Enhancing NiS Performance: Na-Doping for Advanced Photocatalytic and Electrocatalytic Applications

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To compare the various factors influencing the photocatalytic degradation of 2,4-DCP, degradation experiments were conducted using the NiS catalyst by varying the catalyst concentration, pollutant concentration and solution pH. The results are presented in Figure S1. It is evident that increasing the catalyst concentration provides more active sites, thereby enhancing the degradation efficiency. The pollutant concentration was fixed at 20 ppm and the catalyst concentration was varied from 10 mg to 40 mg. The degradation efficiency significantly improved up to 30 mg of catalyst, but the variation became negligible between 30 mg and 40 mg. Similarly, the pollutant concentration was varied from 10 ppm to 40 ppm. The catalyst exhibited only a negligible decrease in degradation efficiency with increasing pollutant concentration, indicating its ability to handle higher pollutant levels effectively. Finally, the solution pH was varied from acidic to basic. Consistent with the observations for Na-NiS, the degradation efficiency was highest in the neutral medium compared to acidic or basic conditions.

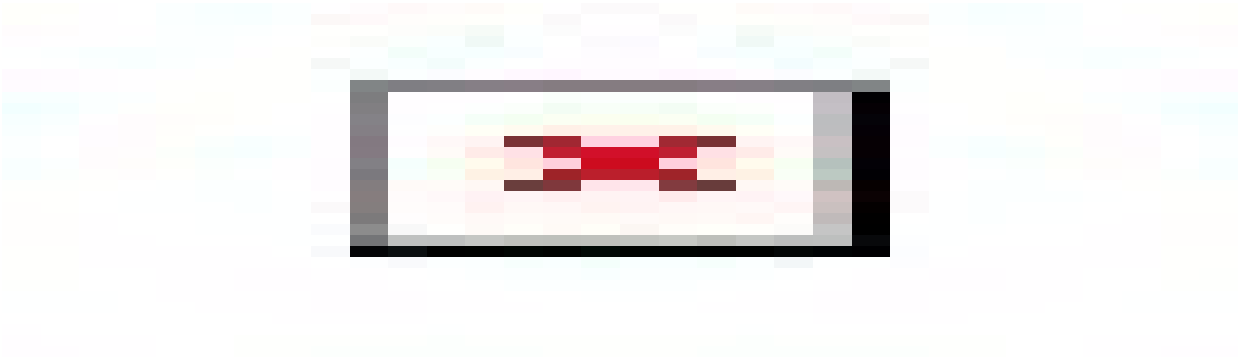

Figure S1: Photocatalytic degradation of 2,4-DCP by NiS catalyst, **(a)** Effect of catalyst concentration [2,4-DCP-20 ppm]; **(b)** Effect of pollutant (2,4-DCP) concentration [NiS-30 mg]; **(c)** Effect of different pH environments on the degradation of 2,4-DCP.

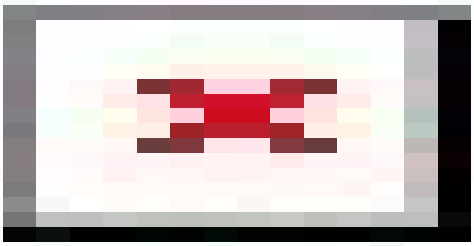

Figure S2. (a) PL analysis showing a gradual increase in fluorescence intensity, signifying the generation of a significant number of hydroxyl radicals and **(b)** EPR spectra showing no significant change in intensity, confirming the absence of singlet oxygen in the analyzed system.

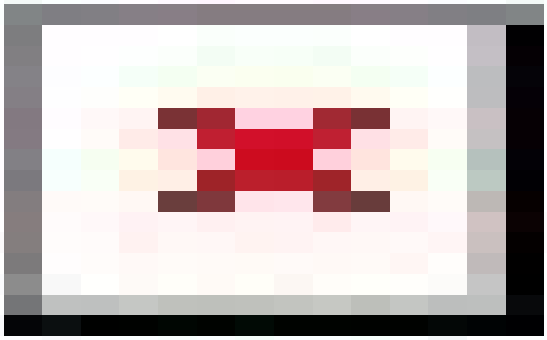

Figure S3. Chronopotentiometry stability studies; **(a)** HER and **(c)** OER for 12 h **(b and d)** LSV curve before and after 12 h time-dependent studies for HER and OER respectively; **(e)** double layer capacitance plot of NiS and Na-NiS.

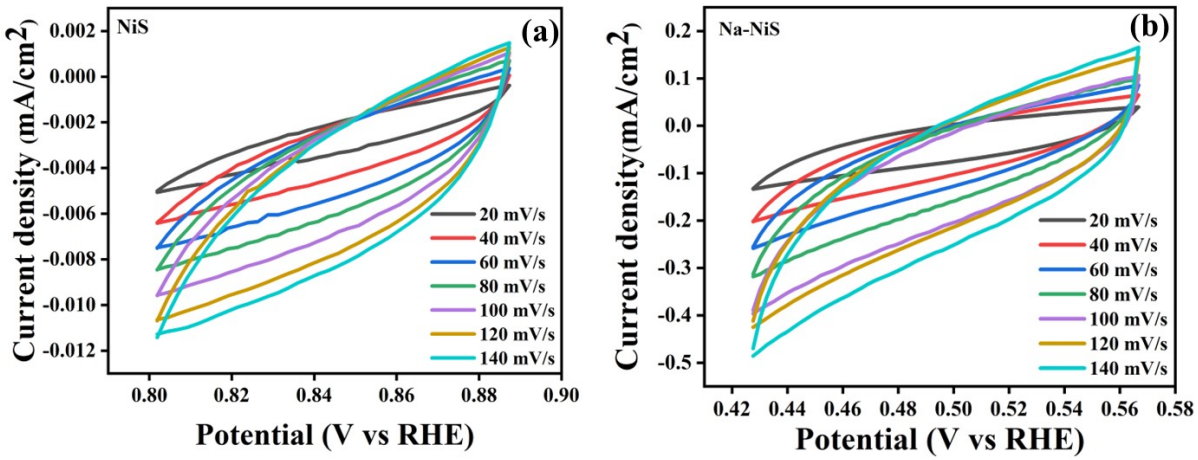

Figure S4. Cyclic voltammetry of **(a)** NiS and **(b)** Na-NiS at different scan rate (20 to 140 mV/s).

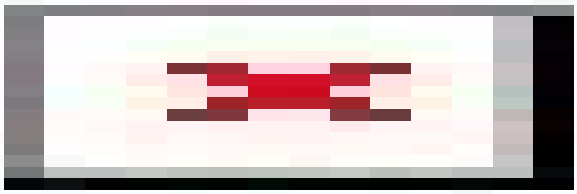

Figure S5. (a) Polarization curve for HER || OER overall water splitting system; **(b)** Chronopotentiometric stability study, **(c)** LSV curves before and after 12 h time-dependent studies for Na-NiS.

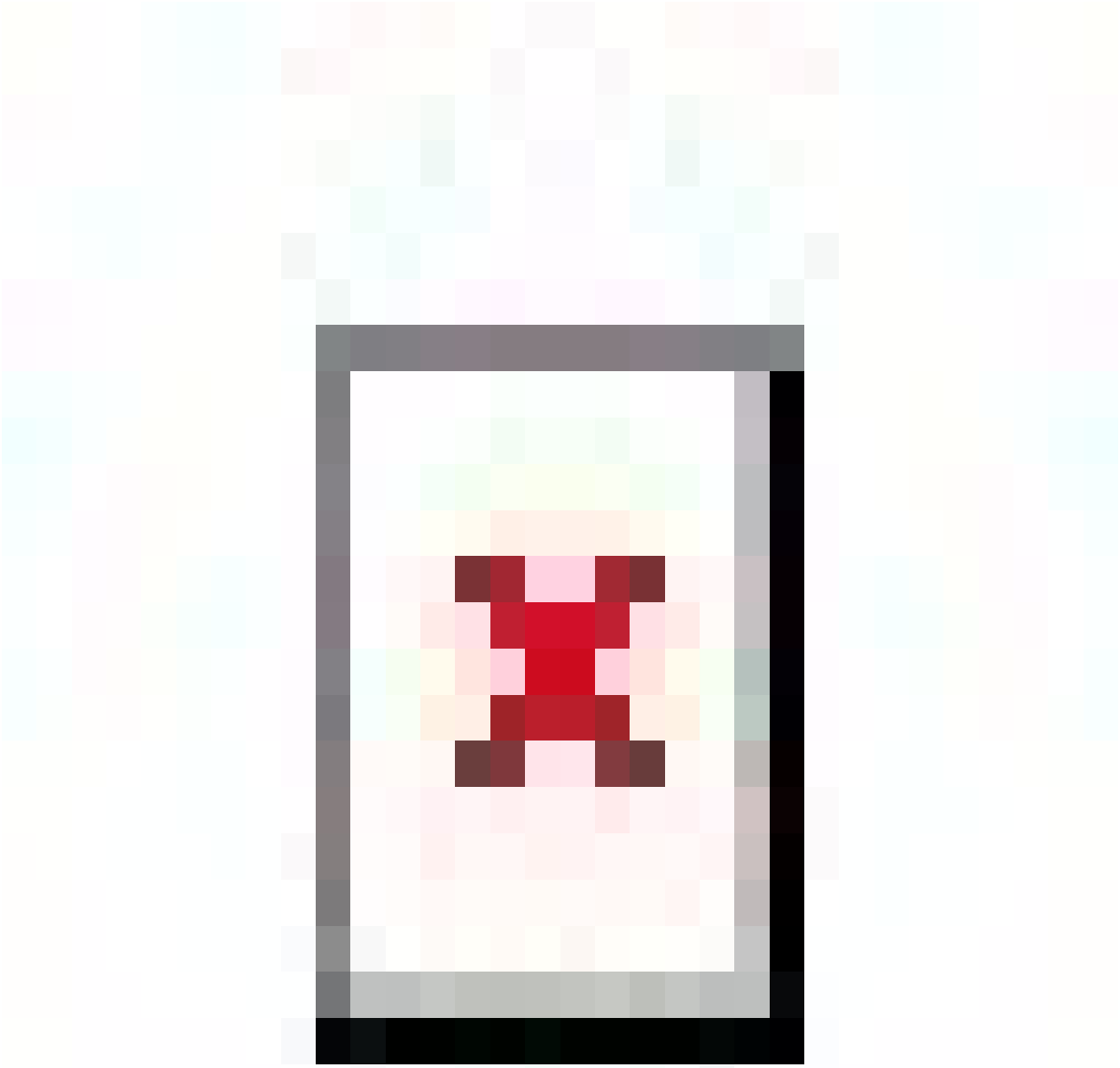

Figure S6. (a-f) TEM, HRTEM, EDAX and elemental mapping of Na-NiS after HER and **(g-l)** TEM, HRTEM, EDAX and elemental mapping of Na-NiS after OER studies representing the materials stability even after cyclic studies.

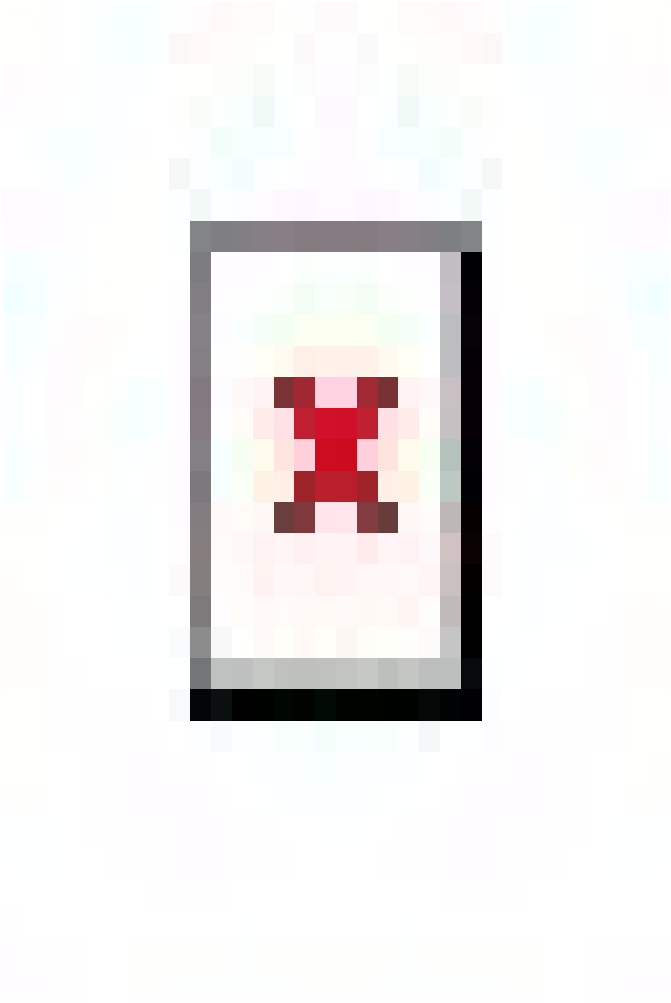

Figure S7. PXRD spectra of Na-NiS after HER and OER cyclic studies representing the same crystal structure of Na-NiS.