Supplementary Information

for

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

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Figure S1. The partially density of states of Ni$_3$(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 Fe$_3$(HHTP)$_2$ and its variations. (a) is the un-adsorbed FeX$_4$. (b)-(c) are OOH, O and OH adsorption systems, respectively.