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Supplementary Materials

Solar desalination charger for water treatment and value-added chemical production

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Fig. S1. FE-SEM images of (a and b) BVO, (c and d) WBVO, and (e and f) Co-WBVO.



Fig. S2. XPS spectra of Bi 4f, V 2p, and O 1s bands for BVO and WBVO samples.

| Sample | Potential (V) | $J_{\rm ph}$ (mA cm ⁻²) | Electrolyte | Light source (mW cm ⁻²) | FE_{CIOR} (%) | Ref. |
|---|------------------------|--|---------------------|--|-----------------|-----------|
| BiVO ₄ /WO ₃ | 1.4 V | 1.25 | 5 M NaCl | 100 mW cm ⁻² L-42 cutoff filter | 81.4 | [1] |
| BiVO ₄ /WO ₃ | $1.42 V_{RHE}$ | 2.61 | 4 M NaCl, pH 1 | 100 mW cm ⁻² | 74 | [2] |
| WO ₃ | $1.46 V_{RHE}$ | 4.78 | Synthetic seawater | 100 mW cm^{-2} | 70 | [3] |
| Co doped BiVO ₄ | $1.1 \ V_{RHE}$ | 0.19 | 1 M NaCl, pH 2.3 | 100 mW cm^{-2} | 92 | [4] |
| CoOx-loaded BiVO ₄ /WO ₃ | $1.0 \ V_{\text{RHE}}$ | 1 | 0.5 M NaCl | 100 mW cm ⁻² L-42 cutoff filter | 95 | [5] |
| BiVO ₄ | | 1.45 | | | 40 | This work |
| W-BiVO ₄ | $1.36 V_{\text{RHE}}$ | 2.4 | 0.171 M NaCl | 100 mW cm ⁻² | 48 | This work |
| W-BiVO ₄ / CoOOH | | 3.55 | | | 91 | This work |

Table S1. Photoelectrocatalytic chloride oxidation activities using various photoanodes

References

- 1. Iguchi, S., Y. Miseki, and K. Sayama, *Efficient hypochlorous acid (HClO) production via photoelectrochemical solar energy conversion using a BiVO*₄*-based photoanode*. Sustainable Energy & Fuels, 2018. **2**(1): p. 155-162.
- 2. Rassoolkhani, A.M., et al., *Nanostructured bismuth vanadate/tungsten oxide photoanode for chlorine production with hydrogen generation at the dark cathode.* Communications Chemistry, 2019. **2**(1): p. 57.
- 3. Jadwiszczak, M., et al., *Highly efficient sunlight-driven seawater splitting in a photoelectrochemical cell with chlorine evolved at nanostructured WO₃ photoanode and hydrogen stored as hydride within metallic cathode. Advanced Energy Materials, 2020. 10(3): p. 1903213.*
- 4. Chauhan, I., et al., *Nanostructured Co-doped BiVO*⁴ for efficient and sustainable photoelectrochemical chlorine evolution from simulated sea-water. Dalton Trans, 2023.
- 5. Okunaka, S., Y. Miseki, and K. Sayama, *Improvement of photoelectrochemical HClO production under visible light irradiation by loading cobalt oxide onto a BiVO4 photoanode*. Catalysis Science & Technology, 2021. **11**(16): p. 5467-5471.



Fig. S3. Linear sweep voltammograms with BVO and W-doped BVO in 0.171 M NaCl solution in the dark and under 1 sun.



Fig. S4. Repetitive linear sweep voltammograms with Co-WBVO in 0.171 M NaCl in the dark and under 1 sun.



Fig. S5. Linear sweep voltammograms with Co-WBVO as a function of Co-electrodeposition charges on WBVO in 0.171 M NaCl solution in the dark (dashed curves) and under 1 sun (solid curves).



Fig. S6. UV-Vis diffuse reflectance absorption spectra of BVO, WBVO, Co-WBVO films.



Fig. S7. Time-profiled J_{ph} changes at E = 1.36 V_{RHE} (0.73 V_{SCE}) in 0.171 M NaCl under AM 1.5 (100 mW cm⁻²).



Fig. S8. Chlorate production during photoelectrochemical chloride oxidation using bare and modified BVO electrodes at E = 1.36 V vs. RHE in 0.171 M NaCl under 1 sun.



Fig. S9. (a) Linear sweep voltammograms with Co-WBVO photoanode coupled with different number of Na_xC electrode and (b) concurrent changes in E_{cell} of the Co-WBVO and Na_xC array pairs as a function of number of Na_xC electrode in 0.171 M NaCl under 1 sun. Na_xC electrodes were connected in parallel.



Fig. S10. Changes in the photopotential (E_{ph}) of WBVO and Co-WBVO photoelectrode coupled to Na_xC electrode in 0.171 M NaCl containing As(III) (1 mM) and NH₃ (1 mM) under 1 sun. While J_{ph} of 1 mA cm⁻² was constantly maintained to the photoelectrodes, E_{cells} of the photoelectrode and Na_xC electrode pairs were recorded. Note that the solution pH changed with time and hence the SCE scale was used.



Fig. S11. Changes in discharging potentials (V vs. RHE) of CNTs, NiMoS, and Bi connected to the charged Na_xC with 8 mAh in 0.1 M K₂SO₄ (pH 6.5) purged with O₂, 0.1 M KOH (pH 13) purged with N₂, and 0.1 M KHCO₃ (pH 6.8) purged with CO₂, respectively. Constant *J* values of (a) -1 mA cm⁻² and (b) -3 mA cm⁻² were applied to the electrocatalysts, while *E*_{cells} of the electrocatalyst and Na_xC pairs were recorded.



Fig. S12. Simultaneous productions and FEs of H₂O₂ via O₂ reduction with CNTs, H₂ via water reduction with NiMoS, and HCOOH via CO₂ reduction with Bi during the discharging stages. $J = -3 \text{ mA cm}^{-2}$. See Fig. S11 for experimental conditions.



Fig. S13. A solar charging process with desalination of saline water (0.171 M NaCl) and oxidation of water contaminants (mixed As(III) and NH₃, each 1 mM). A WBVO photoelectrode (with SCE electrode) and Na_xC electrode were immersed in 0.171 M NaCl solutions. See **Scheme 1b** for the experimental setup. (a) Changes in E_{ph} of WBVO, and E_{cell} of WBVO and Na_xC pair at J_{ph} of 1 m A cm⁻². (b) Changes in the amounts of Na⁺ and Cl⁻ in the saline water, Na⁺ in the catholyte, and Cl⁻ in the anolyte. Inset shows ITEs. (c) Changes in As(V) and NH₃ concentrations.