

## Supplementary information

# Effect of Functionalized Benzene Derivatives as Potential Hole Scavengers for BiVO<sub>4</sub> and rGO-BiVO<sub>4</sub> Photoelectrocatalytic Hydrogen Evolution

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## **Supplemental Materials and Methods**

Thermogravimetric analysis (TGA) was performed using a Q500 thermogravimetric analyzer (TA Instruments, USA). For this purpose, ~5 mg of samples were weighed onto clean Pt pans and covered with a pierced Pt lid. Thermogravimetric analysis was performed in the temperature range of 40 °C to 800 °C at a ramp of 20 °C min<sup>-1</sup> and a nitrogen furnace purge flow rate of 40 mL min<sup>-1</sup>.

## Figure captions

Figure S1. Isosurface plots of HOMO and LUMO frontier orbitals of PH, BA, BA<sup>-</sup>, SA<sup>-</sup>, 5-ASA, and 5-ASA ZW

Figure S2. Thermogravimetric analysis (TGA) of GO and rGO samples in (A) N<sub>2</sub> atmosphere and (B) air

Figure S3. Powder X-ray diffraction (XRD) patterns of GO and rGO

Figure S4. LSV of BiVO<sub>4</sub> and rGO-BiVO<sub>4</sub> photoelectrodes in NaCl solution (0.1 M) containing different concentrations of SFBDs; PH (A and B), BA (C and D), SA (E and F), and 5-ASA (G and H) in the dark and under illumination

Figure S5. OCP of BiVO<sub>4</sub> (A, C, E, G) and rGO-BiVO<sub>4</sub> (B, D, F, H) photoelectrodes in NaCl solution (0.1 M) with simple functionalized benzene derivatives

Figure S6. EIS of BiVO<sub>4</sub> (A, C, E, G) and rGO-BiVO<sub>4</sub> (B, D, F, H) in the dark and under light illumination in NaCl (0.1 M) with simple functionalized benzene derivatives, with inlays corresponding to response in NaCl (0.1 M) alone

Figure S1

Compound	Structure	HOMO isosurface map	$E(\text{HOMO})$ , eV	LUMO isosurface map	$E(\text{LUMO})$ , eV
phenol (PH)			-6.422		-0.490
benzoic acid (BA)			-7.483		-1.714
benzoate (BA <sup>-</sup> )			-5.742		-0.544
salicylic acid (SA)			-6.721		-1.605
salicylate (SA <sup>-</sup> )			-5.850		-0.626
5-aminosalicylic acid (5-ASA)			-5.660		-1.551
5-aminosalicylic acid zwitterion (5-ASA ZW)			-5.850		-1.061

Figure S2

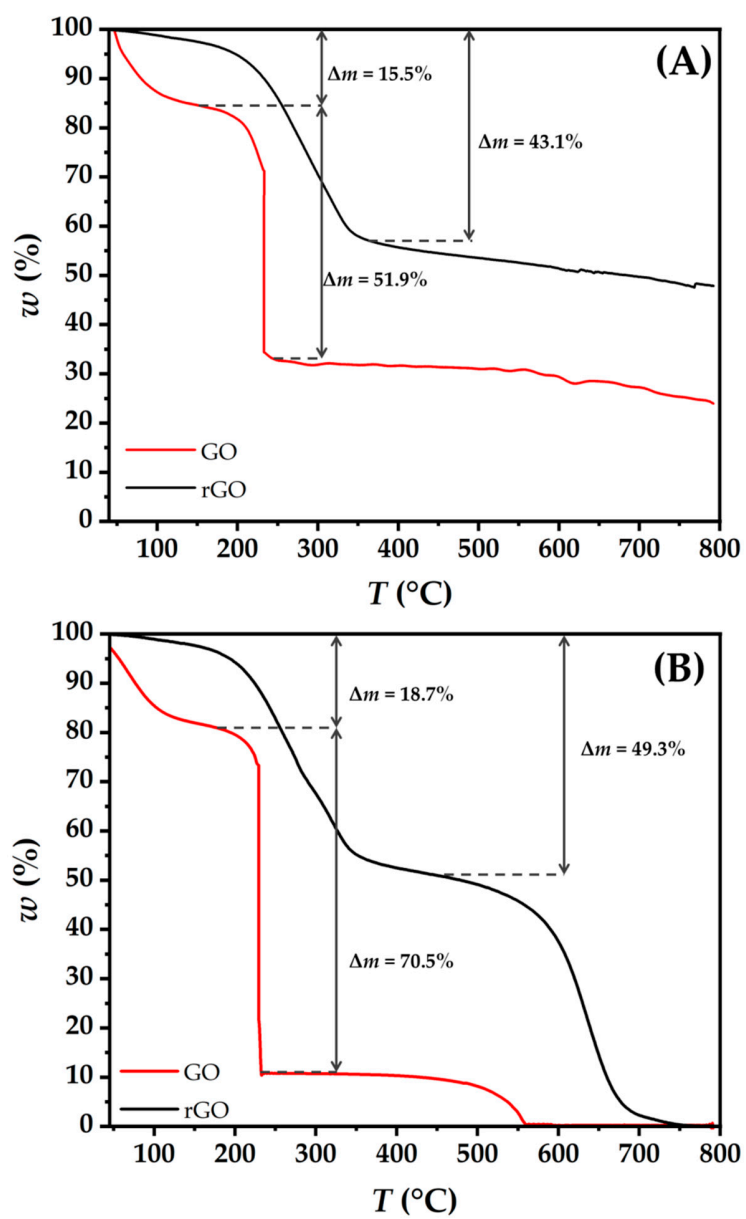


Figure S3

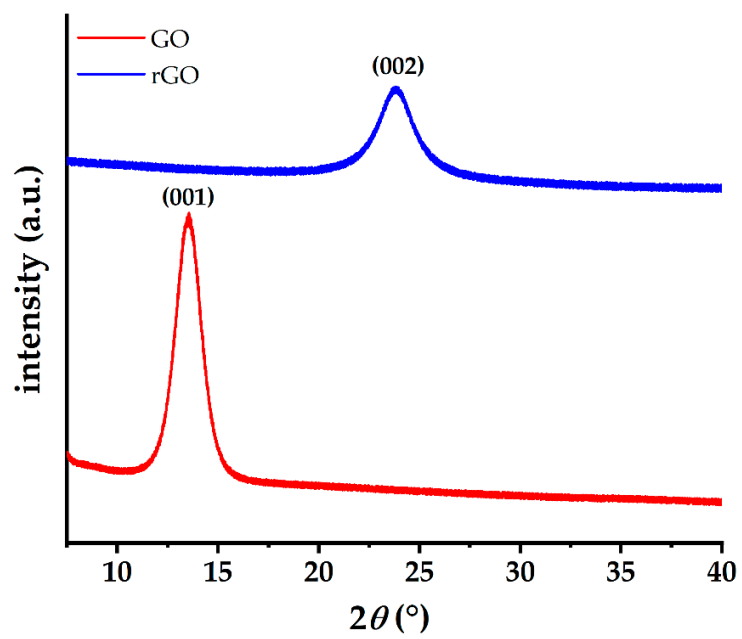


Figure S4

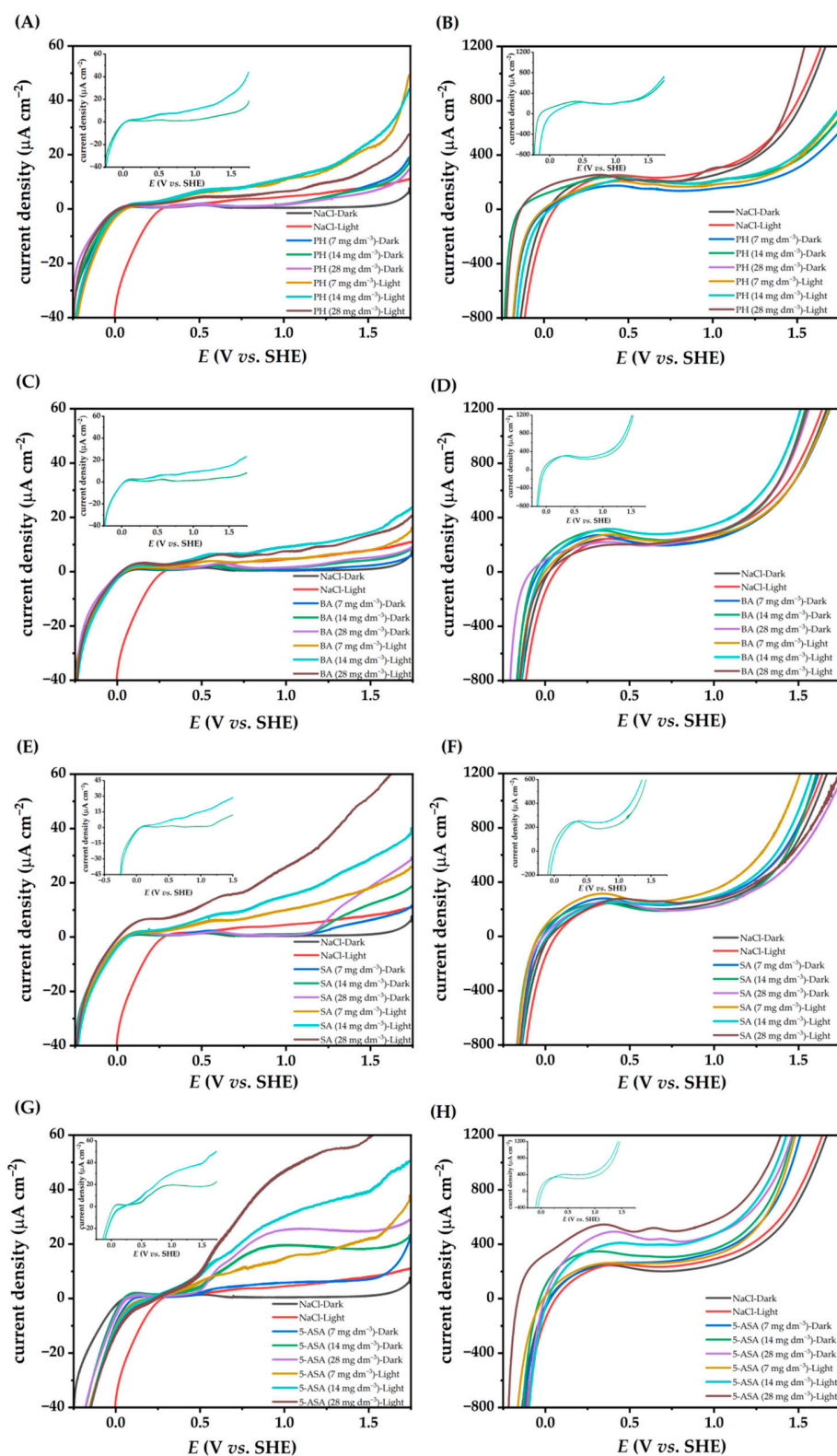


Figure S5

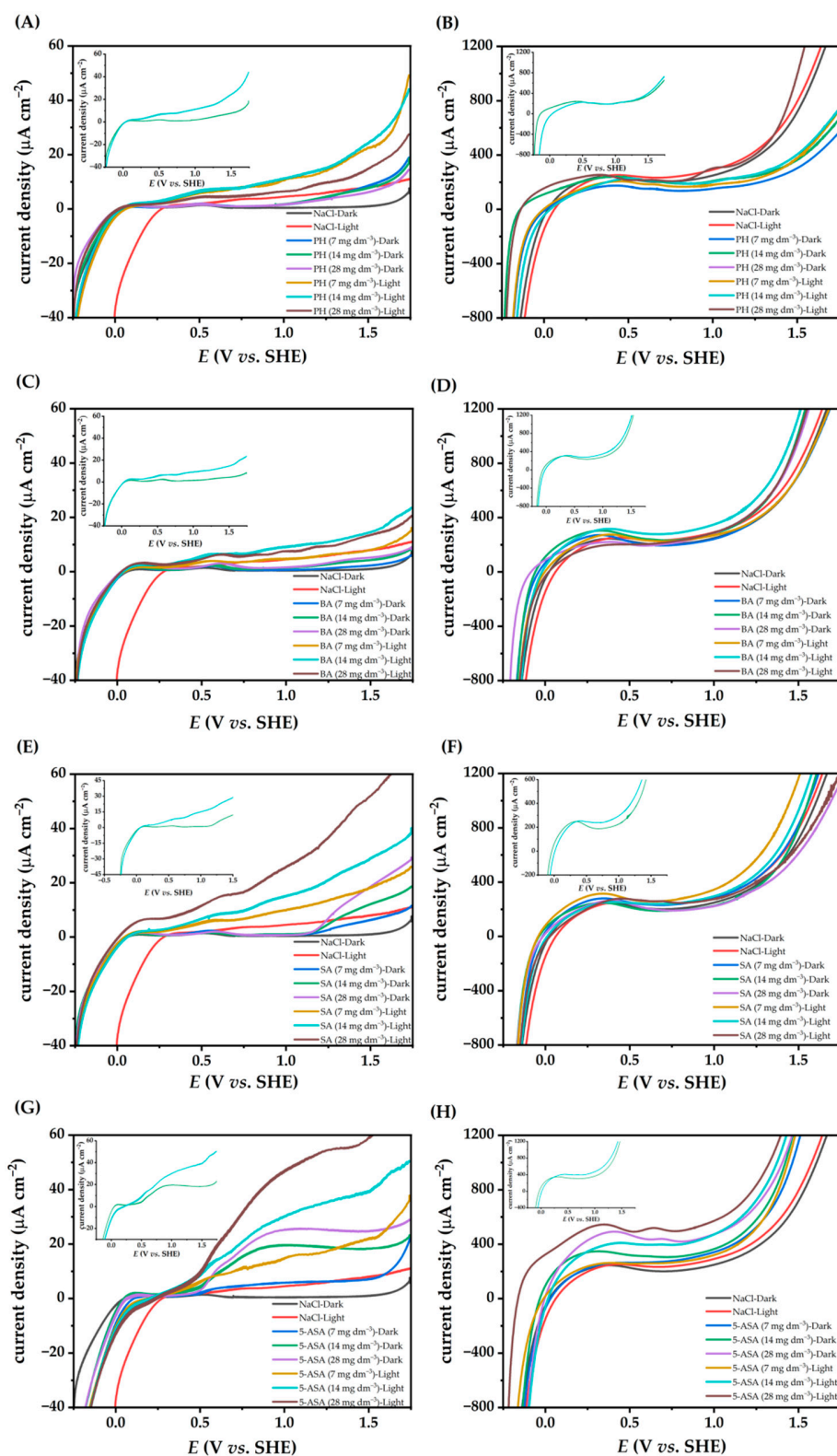




Figure S6

