Electronic Supplementary Information for New Journal of Chemistry

Supporting Information

Theoretical study of two-dimensional bis(iminothiolato)metal monolayers as promising electrocatalysts for carbon dioxide reduction

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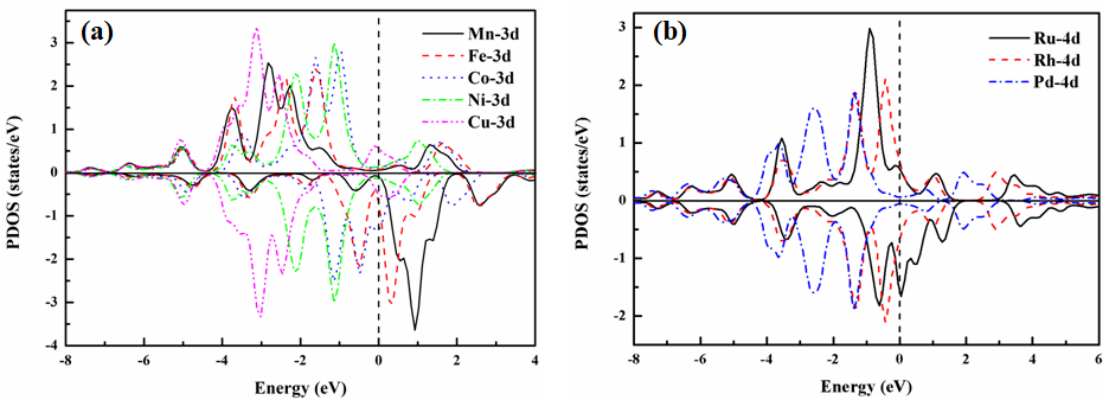

Fig. S1 Density of states for 3d and 4d orbitals of the studied compounds.

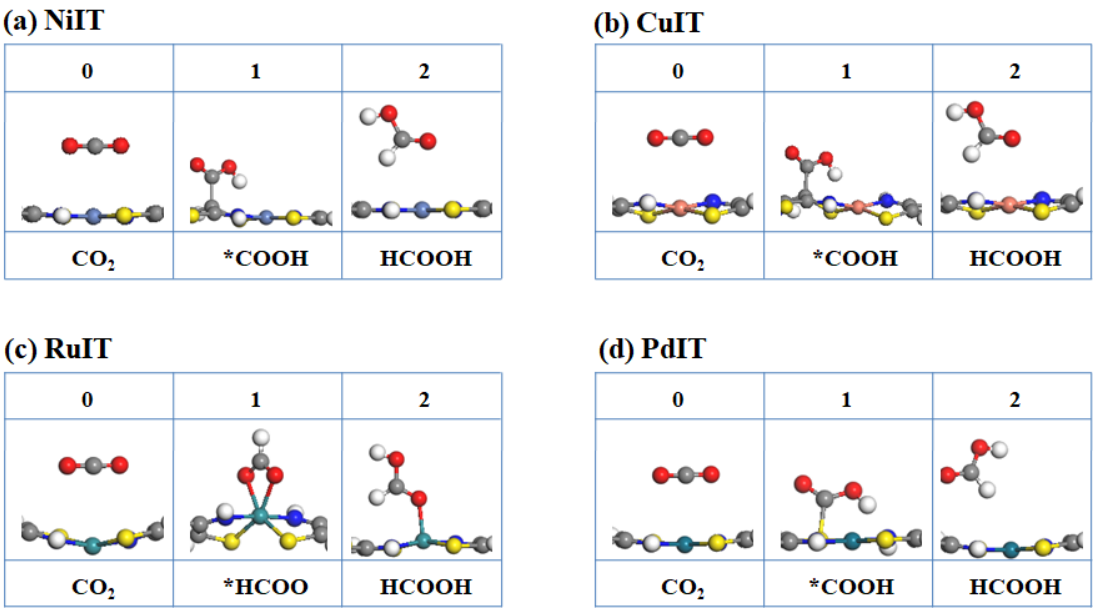

Fig. S2 The most stable structures for the favorable pathway. (a), (b), and (d) are the formation of HCOOH via *COOH on NiIT, CuIT, and PdIT, respectively. (c) is the formation of HCOOH via *HCOO on RuIT. The numbers on top of each column are the transferred numbers of (H^+ + e^-) pairs.

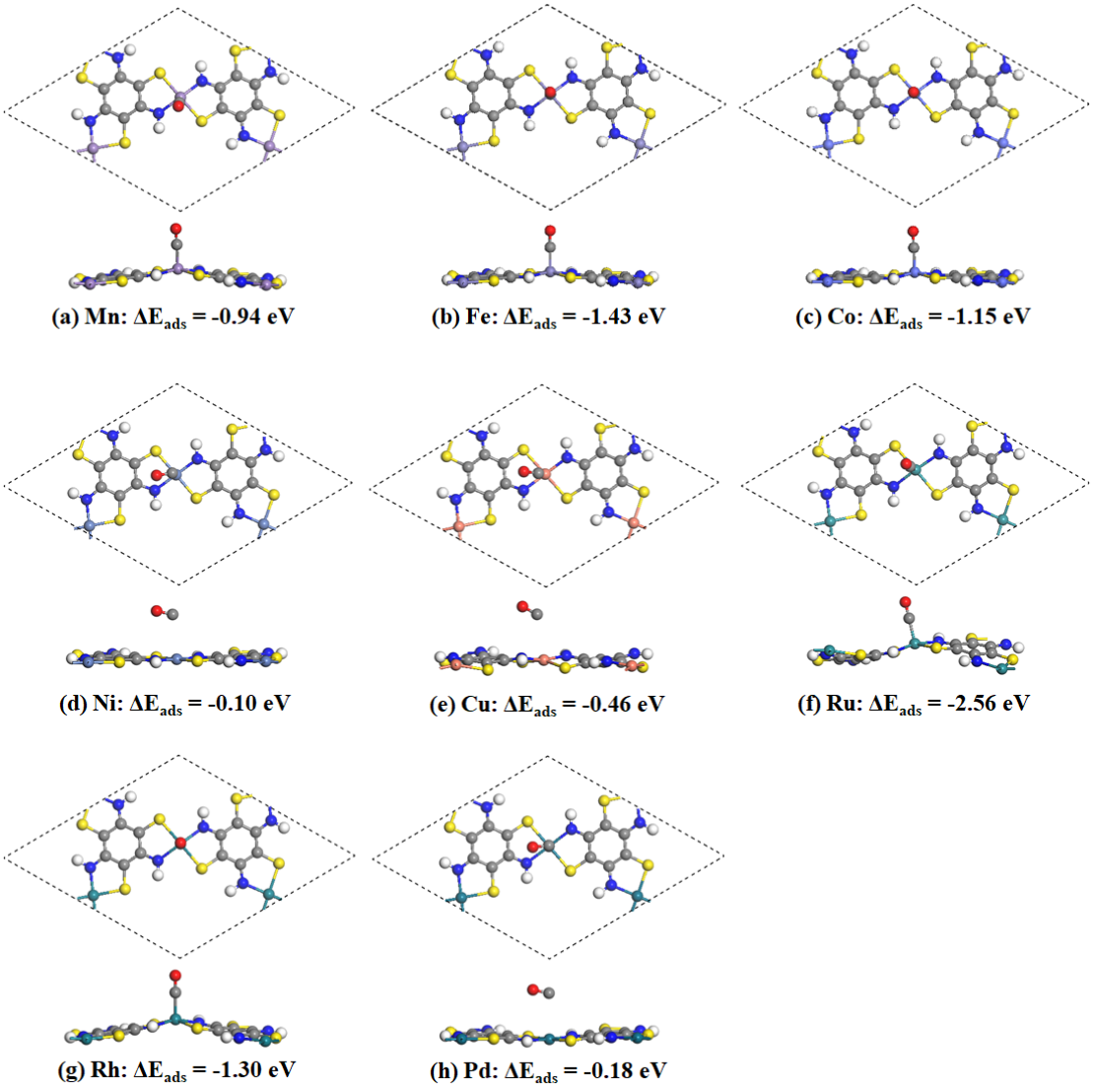

Fig. S3 The most stable adsorption configurations of CO on TMIT. ΔE_{ads} is the adsorption energy (eV).

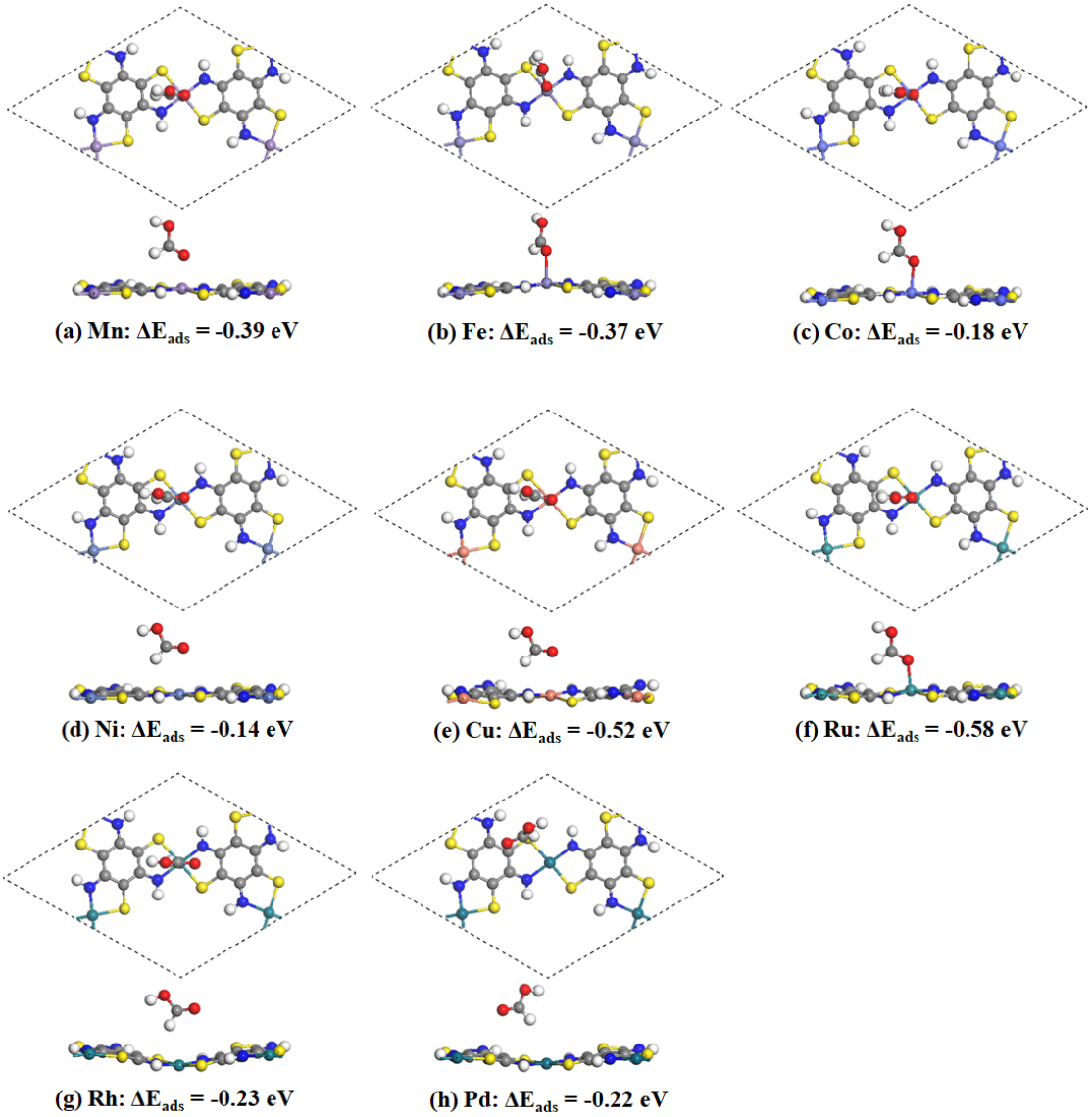

Fig. S4 The most stable adsorption configurations of HCOOH on TMIT. ΔE_{ads} is the adsorption energy (eV).