Enhancing charge separation efficiency in photocatalytic hydrogen evolution via synergistic strategy based on point/interface dual defect engineering in Schottky heterojunctions

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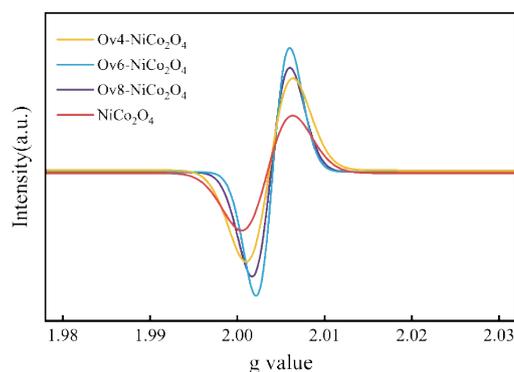*Corresponding author: li_mei@nun.edu.cn (M. Li)

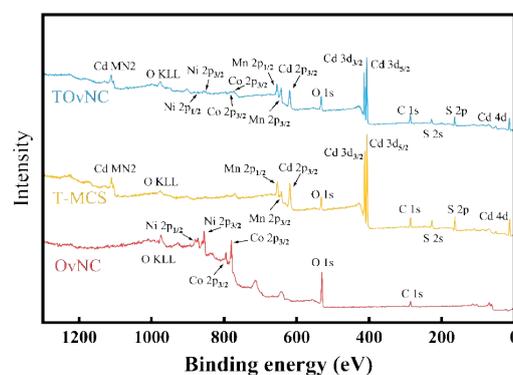Fig. S1 ESR images with different concentrations of oxygen vacancies

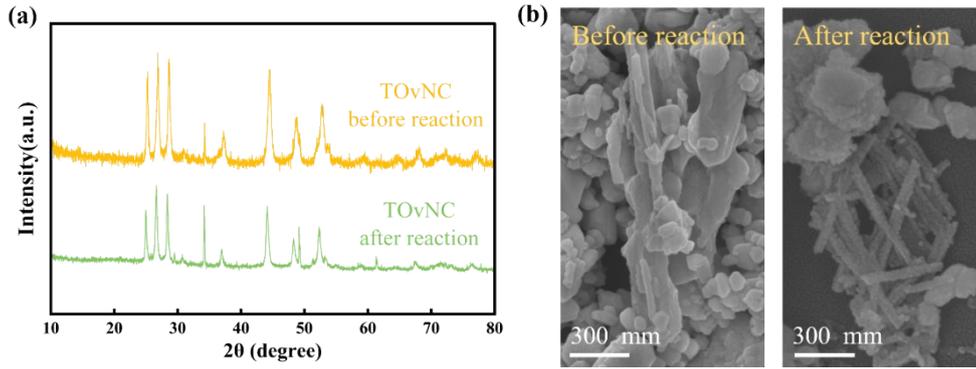Fig. S2 XPS survey spectra of TOvNC, T-MCS and OvNC.

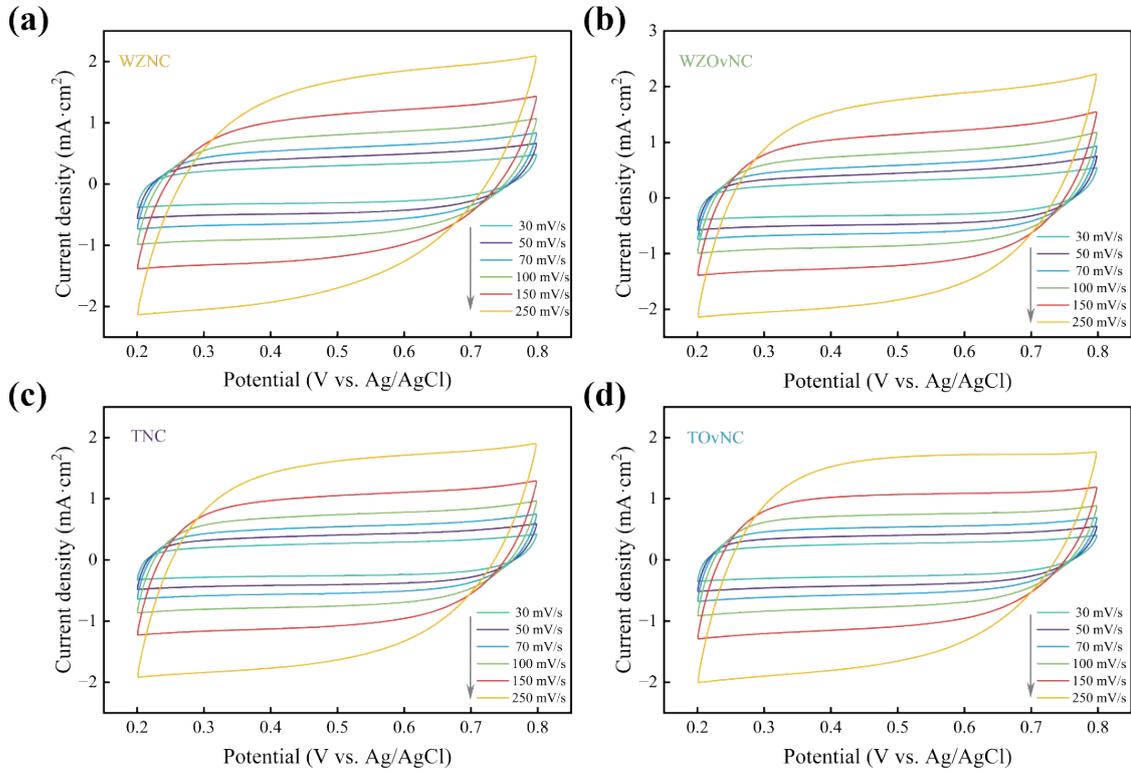Fig. S3 (a) XRD patterns of TOvNC before and after reaction, (b) SEM images of TOvNC before and after reaction

Fig S4. CV plots of (a) WZNC, (b) WZOvNC, (c) TNC, and (d) TOvNC at different scanning speeds

Calculation of charge separation efficiency:

$$\xi Na_2SO_4 = \xi max\ \eta abs \eta sep \eta trans \qquad \text{S-1}$$

ξNa_2SO_4— The photocurrent density in Na_2SO_4、ξmax — The theoretical maximum photocurrent density、ηabs— Light absorption efficiency、ηsep— Surface charge separation efficiency、$\eta trans$— Surface charge transfer efficiency.

$$\xi Na_2SO_3 = \xi max\ \eta abs\eta sep \qquad\qquad \text{S-2}$$

$\xi\,Na_2SO_3$ — The photocurrent density in Na_2SO_3、 ξmax — The theoretical maximum photocurrent density、 ηabs — Light absorption efficiency、 ηsep- Surface charge separation efficiency.

Therefore, the surface charge transfer efficiency of the catalyst can be expressed by the S-3 formula:

$$\eta trans = \xi Na_2SO_4/\xi Na_2SO_3 \qquad\qquad \text{S-3}$$

Calculation of carrier concentration:

$$N_d = \left(\frac{2}{e \times \varepsilon_r \times \varepsilon_0}\right)\left[\frac{d(1/c^2)}{dV}\right]^{-1} \qquad\qquad \text{S-4}$$

e — The electric charge; ε_r — The dielectric constant of the material; ε_0 — Vacuum dielectric constant; $\dfrac{d(1/c^2)}{dV}$ — The slope of the straight line in the Mott-Schottky curve.