Supporting Information

Enhanced reduction of CO to C_2 products on MoS_2 nanoribbon by edge engineering

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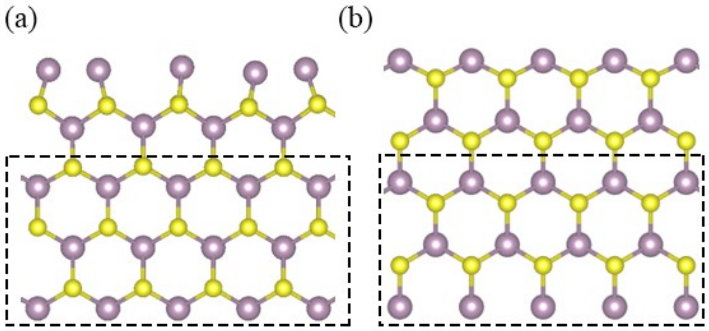

Fig.S1 (a) and (b)Two edge structures of MoS_2 terminated with Mo atoms after structural relaxation. The dashed boxes show the fixed atoms.

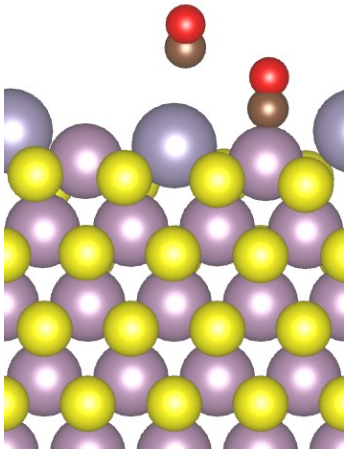

Fig.S2 The optimized structure with two CO adsorbed on the Sn-incorporated edge.

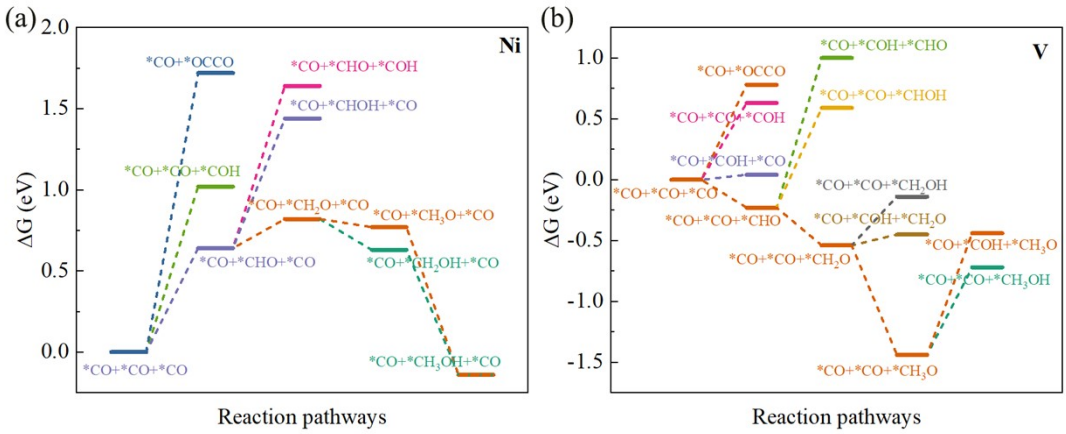

Fig.S3 The reduction pathways of CO on: (a) Ni- and (b) V-incorporated edges.

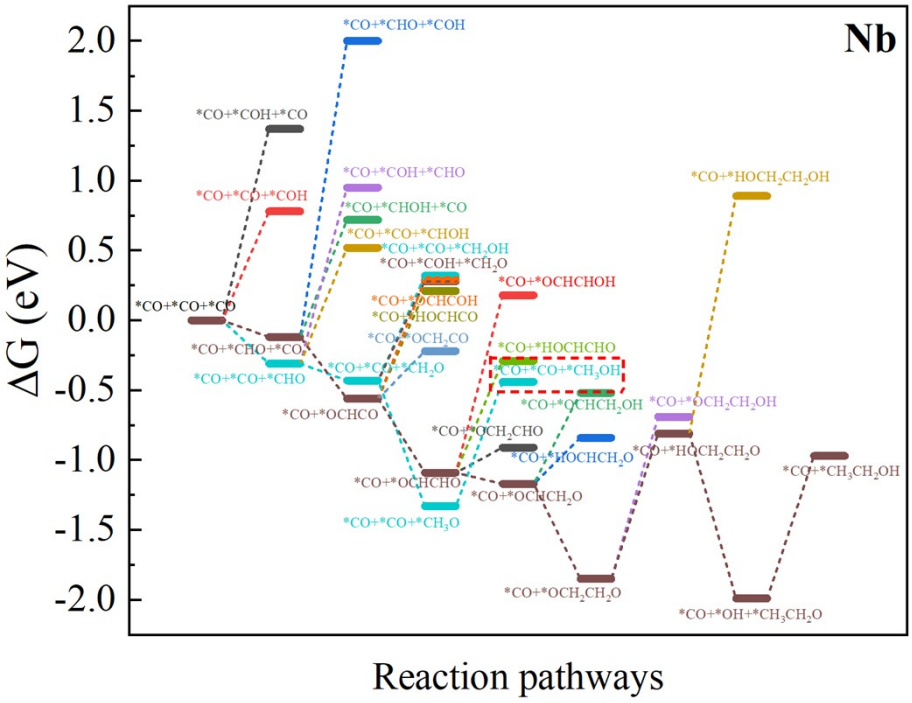

Fig.S4 The reduction pathways of CO on Nb-incorporated edge.

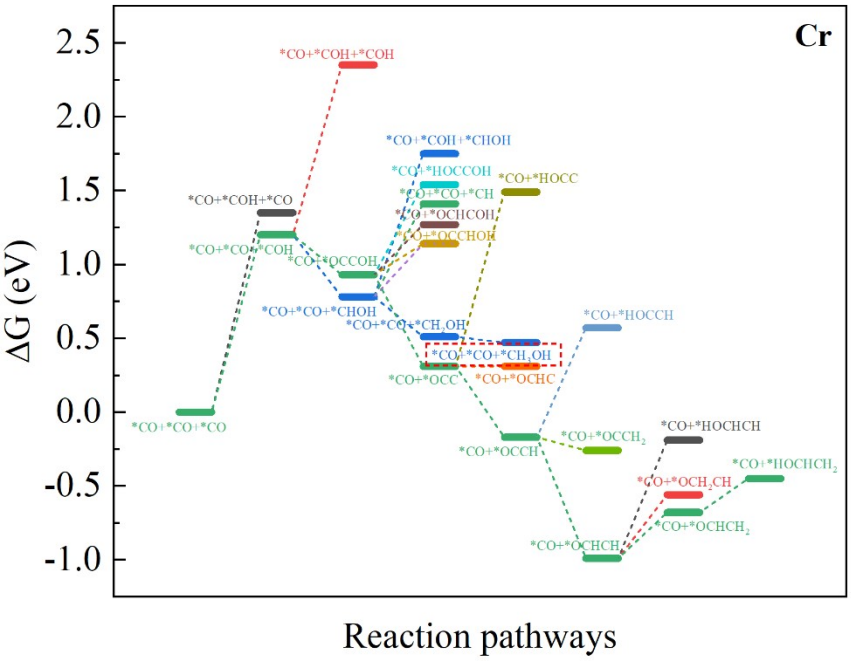

Fig.S5 The reduction pathways of CO on the Cr-incorporated edge.

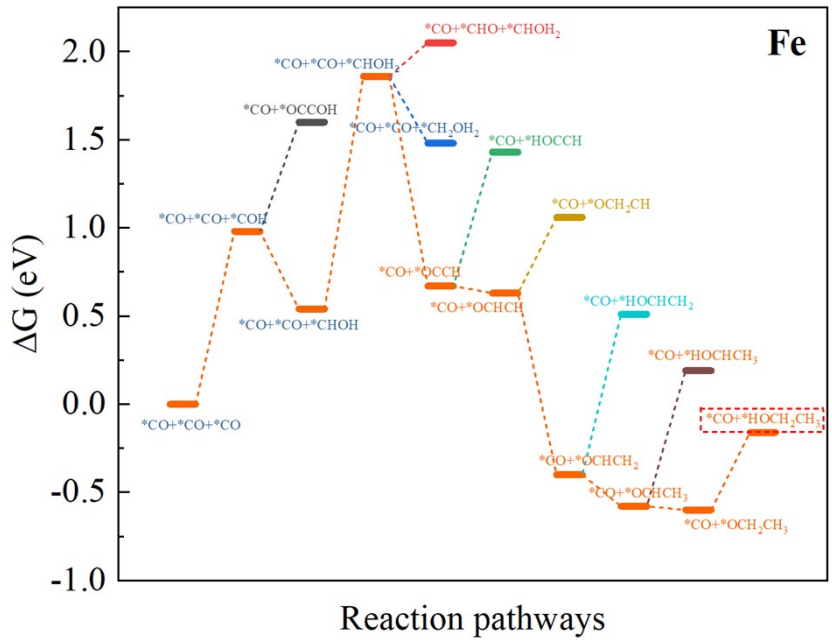

Fig.S6 The reduction pathways of CO on the Fe-incorporated edge.

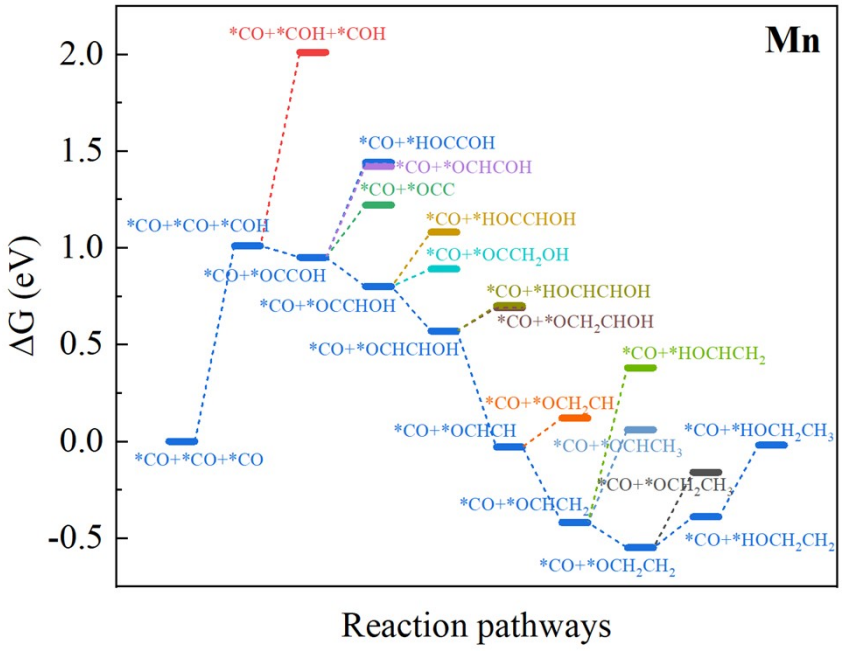

Fig.S7 The reduction pathways of CO on the Mn-incorporated edge.

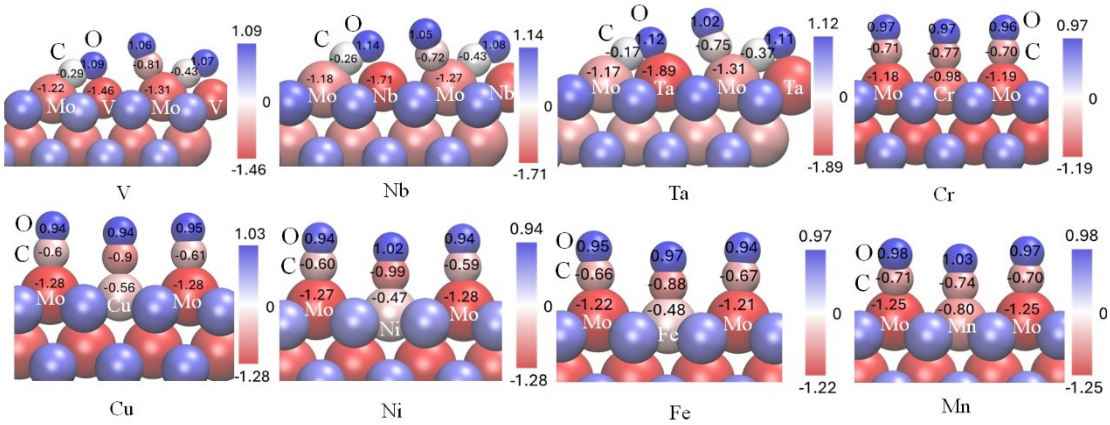

Fig.S8 Charge transfer for the adsorbed CO and active sites at the incorporated edges as obtained from the Bader charge analysis.

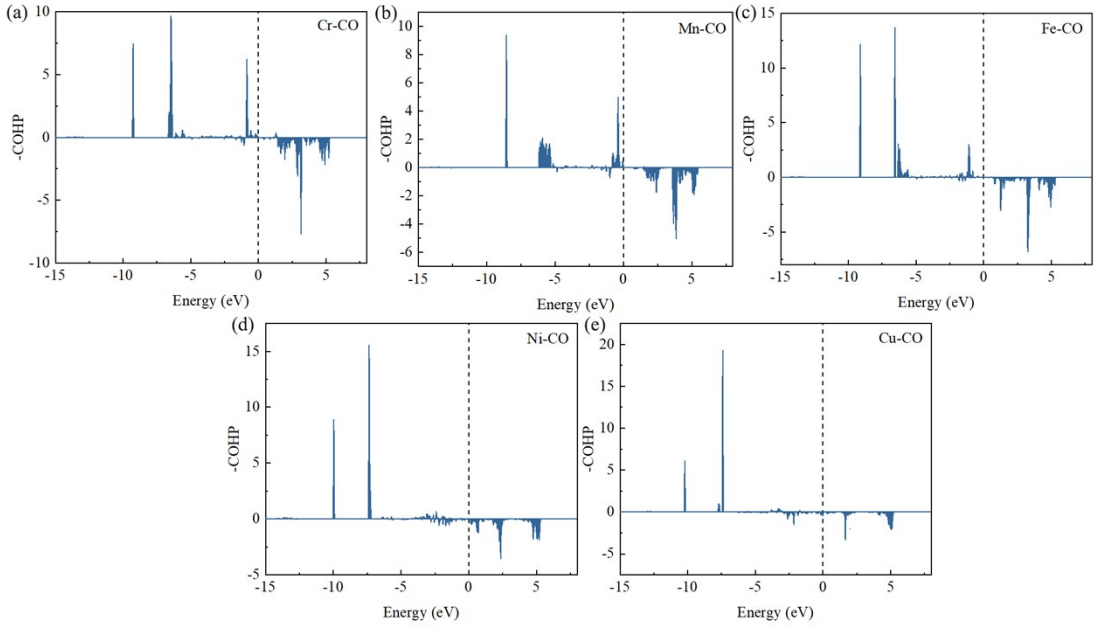

Fig.S9 (a)-(e) The crystal orbital Hamilton populations (COHPs) of C atom in adsorbed CO on the dopant site and the dopant.

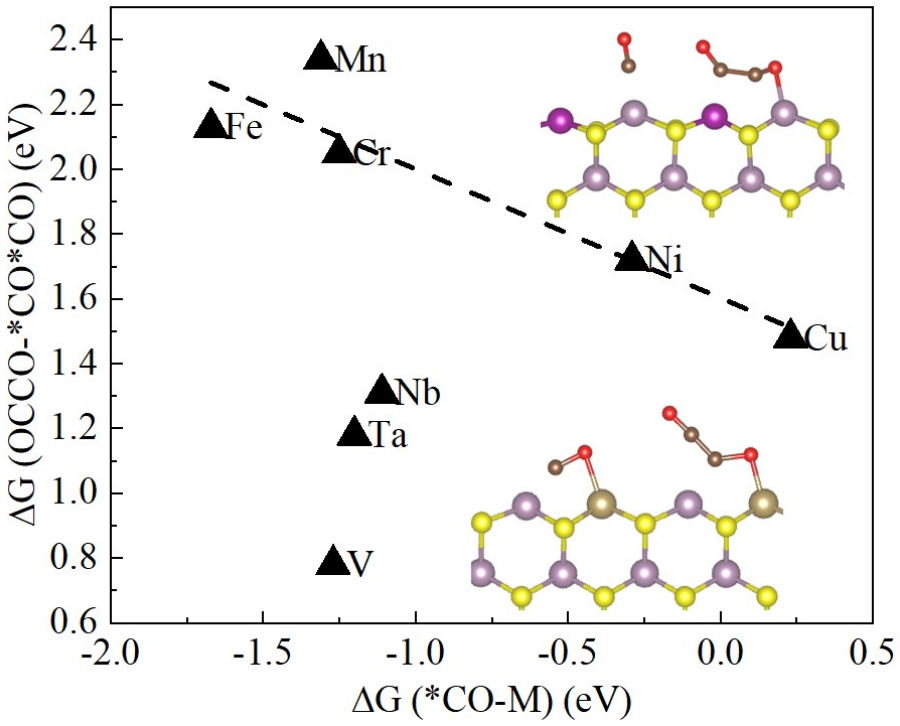

Fig.S10 The Gibbs free energy changes for the coupling of CO molecules adsorbed on the neighboring asymmetric active sites of the different incorporated edges, and the adsorption of CO on the dopant sites.

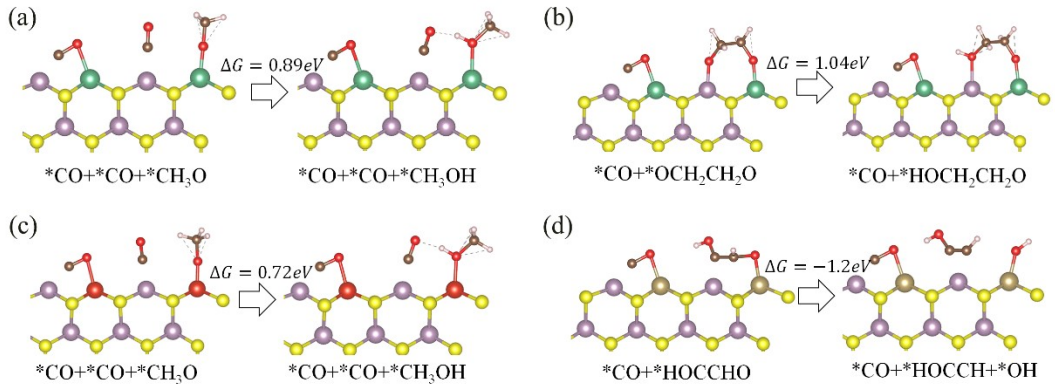

Fig.S11 The hydrogenation of (a) *CH_3O on the Nb site, (b) *OCH_2CH_2O on the Nb-incorporated edge, (c) *CH_3O on the V site, and (d) *HOCCHO on the Ta-incorporated edge.