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

Supporting Infromation:

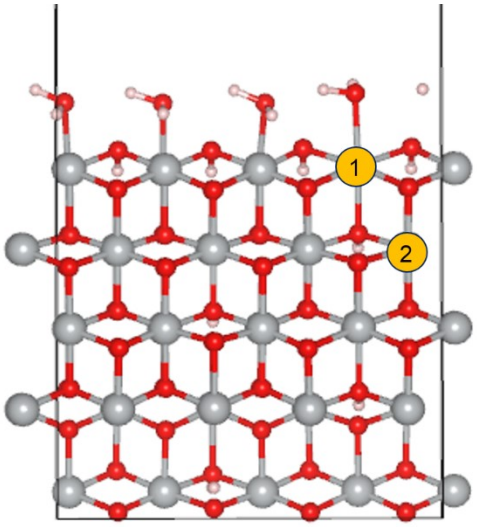

Fig. S1. Dopant site search of Fe dopant on γ-NiOOH surface. Here we considered two different possible dopant sites on NiOOH (see above) and found that Fe prefers to substitute the Ni^{δ} (site 1). Red, gray, white, and brown balls represent O, Ni, H, and Fe, respectively.

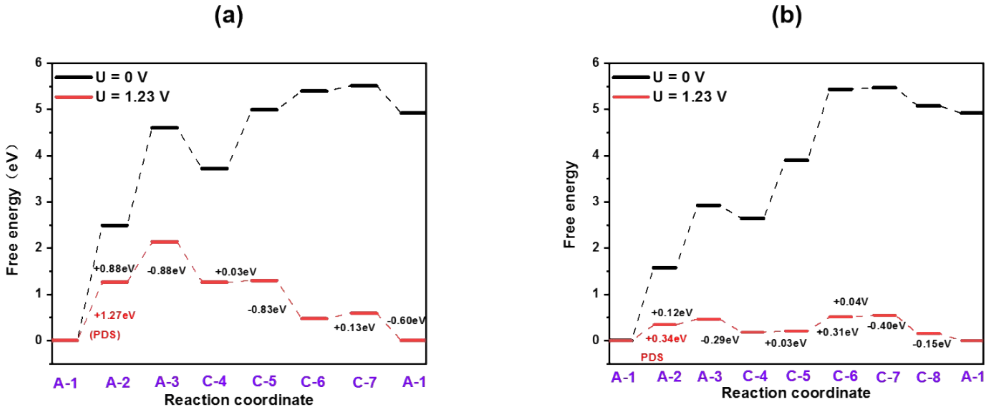

Fig. S2. Free energy diagram corrected for implicit solvation of NiOOH and NiFeOOH models toward OER. Pathway C (the designed MDSM mechanism) for NiOOH (a) and NiFeOOH (b).

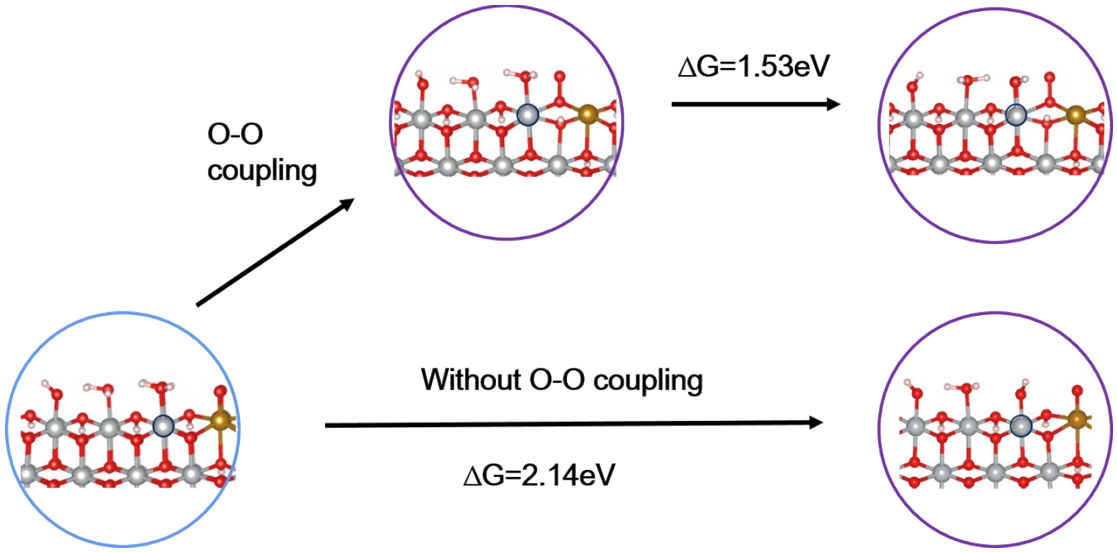

Fig. S3. Schematic diagram of the Ni^{γ} site deprotonation process. The dark cycles represents the Ni^{γ} that will participate in the reaction.

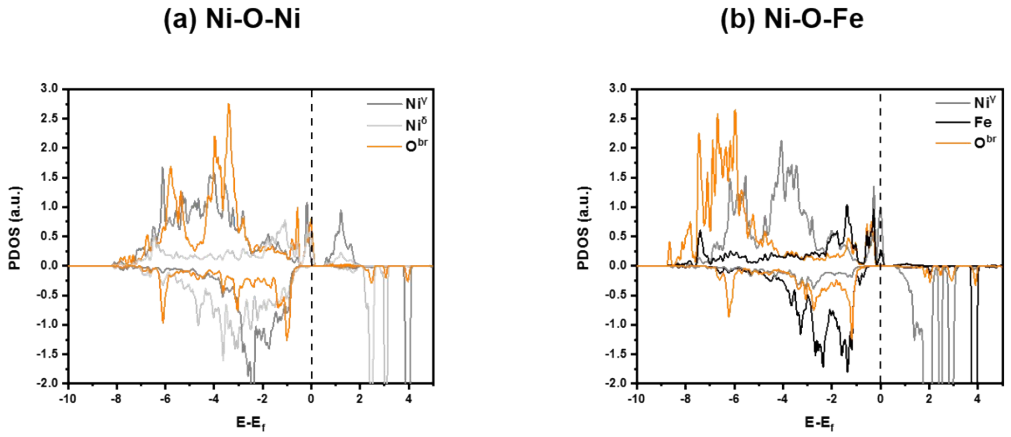

Fig. S4. PDOS of O^{br} 2*p* and M 3*d* orbit in state A-1 for NiOOH (a) and NiFeOOH (b) models. The black dash line represents the Fermi level.

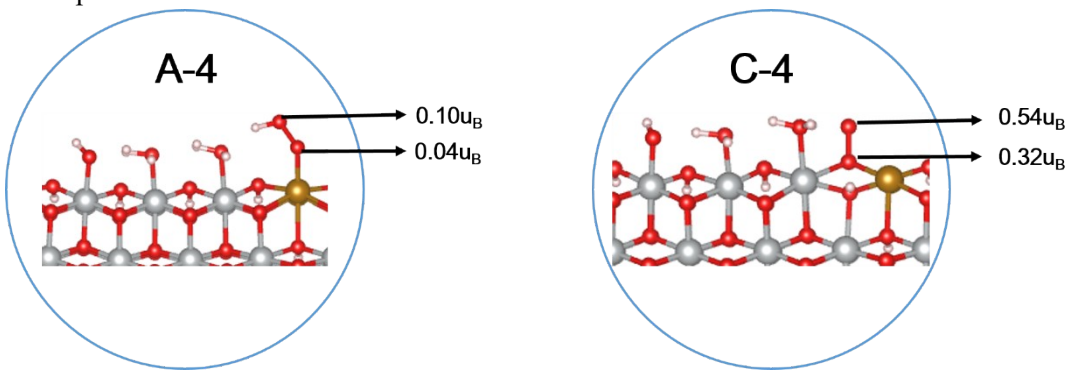

Fig. S5. Schematic diagram of magnetic moments (μ_B) of O species.