

Supplementary

Porous BiVO₄/Boron-doped Diamond Heterojunction Photoanode with Enhanced Photoelectrochemical Activity

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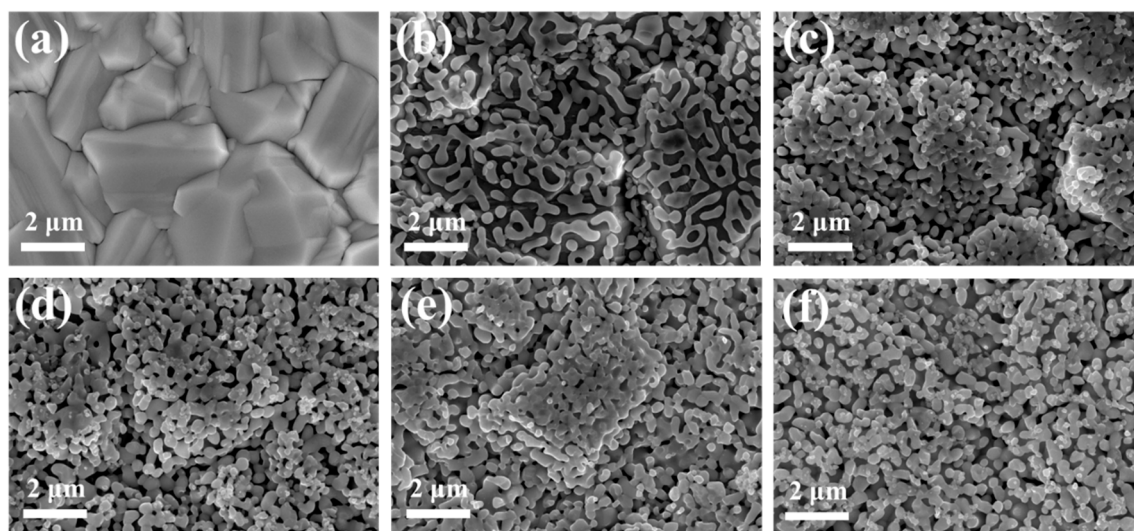


Figure S1. SEM images of BiVO₄/BDD heterojunction photoanodes:(a) bare BDD film, (b) M15, (c) M30, (d) M45, (e) M60 and (f) M75, respectively.

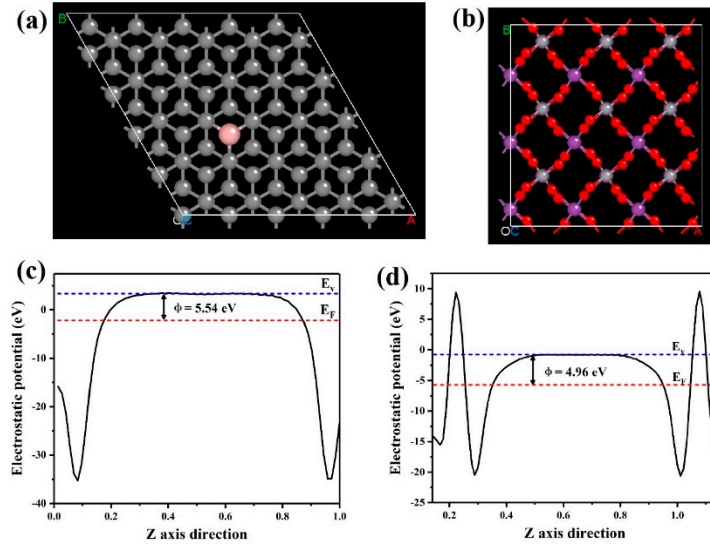


Figure S2 The crystal structures and electrostatic potentials of (a, c) BDD and (b, d) BiVO₄ (001) planes. The gray, pink, red, purple and light gray spheres represent for C, B, V, Bi and O atoms. The red and blue dashed lines stand for the Fermi potential and vacuum energy potential, respectively.

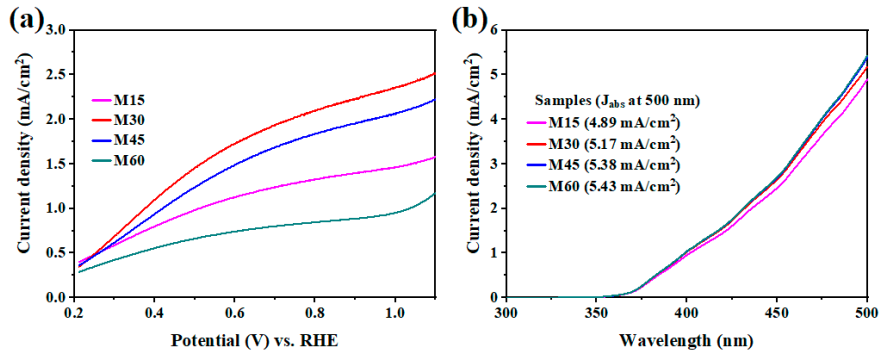


Figure S3. (a) LSVs for the M15 - M60 measured in 0.1 M Na₂SO₄ containing 0.2 M Na₂SO₃ under AM 1.5 irradiation; (b) theoretical current densities calculated based on wavelength of 300 - 500 nm for M15-M60.

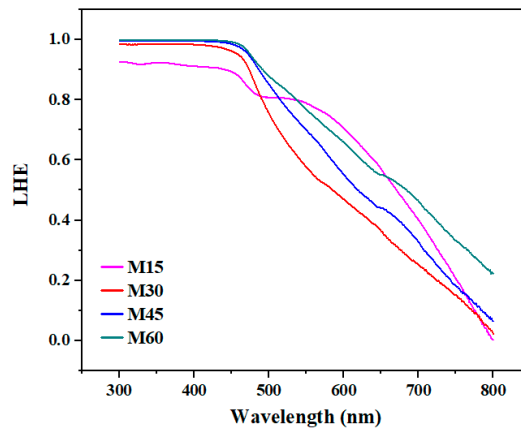


Figure S4. Light harvesting efficiency (LHE) of BiVO₄/BDD heterojunction photoanode for the M15 - M60. LHE was obtained based on the equation: $LHE = 1 - 10^{-A(\lambda)}$, where $A(\lambda)$ is absorbance corresponding to the wavelength (λ) [24].

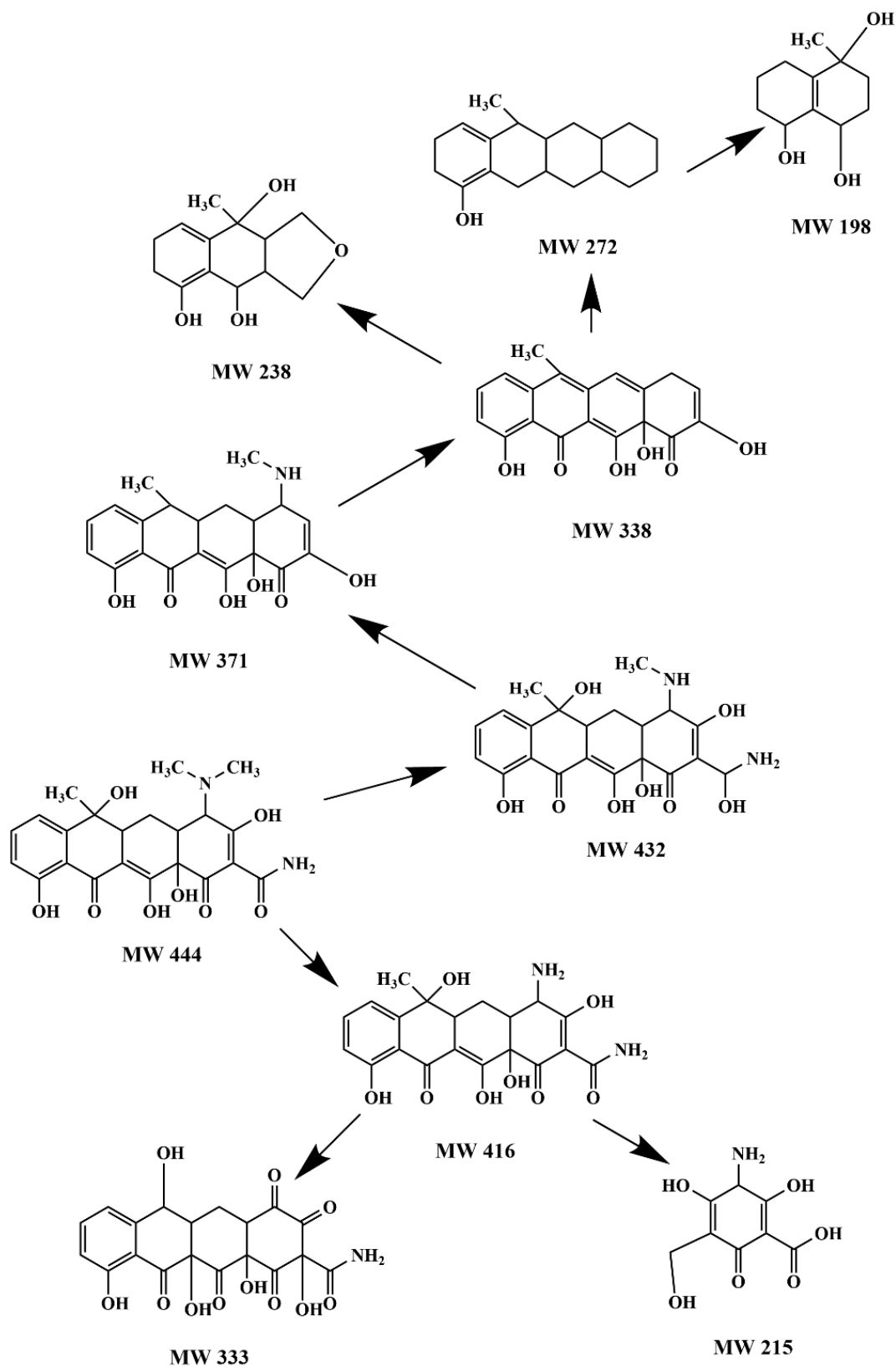


Figure S5. The degradation products and possible degradation pathways of TCH degradation.

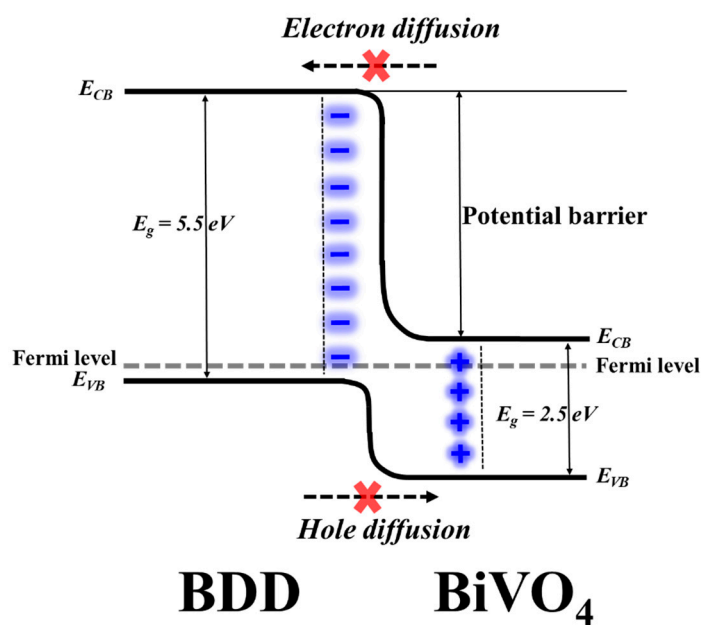


Figure S6. Schematic of the energy band structure of a BiVO₄/BDD heterojunction in an equilibrium state.

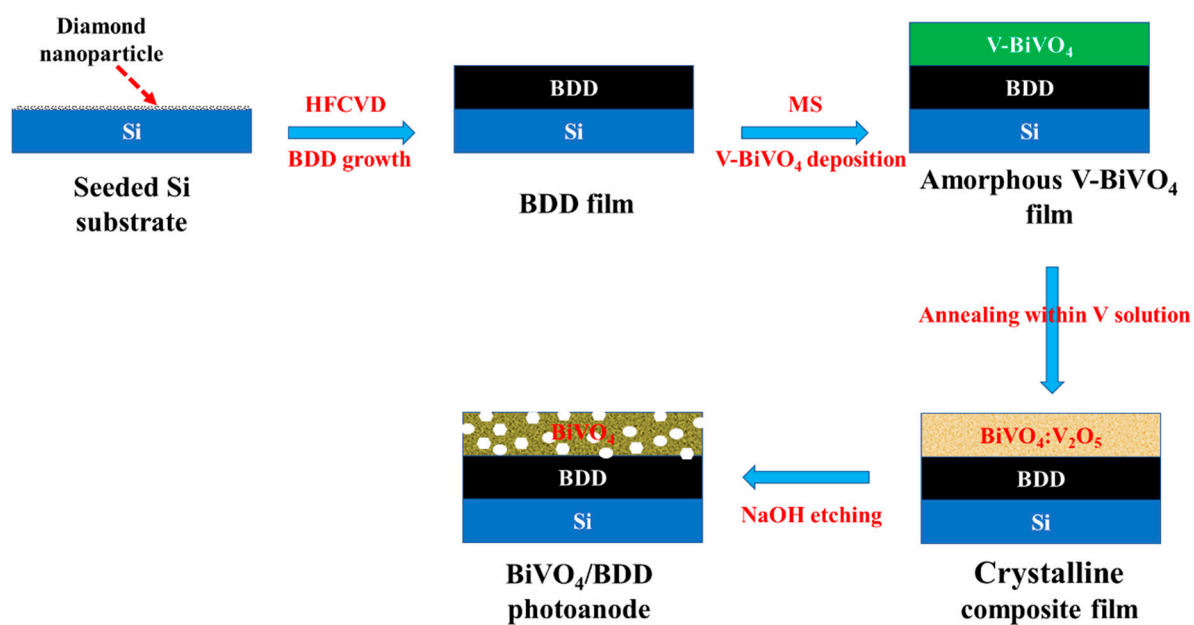


Figure S7. Schematic illustration for the synthesis of porous BiVO₄/BDD heterojunction photoanodes.

Table S1. Comparison of energy values and band gap for BiVO₄ and BDD.

	BiVO ₄	BDD
Valence band maximum (E _{VB}) (eV)	-8.17	-6.57
Conduction band minimum (E _{CB}) (eV)	-5.67	-1.07
Work function (Φ) (eV)	6.09	6.14
Band gap (E _g) (eV)	2.5	5.5 [24]

Table S2. Parameters of BDD film growth.

Growth parameters	Values/Unit
Background pressure (Torr)	6.0E-6
Working pressure (Torr)	30
H ₂ flow (sccm)	500
CH ₄ flow (sccm)	20
TMB flow (99.9% Hydrogen dilution) (sccm)	20
Substrate-to-filament distance (mm)	10
Deposition time (hour)	8
Substrate temperature (°C)	820±15

Table S3. Parameters for BiVO₄ films deposition.

	Duration of deposition (T _d) (min)	Flow ratio O ₂ /Ar (%)	Power of V target (W)	Power of BiVO ₄ target (W)	Working pressure (Torr)
M15	15	40	250	250	0.015
M30	30				
M45	45				
M60	60				
M75	75				