Controlled synthesis of P-Co_3O_4@NiCo-LDH/NF nanoarrays as binder-free electrodes for water splitting

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DFT calculation

In this work, the Cambridge Serial Total Energy Package module of Materials Studio was employed for DFT calculation. The interactions of electrons were assessed by the generalized gradient approximation functions of Perdew-Burke-Emzerh (GGA-PBE). The (003) and (111) plane optimal structures of NiOOH and P-Co_3O_4 were calculated by setting a cutoff energy of 500 eV and 7×7×1 k-points grid. The structures were also optimized for energy and force convergence choosing as 2.0×10^{-5} eV/atom and 0.05 eV/A, respectively. The vacuum space was up to 0.002 A to eliminate periodic interactions.

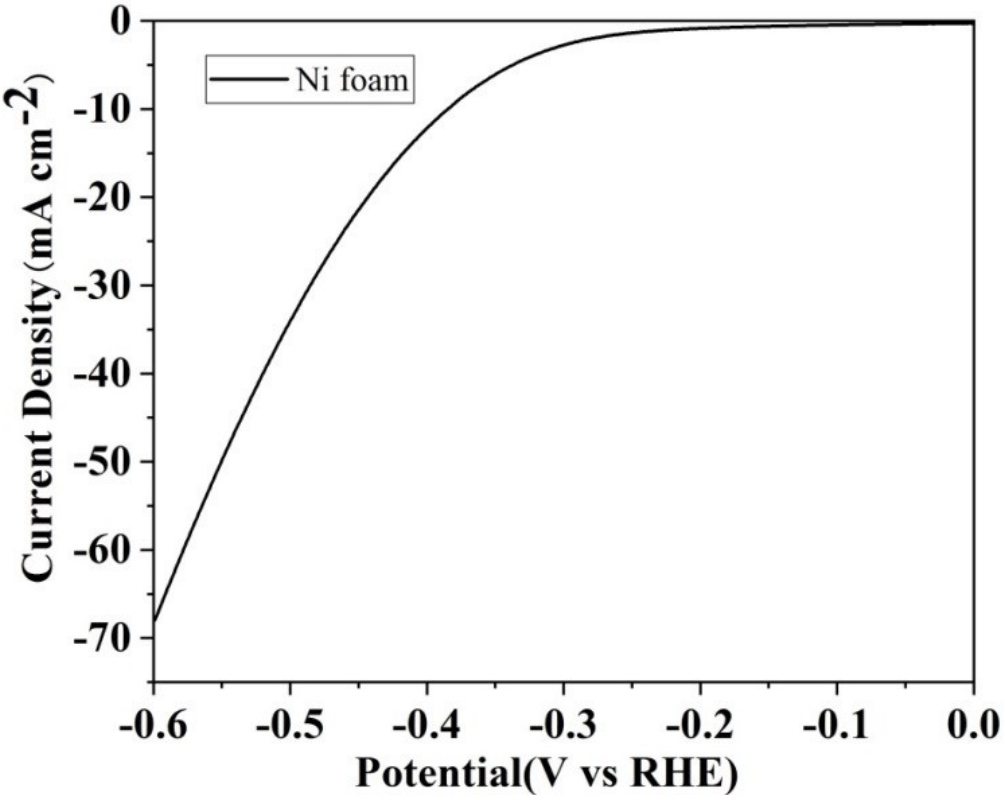

Fig. S1 Polarization curves of NF in 1.0 M KOH at a potential sweep rate of 5 mV s^{-1}.

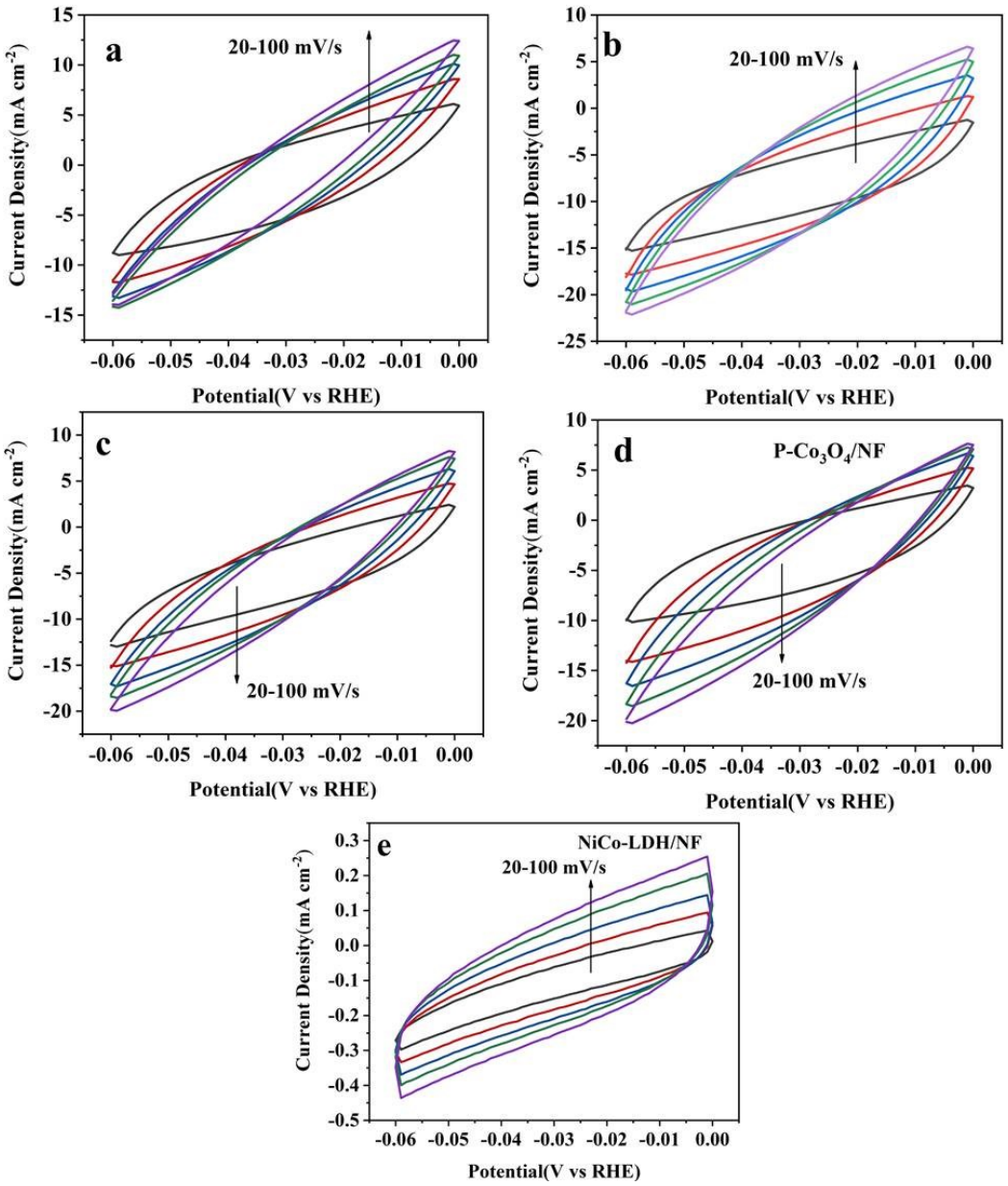

Fig. S2 CVs of P-Co_3O_4@NiCo-LDH-1/NF, P-Co_3O_4@NiCo-LDH-2/NF, P-Co_3O_4@NiCo-LDH-3 /NF, P-Co_3O_4/NF and NiCo-LDH/NF.

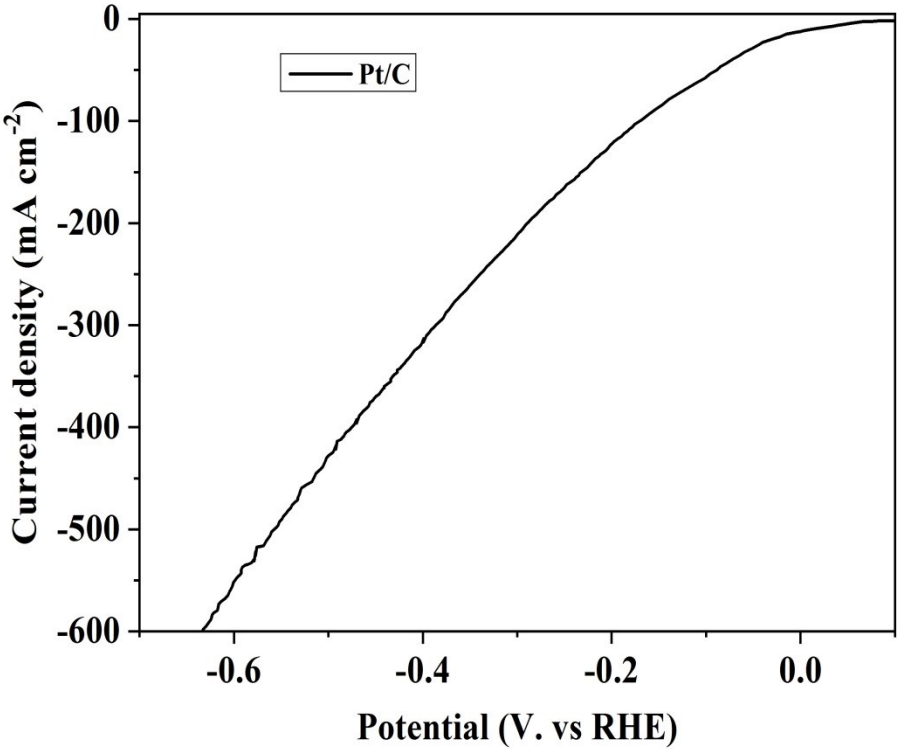

Fig. S3 Polarization curve of the Pt/C for HER with a scan rate of 5 mV s^{-1} in 1 M KOH.

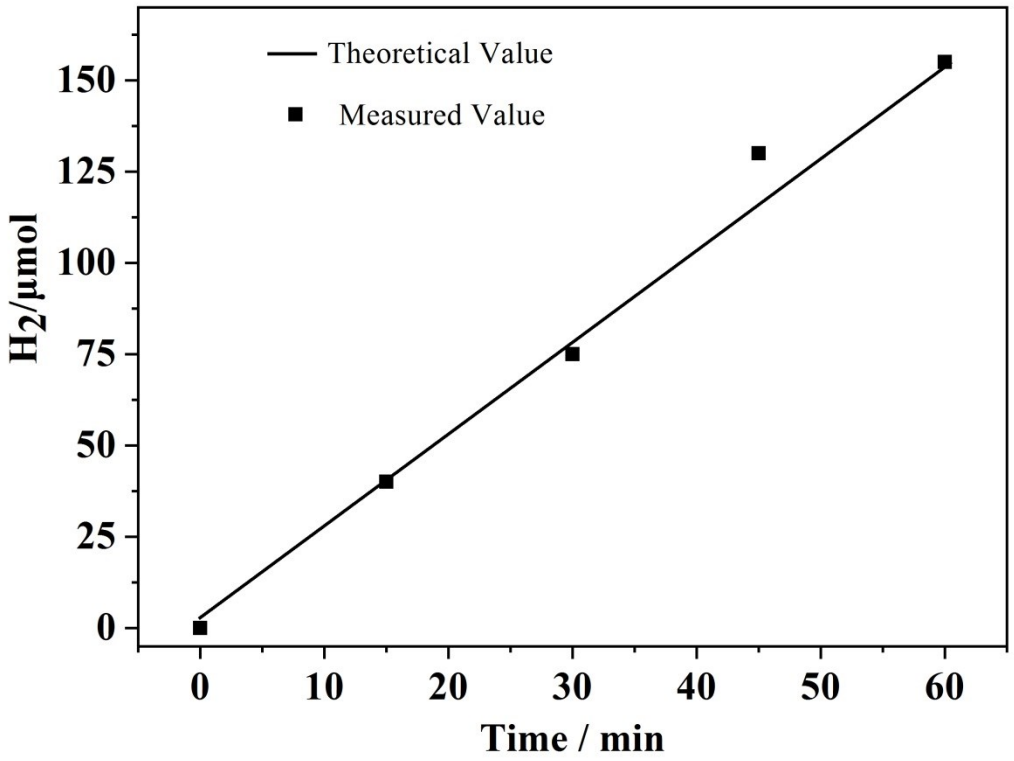

Fig. S4 Electrocatalytic efficiency of H_2 production over P-Co_3O_4@NiCo-LDH-2 /NF.

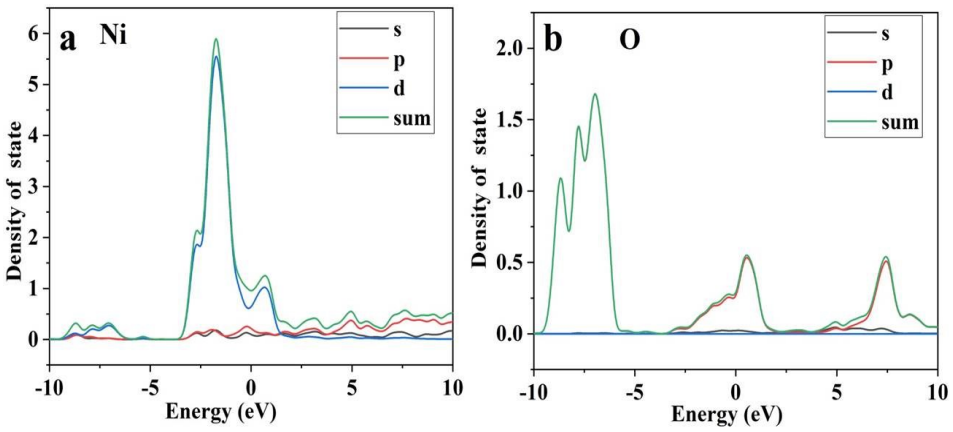

Fig. S5 Density of states for NiOOH, (a) Ni and (b) O.

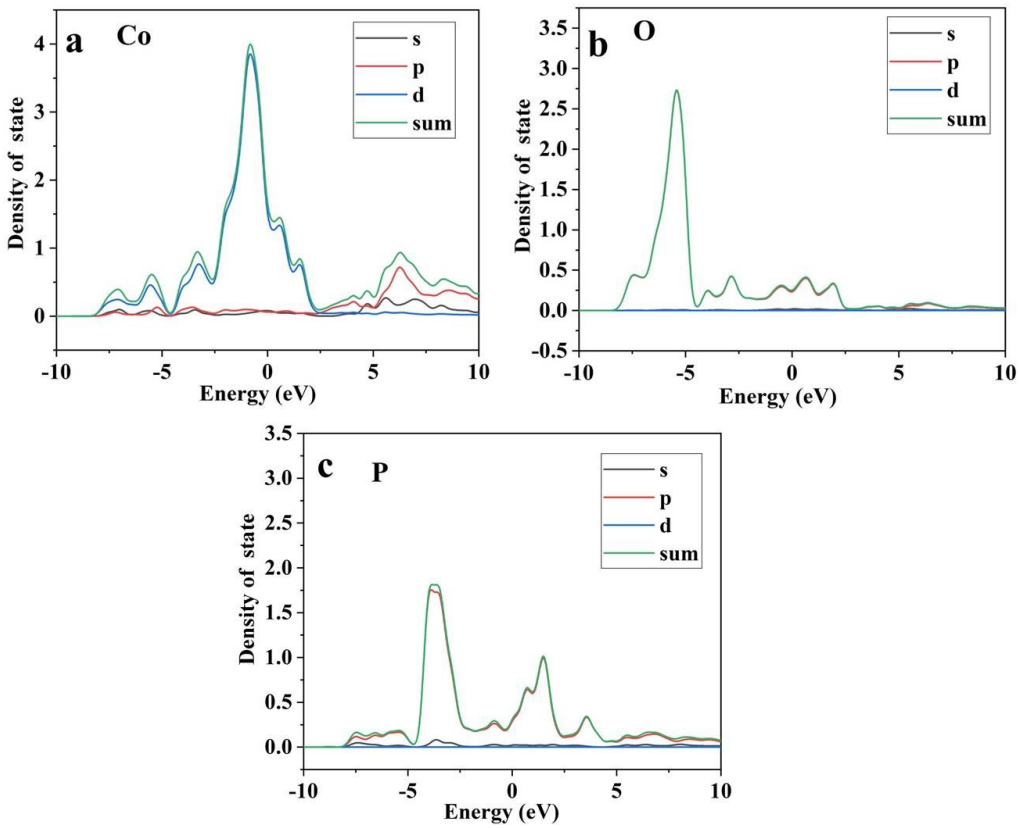

Fig. S6 Density of states for P-Co_3O_4, (a) Co, (b) O and (c) P.