

Supplementary Information

for

A Bifunctional Two Dimensional $\text{TM}_3(\text{HHTP})_2$ monolayer and its variations for Oxygen Electrode Reactions

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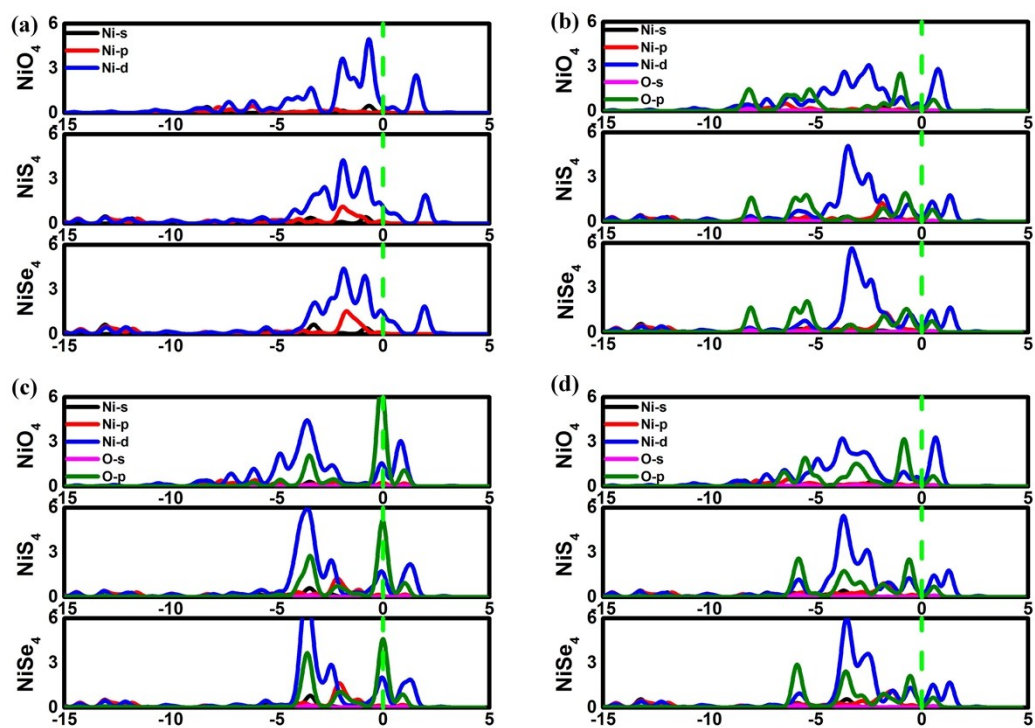


Figure S1. The partially density of states of $\text{Ni}_3(\text{HHTP})_2$ and its variations. (a) is the un-adsorbed NiX_4 . (b)-(c) are OOH, O and OH adsorption systems, respectively.

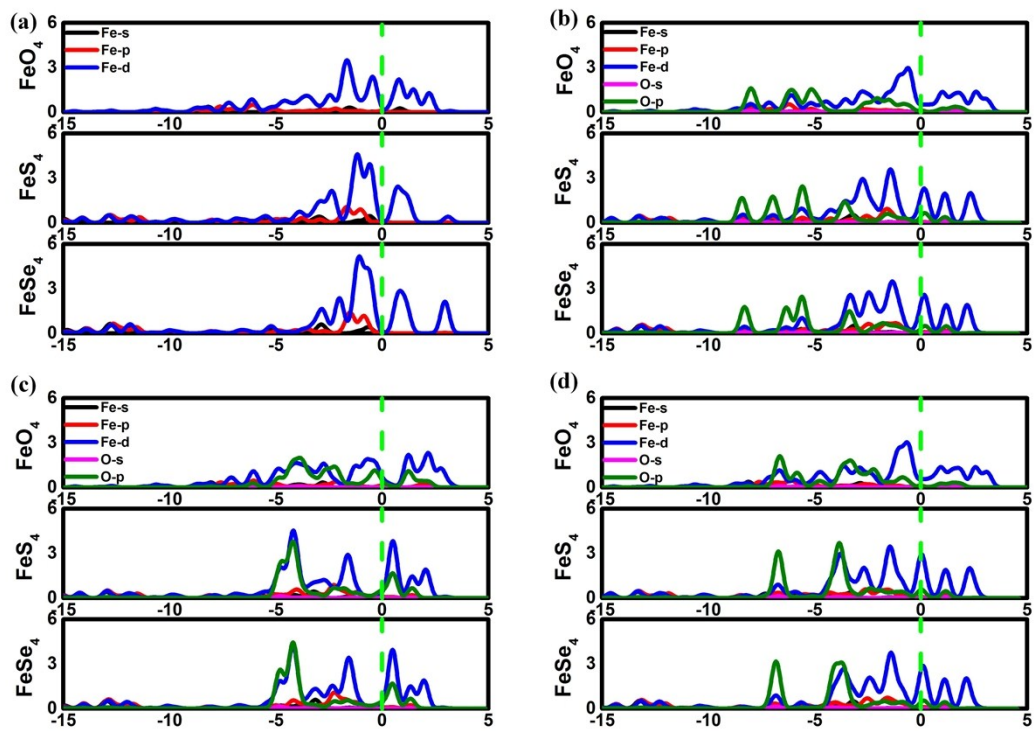


Figure S2. The partially density of states of $\text{Fe}_3(\text{HHTP})_2$ and its variations. (a) is the un-adsorbed FeX_4 . (b)-(c) are OOH, O and OH adsorption systems, respectively.