

[b] College of Foreign Languages, Shihezi University, Shihezi 832003, China

Corresponding Author
***Email:** geguixian@126.com (G.X.G.)
***Email:** yangxiaodong1209@hotmail.com (X.D.Y.)

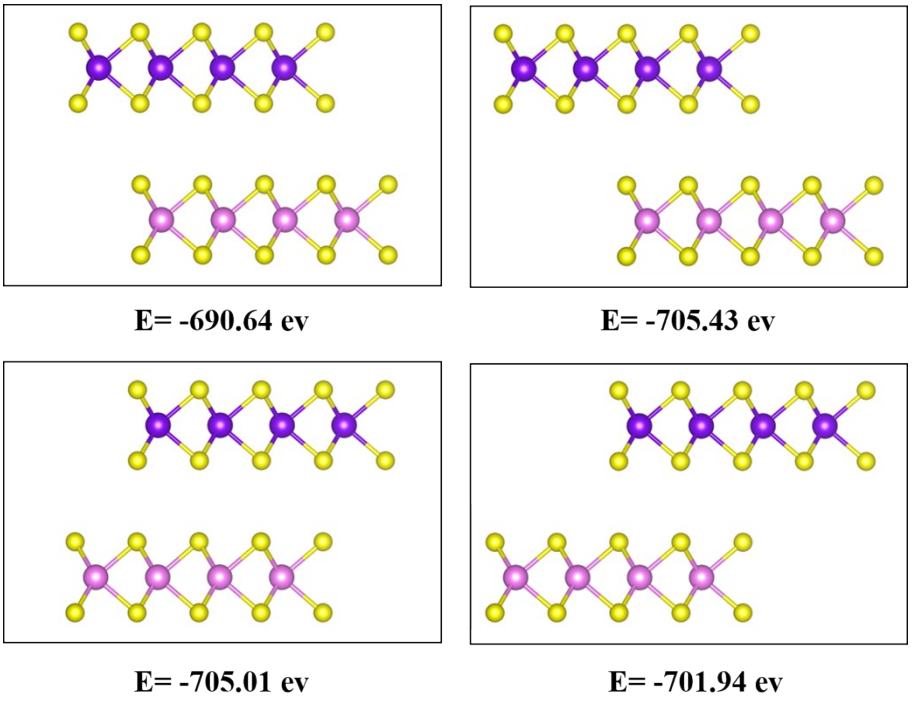

Fig.S1 The structure and energy of different stacking modes.

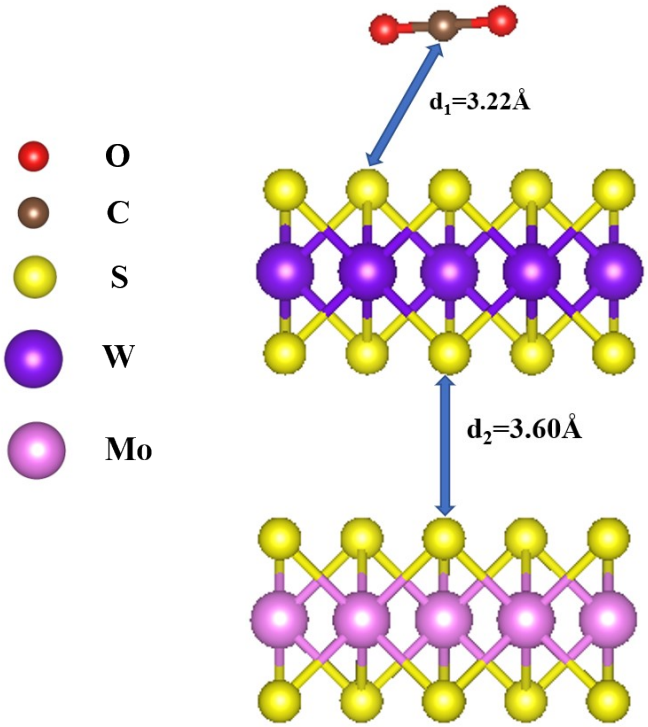

Fig.S2 Adsorbed CO_2 molecule on MoS_2/WS_2 surface.

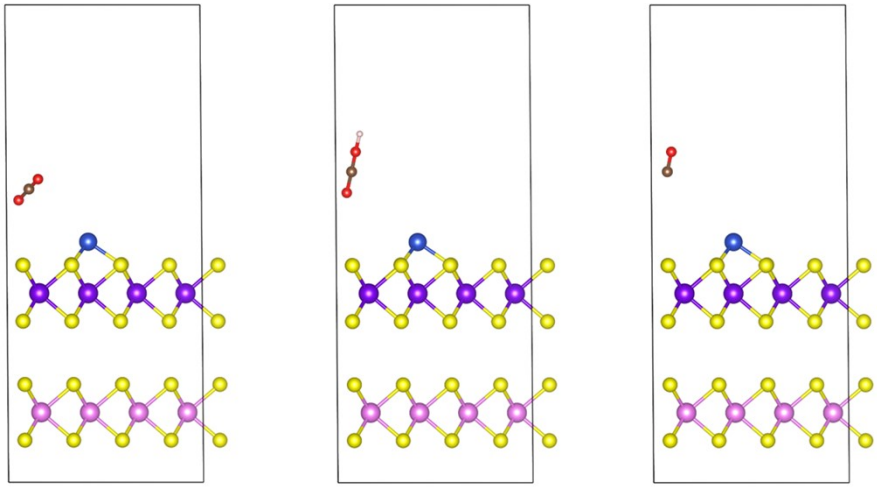

Fig.S3 The optimized structure diagram of S atom in different intermediate states.

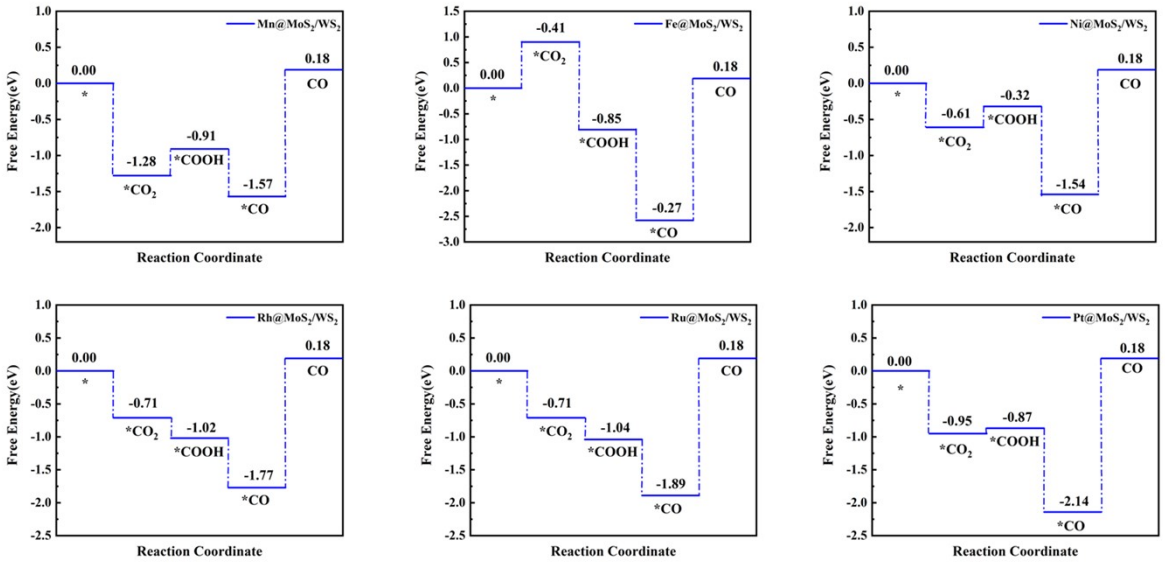

Fig.S4 Energy variation of different adsorbed metal structures during the whole reaction process. (Mn, Fe, Ni, Rh, Ru, Pt).

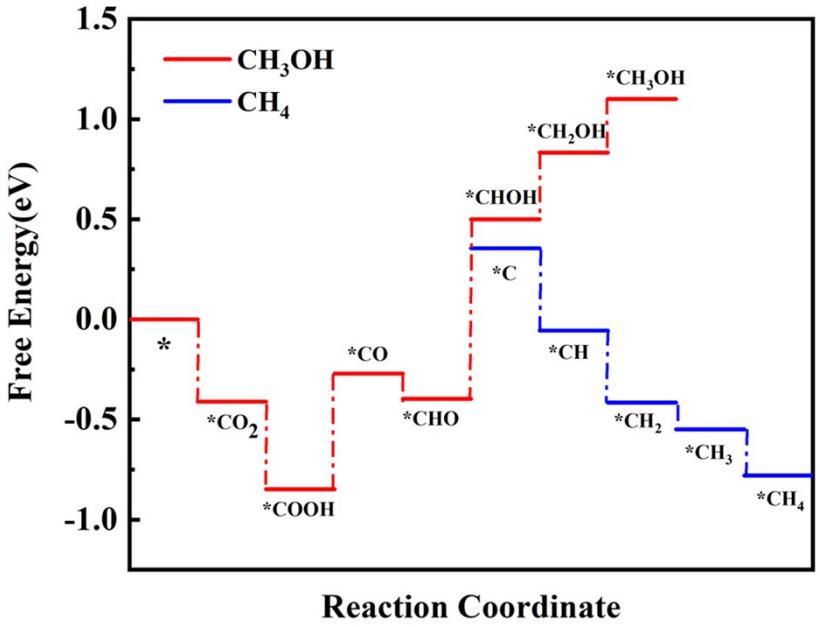

Fig.S5 Free-energy profiles for CO_2RR on Cu@MoS_2/WS_2.