Electronic supplementary information (ESI) for

A Facile Approach for Preparing Densely-Packed Individual *p*-NiO/*n*-Fe_2O_3 Heterojunction Nanowires for Photoelectrochemical Water Splitting

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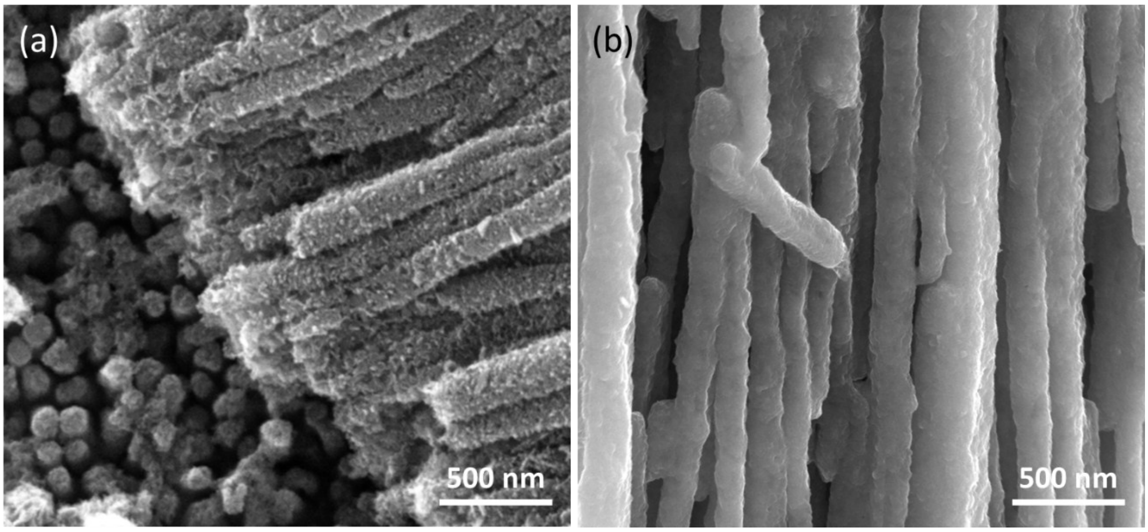

Fig. S1 FESEM images of individual (a) α-Fe_2O_3 NWs as well as (b) NiO NWs grown using the process same as fabricating heterojunction NWs.

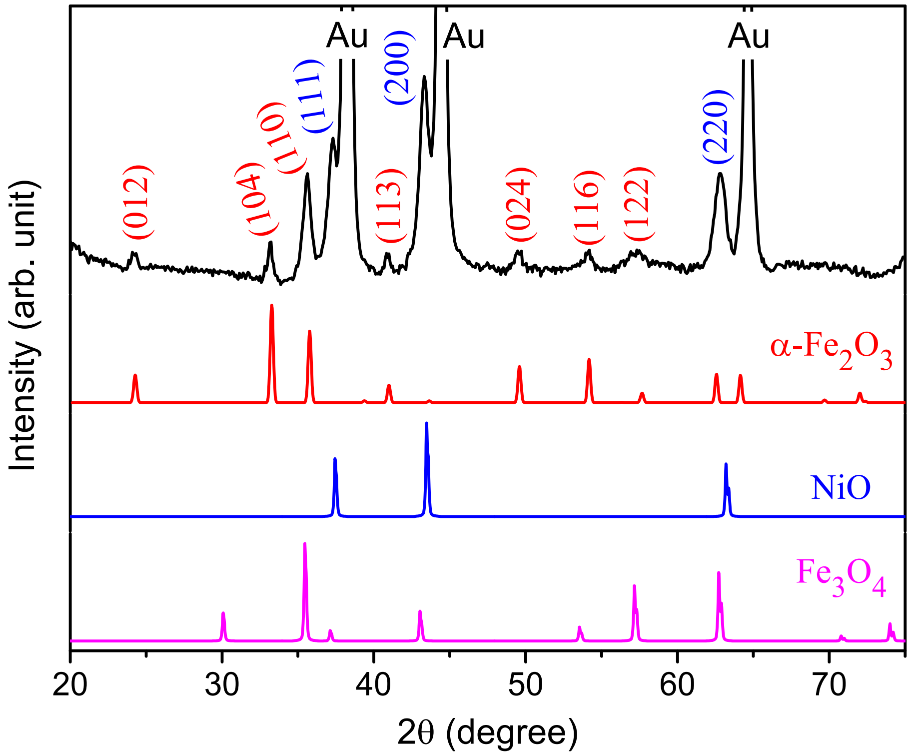

Fig. S2 X-ray diffraction (XRD) spectrum for the NiO/α-Fe_2O_3 heterojunction NW arrays (black), along with the reference patterns of α-Fe_2O_3 (red), NiO (blue) and Fe_3O_4 (magenta).

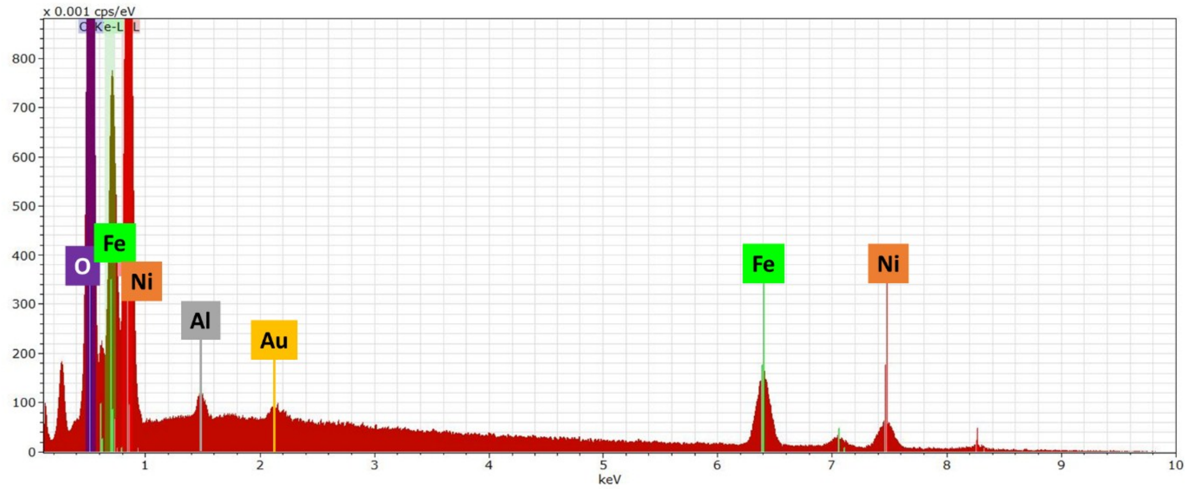

Fig. S3 Energy dispersive spectrum (EDS) recorded from the p-NiO/n-Fe_2O_3 heterojunction NW arrays.

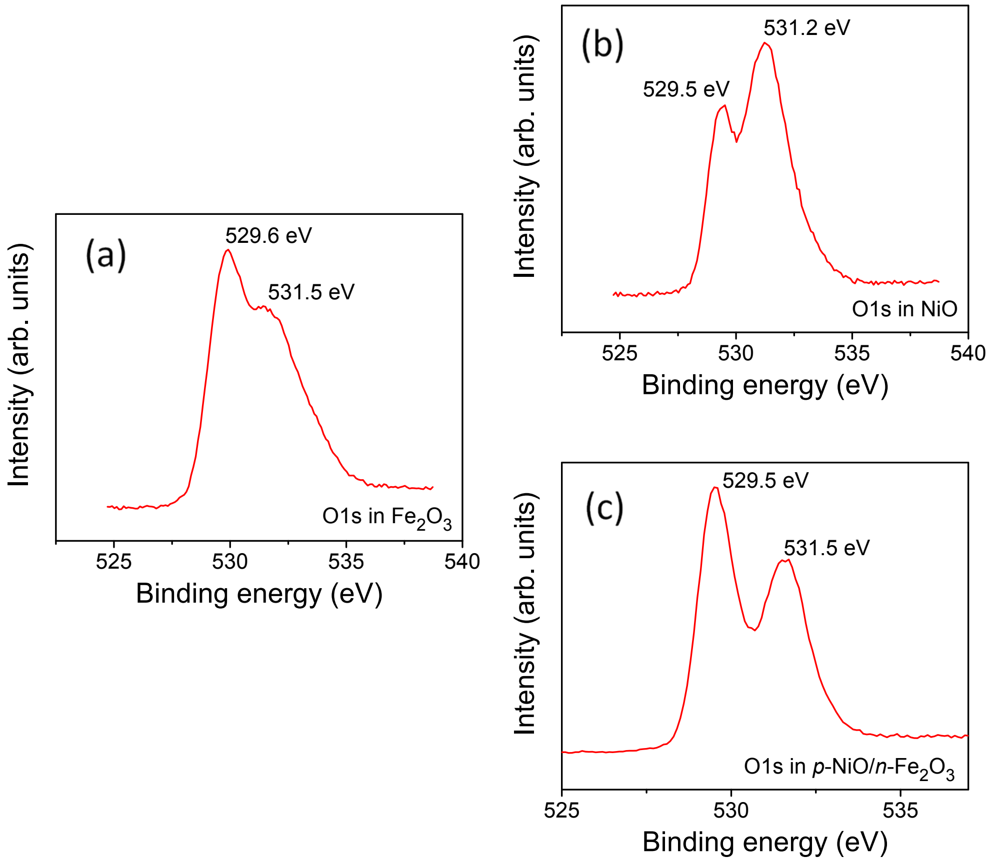

Fig. S4 O1s core level XPS spectrum obtained from the pristine Fe_2O_3 (a), NiO (b) NWs and from the p-NiO/n-Fe_2O_3 heterojunction NW (c) arrays.

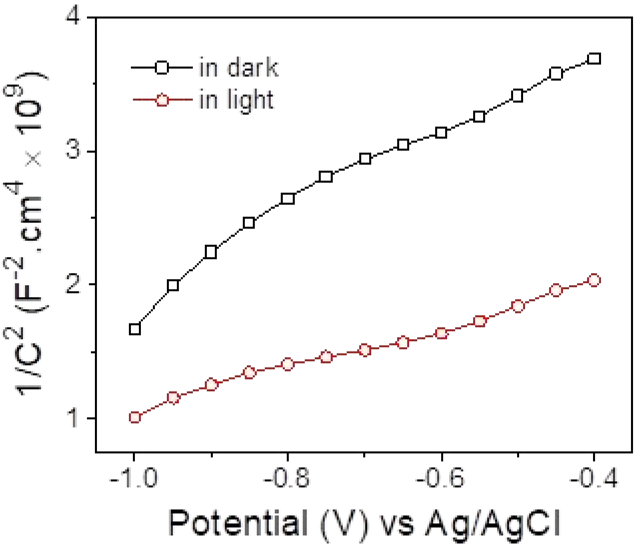

Fig. S5 Mott-Schottky plot for the pristine α-Fe_2O_3 NW electrode measured at an AC field frequency of 10 kHz.

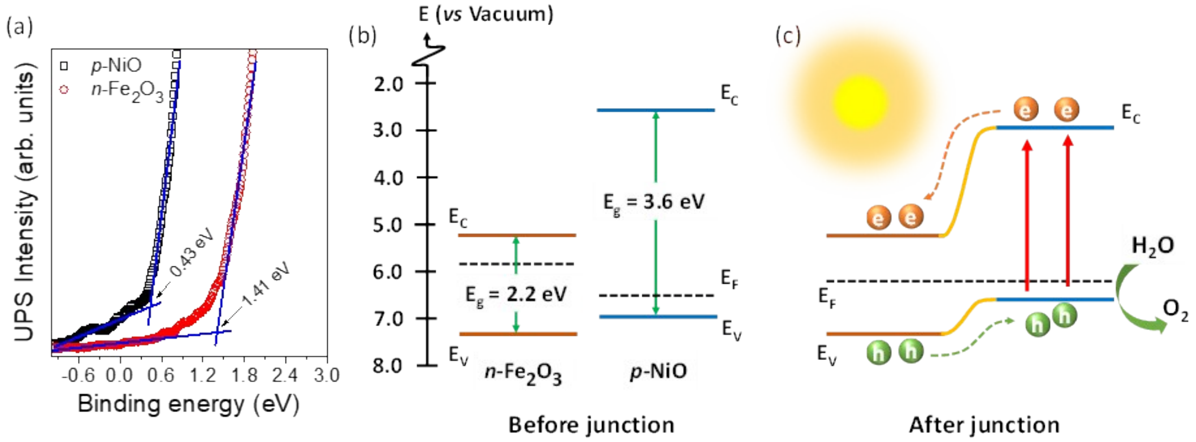

Fig. S6 (a) Valence band spectra of the pristine Fe_2O_3 and NiO NWs recorded utilizing ultraviolet photoelectron spectroscopy (UPS), (b) shows schematic diagram of the band positions of *p*-NiO and *n*-Fe_2O_3 before the formation of the heterojunction along with the possible band alignment at the interface after the formation of the heterojunction (c).

Fig. S6 depicts interfacial band configuration before and after the formation of heterojunction interface. However, the valence band positions for pristine NiO and Fe_2O_3 have been estimated using ultraviolet photoelectron spectroscopy (UPS) and corresponding valence band (VB) spectra are shown in Fig. S6a. The position of the valence band maxima (VBM) with respect to the fermi level are found to be at 0.43 eV and 1.41 eV for the *p*-type NiO and *n*-type Fe_2O_3, respectively, and are in good agreement with the values reported elsewhere.[1-3] Considering the work functions of NiO and Fe_2O_3 to be 6.55 eV and 5.88 eV, respectively,[1, 4] the possible band positions of NiO and Fe_2O_3 before the formation of the heterojunction are schematically demonstrated in Fig. S6b. Now, during the formation of the heterojunction, fermi levels at both sides of the interface will tend to come at equilibrium through diffusion, drift motion followed by recombination of charge carriers across the interface, thus forming a charge depletion layer across the interface. Probable interfacial band alignment after the formation of heterojunction interface is depicted in Fig. S6c.

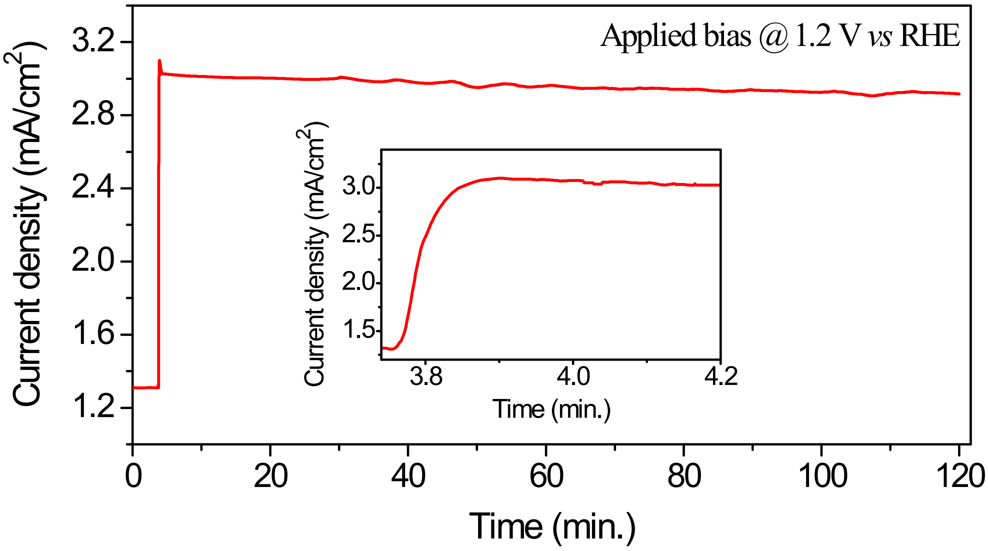

Fig. S7 Photocurrent stability test for *p*-NiO/*n*-Fe_2O_3 heterojunction electrode under an applied bias of 1.2 V *vs* RHE. Inset figure shows photocurrent response during few initial minutes.

References

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