

Supplementary Materials

Enhanced Photodegradation of Antibiotics Using a Novel BiVO₄/P-Doped TiO₂ Heterostructure: Performance Evaluation, Property and Kinetic Modelling

Tanzim Ur Rahman^a, Musfekur Rahman Dihan^a, Abdul Hai^b, Md. Shahinoor Islam^{a*},

^aDepartment of Chemical Engineering, Bangladesh University of Engineering and Technology,
Dhaka- 1000, Bangladesh

^bDepartment of Chemical & Petroleum Engineering, Khalifa University, 127788, Abu Dhabi,
United Arab Emirates. *Corresponding author: Tel: +8801732782120; E-mail:

shahinoorislam@che.buet.ac.bd (Md. Shahinoor Islam)

List of Figures

Figure S1. Graph of Absorbance vs Wavelength for the photocatalyst samples.

Figure S2. Tauc Plots of the prepared photocatalysts.

Figure S3. Particle size distribution of TiO₂ (a), P-TiO₂ (b), BiVO₄ (c), TiO₂/BiVO₄ (d), P-TiO₂/BiVO₄-20 (e), P-TiO₂/BiVO₄-50 (f), and P-TiO₂/BiVO₄-80 (g).

Figure S4. EDX Mapping and Spectra of TiO₂

Figure S5. EDX Mapping and Spectra of P-TiO₂

Figure S6. EDX Mapping and Spectra of BiVO₄

Figure S7. EDX Mapping and Spectra of TiO₂/BiVO₄

Figure S8. EDX Mapping and Spectra of P-TiO₂/BiVO₄-20

Figure S9. EDX Mapping and Spectra of P-TiO₂/BiVO₄-50

Figure S10. Determination of pH at Point of Zero Charge for P-TiO₂/BiVO₄-80.

Figure S11: Degradation Efficiency vs time for (a) CIP, (c) MNZ and Kinetic study for (b) CIP, (d) MNZ for different concentration of H₂O₂ using P-TiO₂/BiVO₄-80. (Experimental Conditions: 20 mg/L of pollutant concentration, 1 g/L of catalyst dosage and natural pH)

27 **List of Tables**

28 Table S1. The two-tailed Pearson correlation matrix for the crystal size and the bandgap of the
29 prepared seven photocatalysts with the elemental composition.

30 Table S2. Summary of kinetic parameters for CIP degradation.

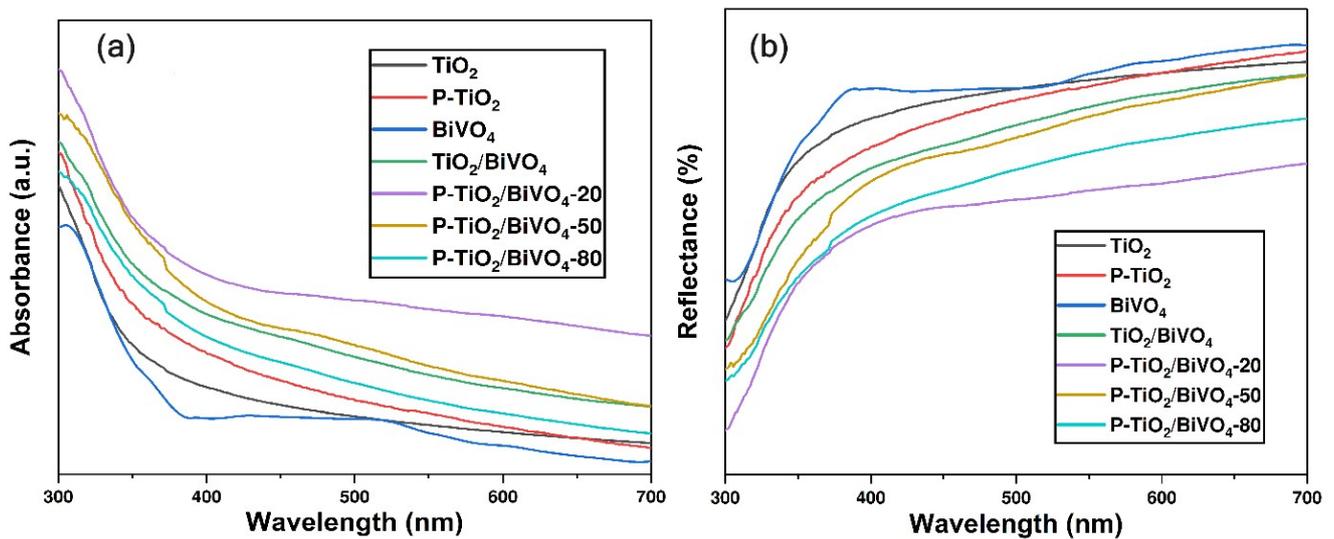
31 Table S3. Summary of kinetic parameters for MNZ degradation.

32 Table S4. Table for rate constant and R^2 -values obtained from first-order kinetics of
33 photodegradation of CIP and MNZ using P-TiO₂/BiVO₄-80 for different experimental
34 conditions.

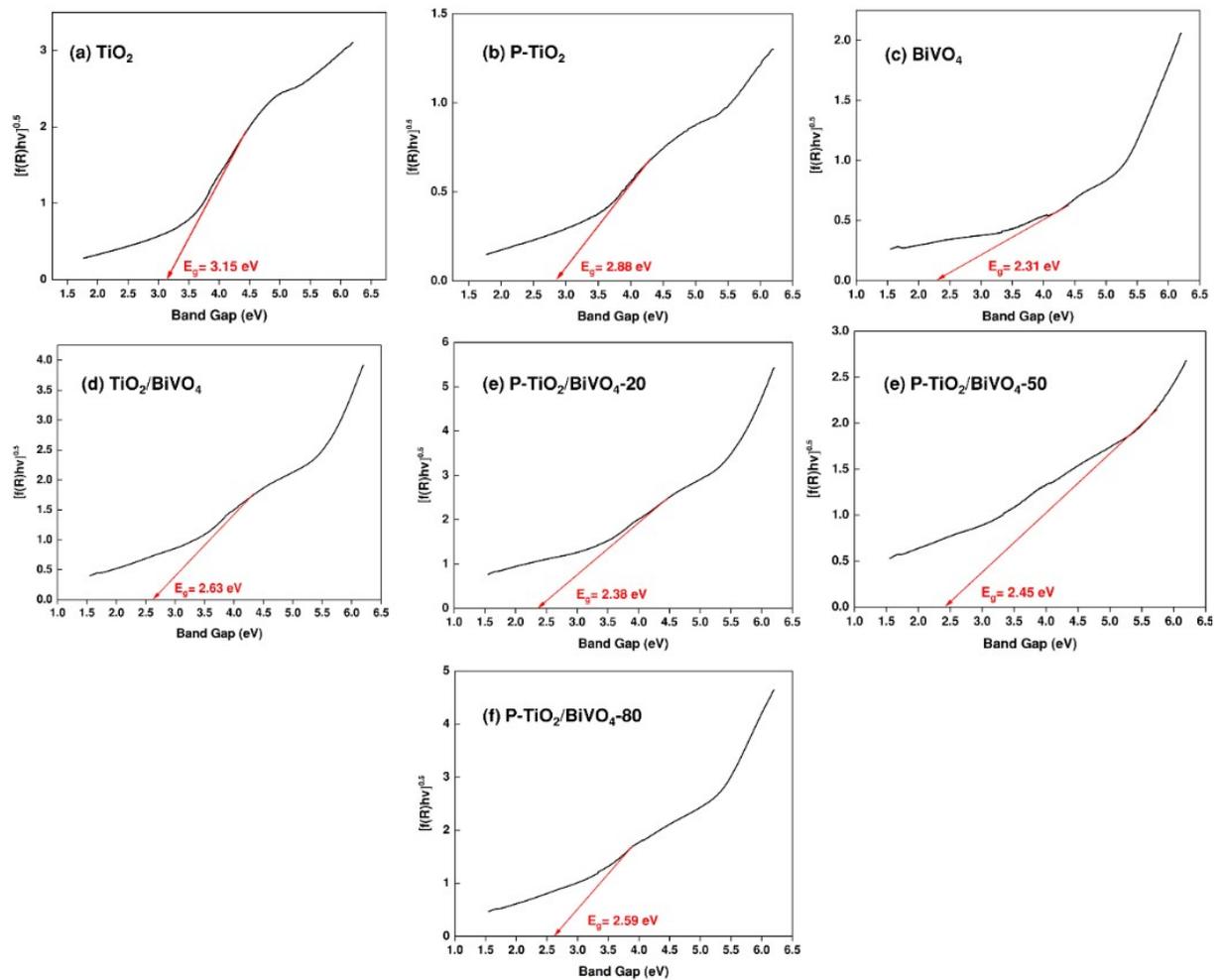
35

36

37



38 Figure S1. Graph of Absorbance vs Wavelength for the photocatalyst sample



40 Figure S2. Tauc Plots of the prepared photocatalysts.

41 The Tauc plots for photocatalysts were developed following the Tauc equation

$$42 (\alpha h\nu)^{1/n} = C \times (h\nu - E_g)$$

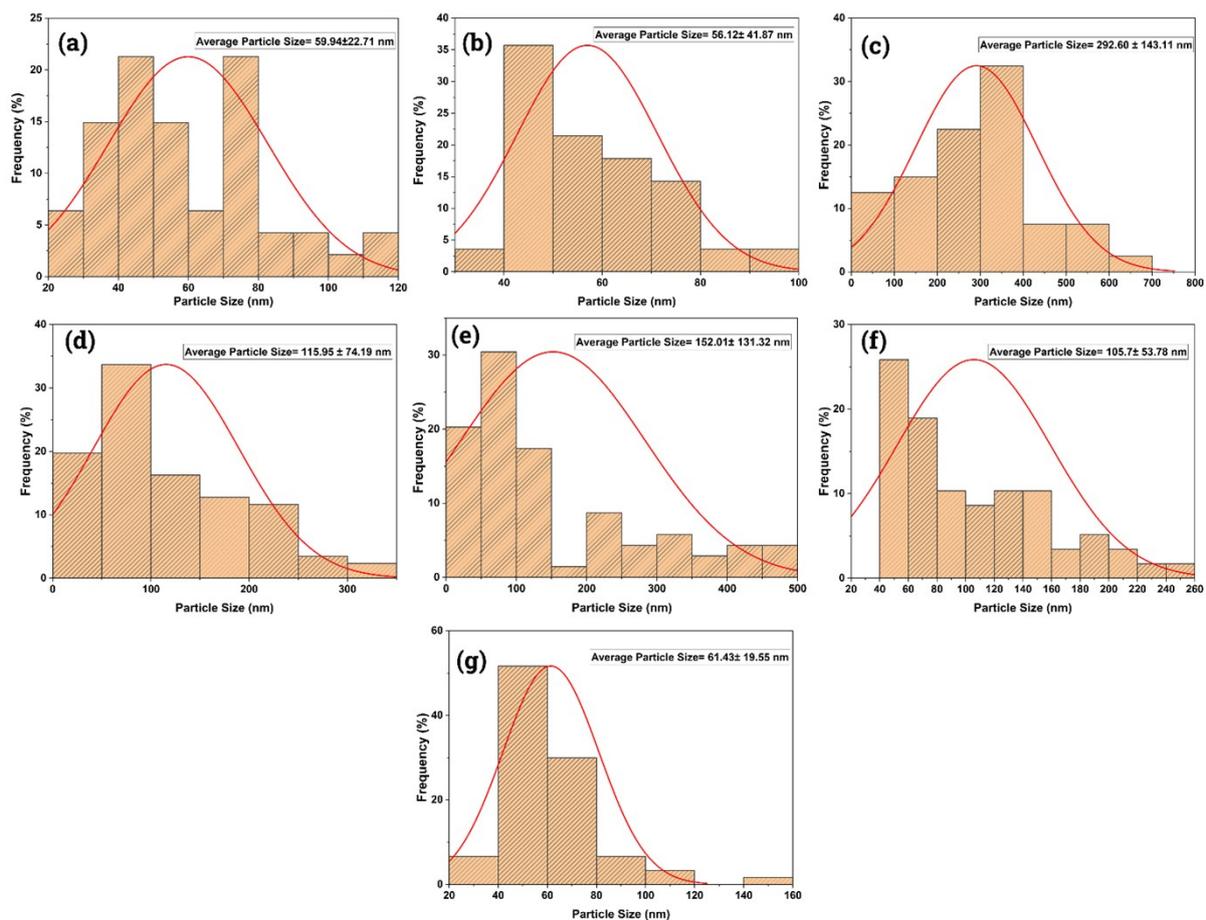
43 Here, for the photocatalyst, indirect electron transition was considered. Thus, the value of the

44 $n=2$. The resulting y-axis is to be $(\alpha h\nu)^{0.5}$ in the Tauc plots.

45

46

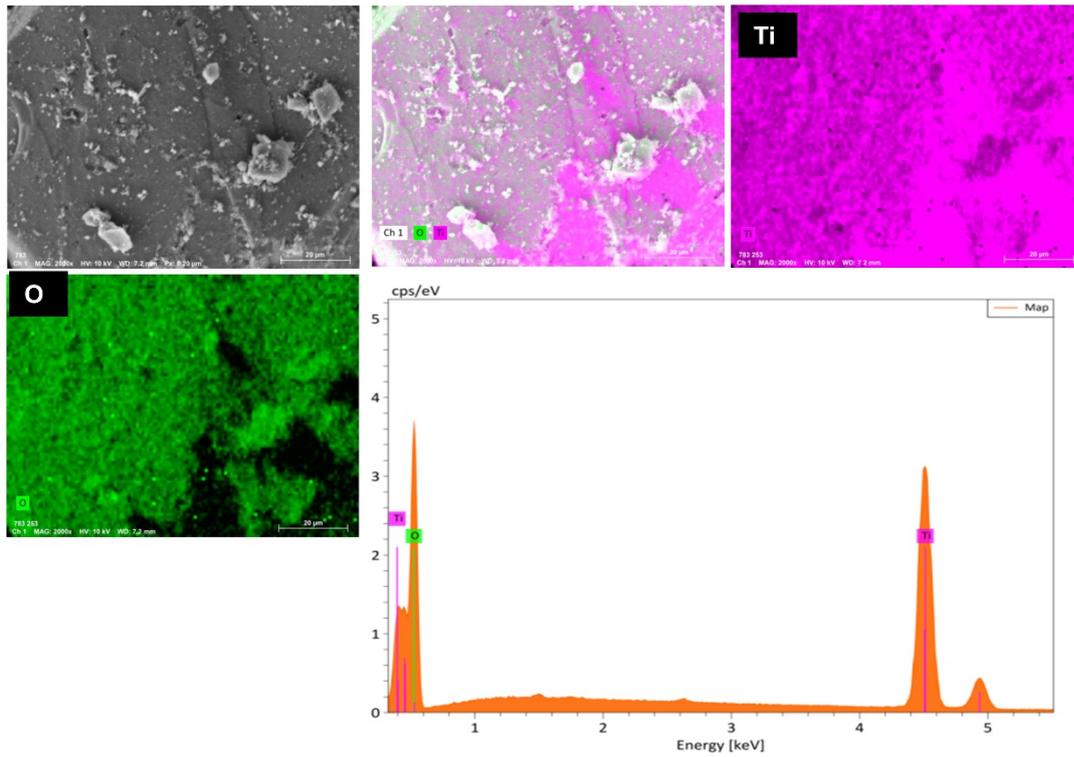
47



48

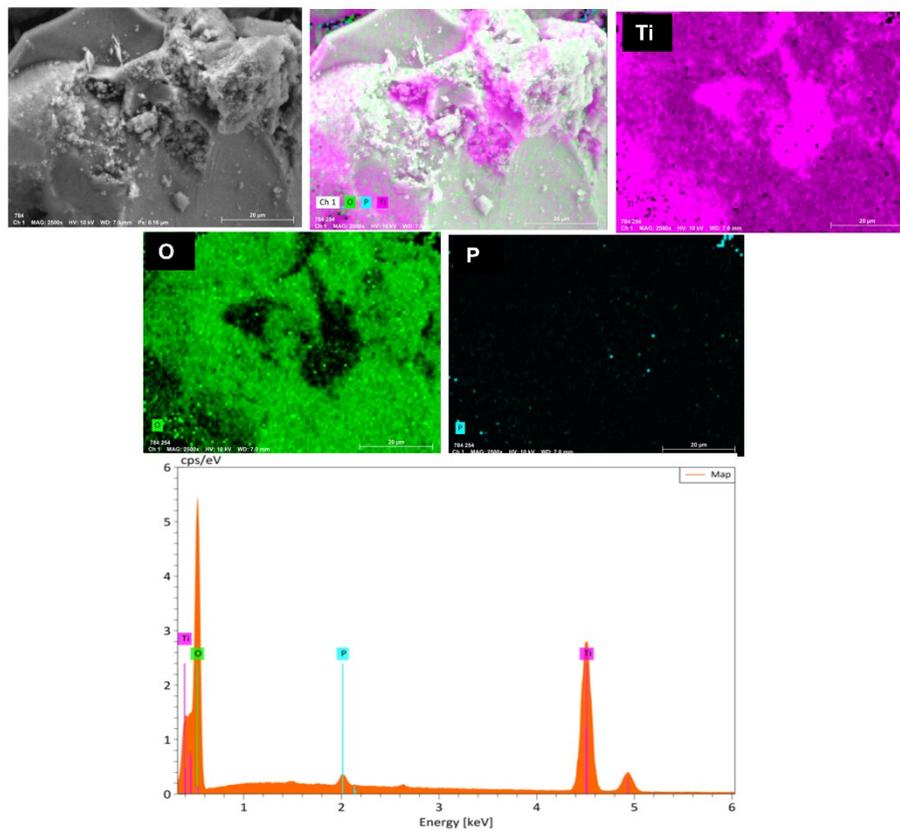
49 Figure S3. Particle size distribution of TiO_2 (a), P- TiO_2 (b), BiVO_4 (c), $\text{TiO}_2/\text{BiVO}_4$ (d), P-
 50 $\text{TiO}_2/\text{BiVO}_4$ -20 (e), P- $\text{TiO}_2/\text{BiVO}_4$ -50 (f), and P- $\text{TiO}_2/\text{BiVO}_4$ -80 (g).

51



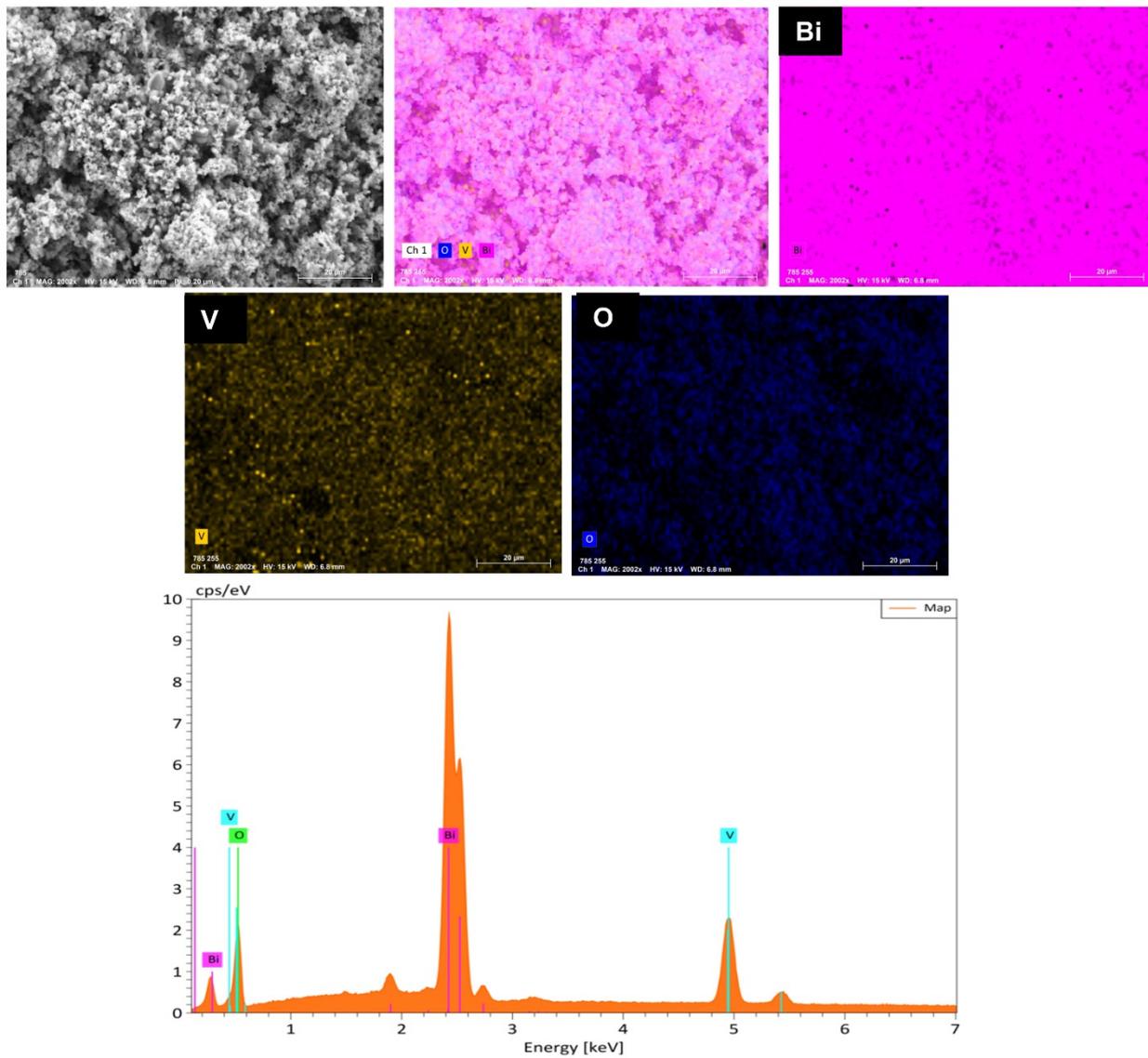
52
53
54

Figure S4. EDX Mapping and Spectra of TiO_2



55
56

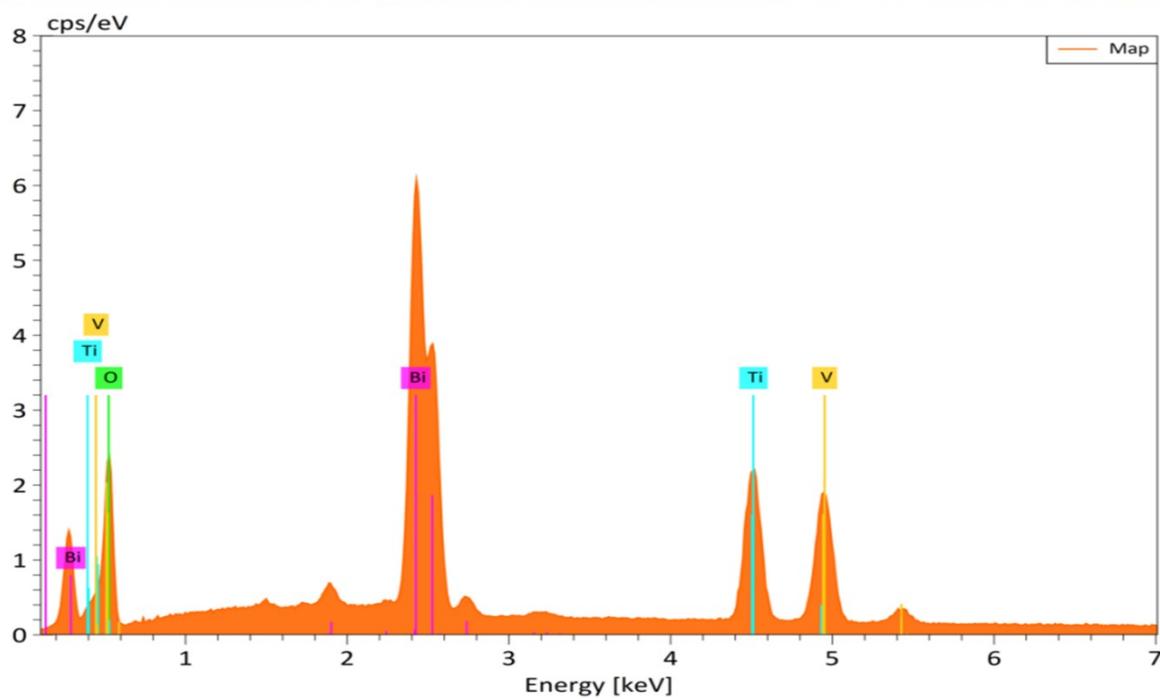
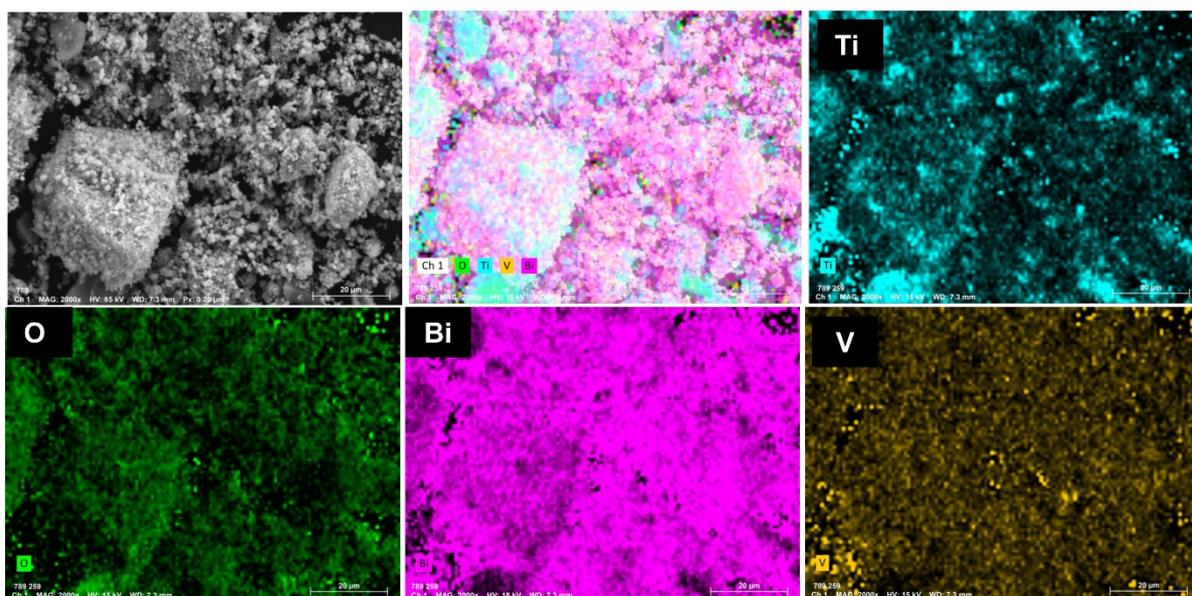
Figure S5. EDX Mapping and Spectra of P-TiO_2



57

58

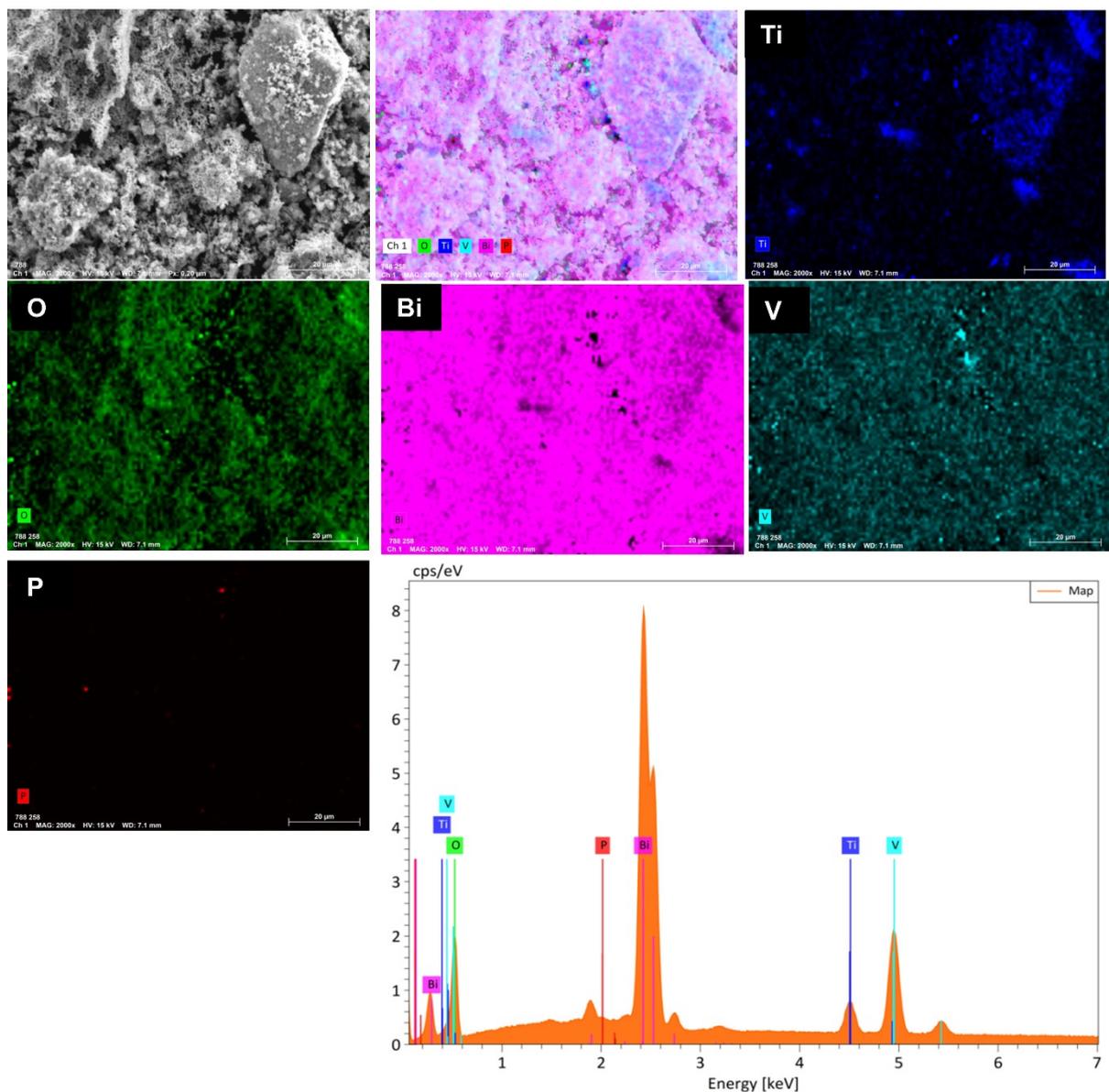
Figure S6. EDX Mapping and Spectra of BiVO₄



59

60

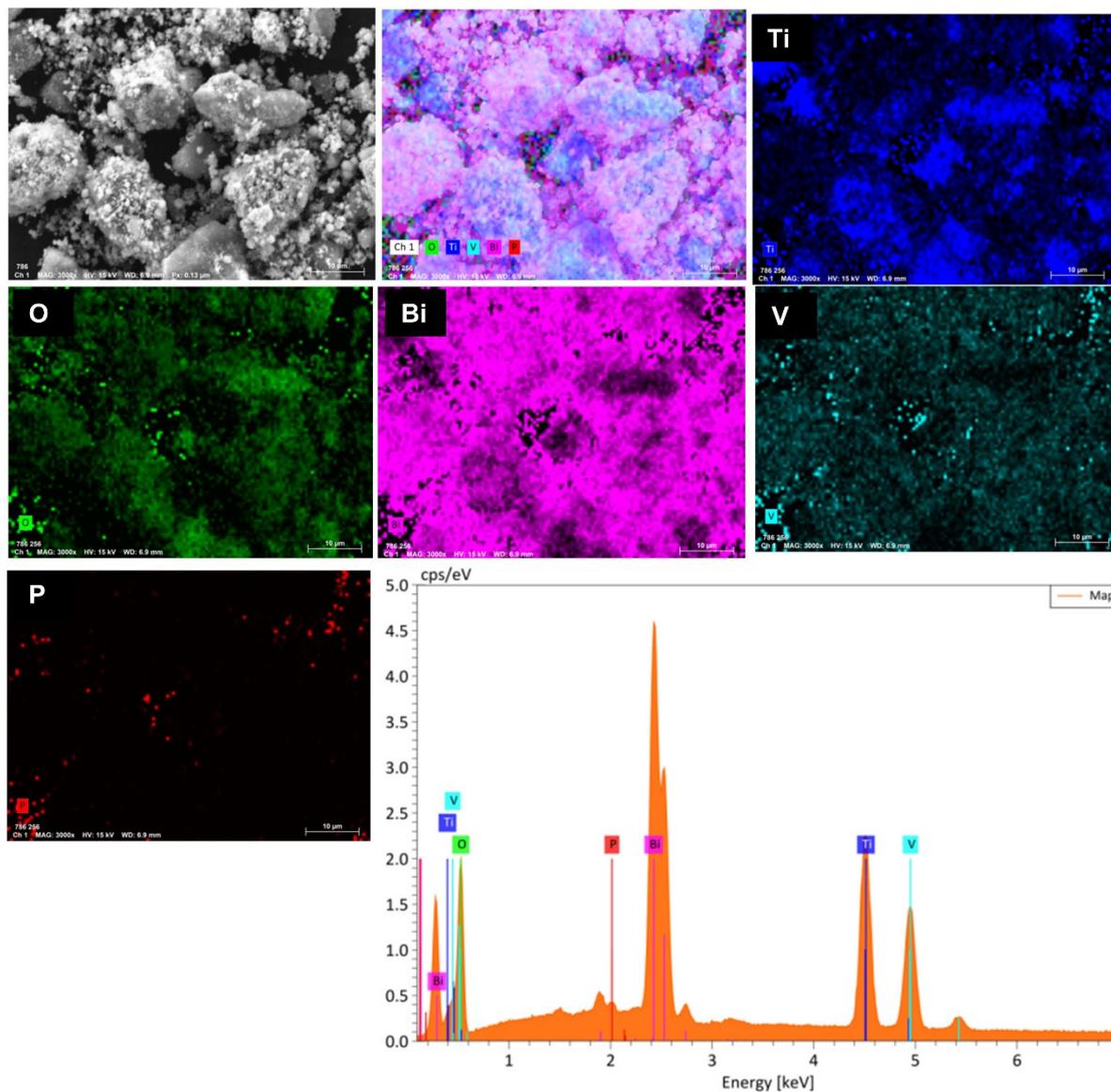
Figure S7. EDX Mapping and Spectra of $\text{TiO}_2\text{-BiVO}_4$



61

62

Figure S8. EDX Mapping and Spectra of P-TiO₂/BiVO₄-20.



63

64

Figure S9. EDX Mapping and Spectra of P-TiO₂/BiVO₄-50

65

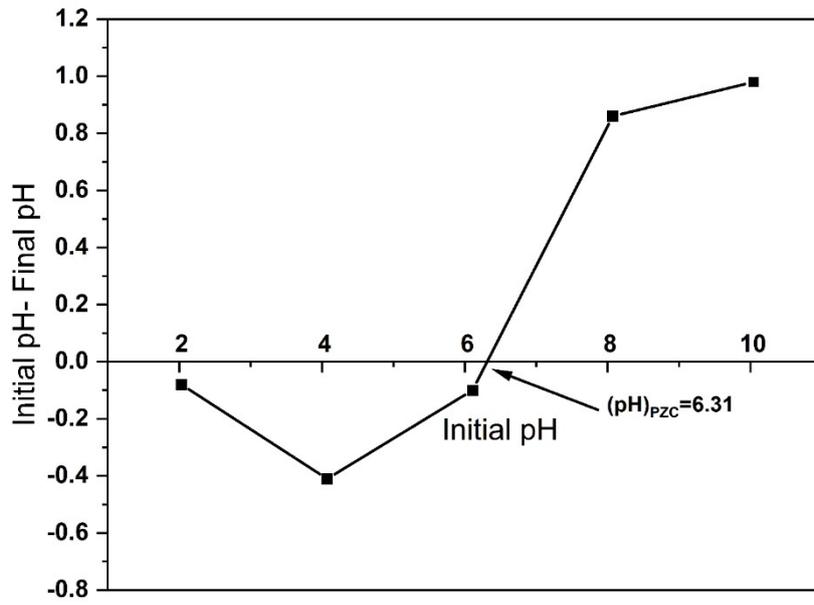


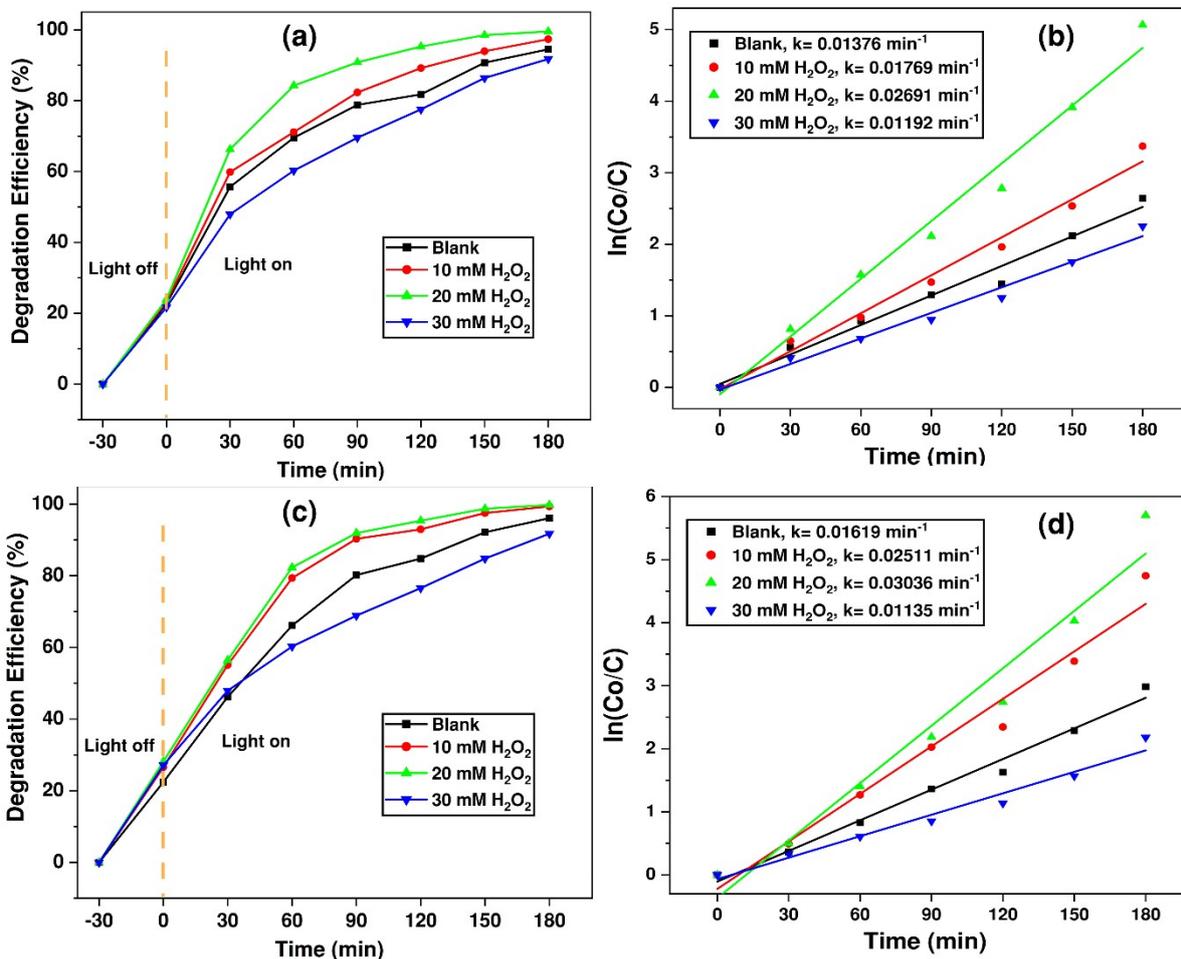
Figure S10. Determination of pH at Point of Zero Charge for P-TiO₂/BiVO₄-80.

67
 68
 69
 70
 71
 72
 73
 74
 75
 76
 77
 78
 79
 80
 81
 82
 83
 84
 85
 86
 87

88

89

90



91

92 Figure S10. Degradation Efficiency vs time for (a) CIP, (c) MNZ, and Kinetic study for (b)
93 CIP, (d) MNZ for different concentrations of H₂O₂ using P-TiO₂/BiVO₄-80. (Experimental
94 Conditions: 20 mg/L of pollutant concentration, 1 g/L of catalyst dosage, and natural pH)

95

96

97

98

99

100

101 **Supporting Tables**

102 Table S1. The two-tailed Pearson correlation matrix for the crystal size and the bandgap of the
 103 prepared seven photocatalysts with the elemental composition. **Correlation is significant at
 104 the 0.01 level (2-tailed).

	Ti	O	P	Bi	V	Crystal Size
Ti	1					
O	0.706	1				
P	0.509	0.530	1			
Bi	-0.992**	-0.685	-0.574	1		
V	-0.990**	-0.680	-0.574	0.996**	1	
Crystal Size	-0.889**	-0.743	-0.579	0.901**	0.865	1
	Ti	O	P	Bi	V	Band Gap
Ti	1					
O	0.706	1				
P	0.509	0.530	1			
Bi	-0.992**	-0.685	-0.574	1		
V	-0.990**	-0.680	-0.570	0.996**	1	
Band Gap	0.899**	0.522	0.147	-0.886**	-0.879**	1

105

106

107

108

109

Table S2. Summary of kinetic parameters for CIP degradation.

Photocatalyst Samples	Zero Order		1 st Order		2 nd Order	
	Rate constant, k_0 (mg.L ⁻¹ .min ⁻¹)	R ²	Rate constant, k_1 (min ⁻¹)	R ²	Rate constant, k_2 (L.mg ⁻¹ .min ⁻¹)	R ²
TiO ₂	0.035	0.979	0.0028	0.989	0.0002	0.989
P-TiO ₂	0.042	0.981	0.0037	0.992	0.0003	0.983
BiVO ₄	0.024	0.910	0.0014	0.988	0.0001	0.959
TiO ₂ / BiVO ₄	0.055	0.938	0.0060	0.981	0.0007	0.969
P-TiO ₂ / BiVO ₄ -20	0.064	0.944	0.0083	0.991	0.0012	0.931
P-TiO ₂ / BiVO ₄ -50	0.068	0.910	0.0105	0.983	0.0021	0.875
P-TiO ₂ / BiVO ₄ -80	0.071	0.859	0.0138	0.981	0.0041	0.831

110

111

Table S3. Summary of kinetic parameters for MNZ degradation.

Photocatalyst Samples	Zero Order		1 st Order		2 nd Order	
	Rate constant, k_0 (mg.L ⁻¹ .min ⁻¹)	R ²	Rate constant, k_1 (min ⁻¹)	R ²	Rate constant, k_2 (L.mg ⁻¹ .min ⁻¹)	R ²
TiO ₂	0.034	0.982	0.003	0.986	0.0002	0.974
P-TiO ₂	0.042	0.986	0.004	0.993	0.0003	0.981
BiVO ₄	0.029	0.944	0.002	0.985	0.0001	0.983
TiO ₂ / BiVO ₄	0.0591	0.971	0.006	0.987	0.0007	0.942
P-TiO ₂ / BiVO ₄ -20	0.0674	0.952	0.009	0.984	0.0014	0.876
P-TiO ₂ / BiVO ₄ -50	0.0725	0.951	0.011	0.980	0.0024	0.803
P-TiO ₂ / BiVO ₄ -80	0.0789	0.905	0.016	0.987	0.0058	0.767

112

113

114

115

116

117

118

119

120

121

122

123

Table S4. Table for rate constant and R²-values obtained from first-order kinetics of photodegradation of CIP and MNZ using P-TiO₂/BiVO₄-80 for different experimental conditions.

Influencing Factors	Values	MNZ		CIP	
		Rate constant, min ⁻¹	R ²	Rate constant, min ⁻¹	R ²
pH	Natural pH	0.0162	0.9868	0.0132	0.9809
	pH 3	0.0089	0.9807	0.0079	0.9847
	pH 10	0.0107	0.9879	0.0088	0.9807
Initial Pollutant Concentration	10 mg/L	0.0162	0.9868	0.0148	0.9860
	20 mg/L	0.0196	0.9743	0.0132	0.9809
	30 mg/L	0.0107	0.9879	0.0088	0.9807
Catalyst Dosage	0.8 g/l	0.0162	0.9868	0.0085	0.9810
	1 g/l	0.0203	0.9778	0.0132	0.9809
	1.2 g/l	0.0098	0.9804	0.0151	0.9816
	1.4 g/l	0.0094	0.9847	0.0099	0.9831
H₂O₂ Concentration	Blank	0.0162	0.9868	0.0138	0.9809
	10 mM	0.0251	0.9711	0.0177	0.9868
	20mM	0.0304	0.9647	0.0269	0.9841
	30mM	0.0113	0.9727	0.0119	0.9838

124

125