

Electronic Supporting information

**Synthesis of highly crystalline LaFeO₃ nanospheres for
phenoxazinone synthase mimicking activity**

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S1. Calculation of CB and VB potentials for LaFeO₃.

$$\text{La} \quad E_{\text{IE}} = 538.1 \text{ kJ/mol} \div 96.48 = 5.577 \text{ eV}$$

$$E_{\text{EA}} = 48 \text{ kJ/mol} \div 96.48 = 0.498 \text{ eV}$$

$$\chi_{\text{La}} = 1/2(5.577+0.498) = 3.0375 \text{ eV}$$

$$\text{Fe} \quad E_{\text{IE}} = 762.5 \text{ kJ/mol} \div 96.48 = 7.9 \text{ eV}$$

$$E_{\text{EA}} = 14.78 \text{ kJ/mol} \div 96.48 = 0.153 \text{ eV}$$

$$\chi_{\text{Fe}} = 1/2(7.9 \text{ eV} + 0.153) = 4.02 \text{ eV}$$

$$\text{O} \quad E_{\text{IE}} = 1313.9 \text{ kJ/mol} \div 96.48 = 13.618 \text{ eV}$$

$$E_{\text{EA}} = 140.97 \text{ kJ/mol} \div 96.48 = 1.461 \text{ eV}$$

$$\chi_{\text{O}} = 1/2(13.618+1.461) = 7.54 \text{ eV}$$

$$\chi_{\text{LaFeO}_3} = (3.0375 \times 4.02 \times (7.54)^3)^{1/5} = 5.54 \text{ eV}$$

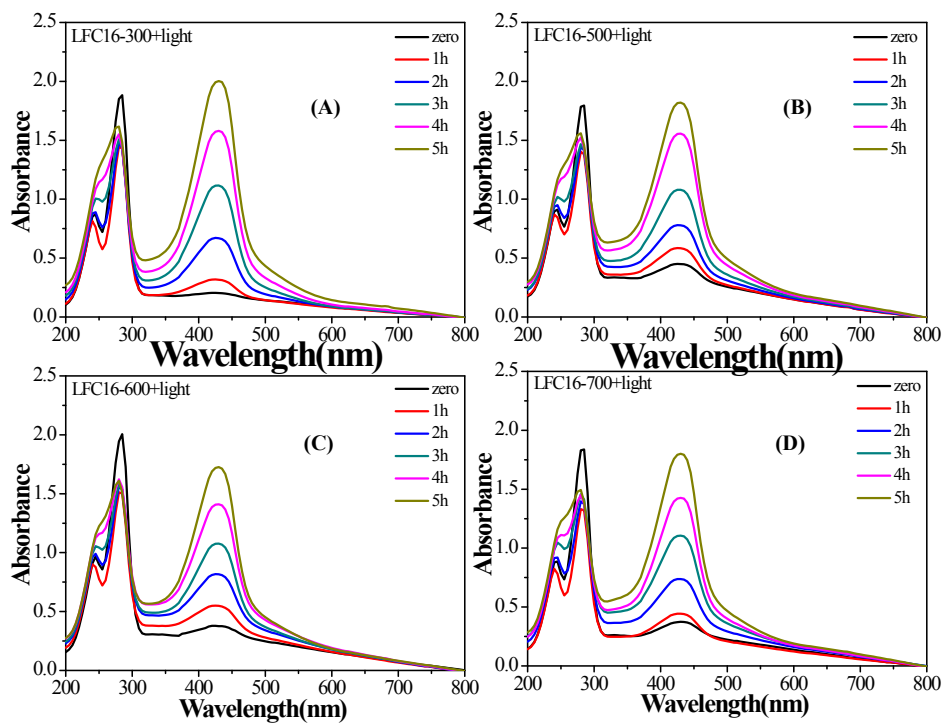


Figure S2. UV/Vis spectra of photocatalytic conversion of OAP over LFC16 at different calcination temperatures (A) 300 °C, (B) 500 °C, (C) 600 °C, and (D) 700 °C in ethanoic solution under nitrogen atmosphere.

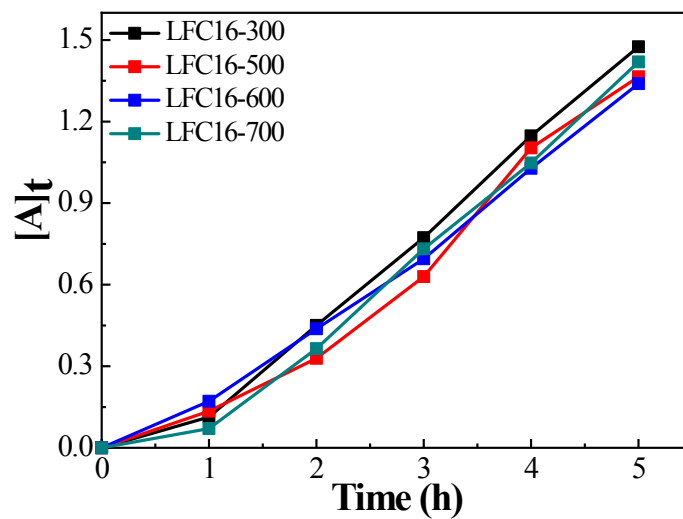


Figure S3. Analysis of absorbance time dependence in ethanol/water under nitrogen atmosphere using LaFeO_3 synthesized at different annealing temperatures under solar irradiation.

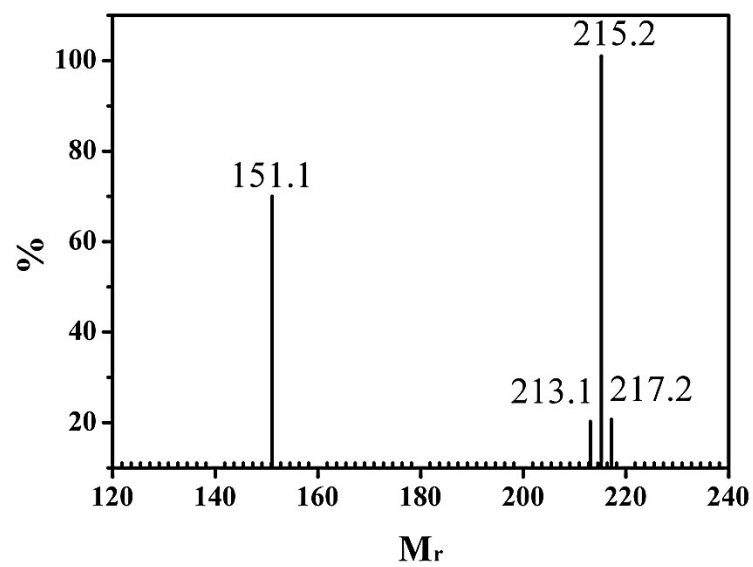


Figure S4. Mass spectra of isolated oxidation reaction products of *o*-aminophenol.

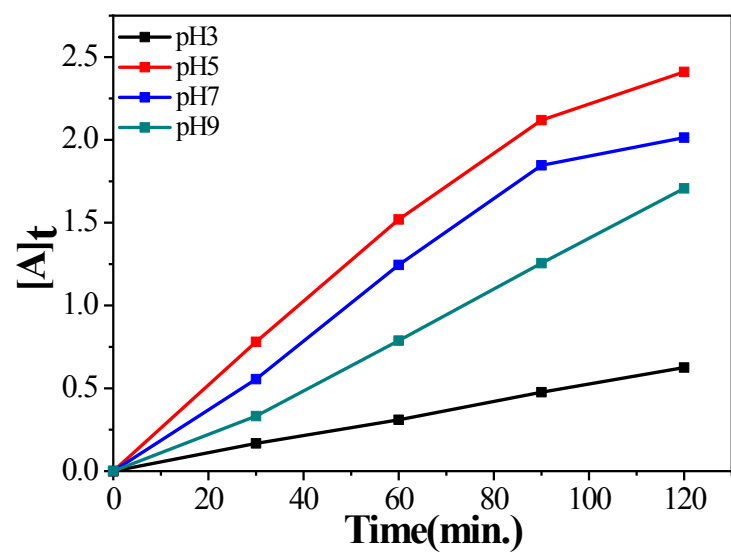


Figure S5. Effect of solution pH on the photocatalytic conversion of OAP to APX over LFC4 in acetonitrile/water solvent under nitrogen atmosphere under solar irradiation.

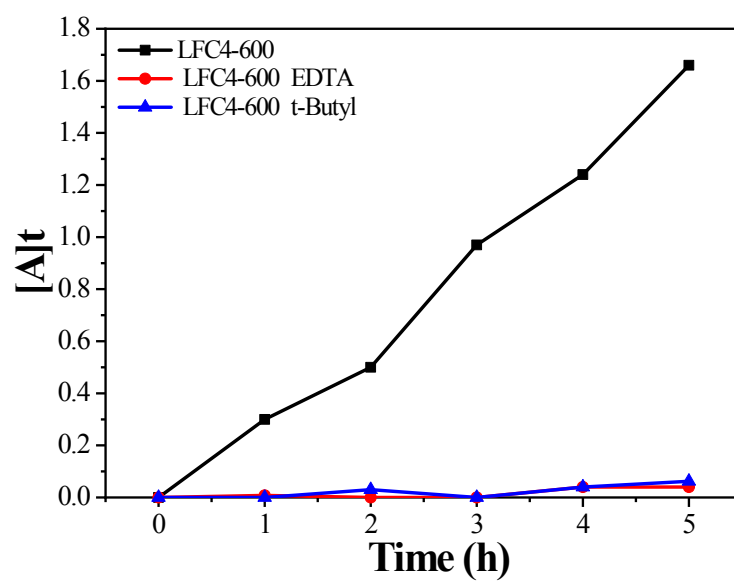


Figure S6. Effect of scavenger on the photocatalytic conversion of OAP to APX over LFC4-600 in acetonitrile/water solvent under nitrogen atmosphere under solar irradiation.

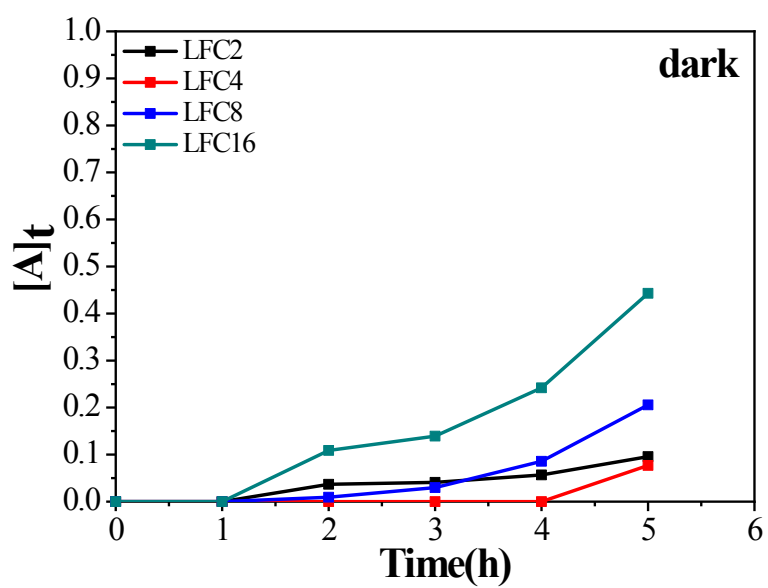


Figure S7. Analysis of absorbance time dependence in acetonitrile/water under nitrogen atmosphere using LaFeO_3 synthesized in dark.

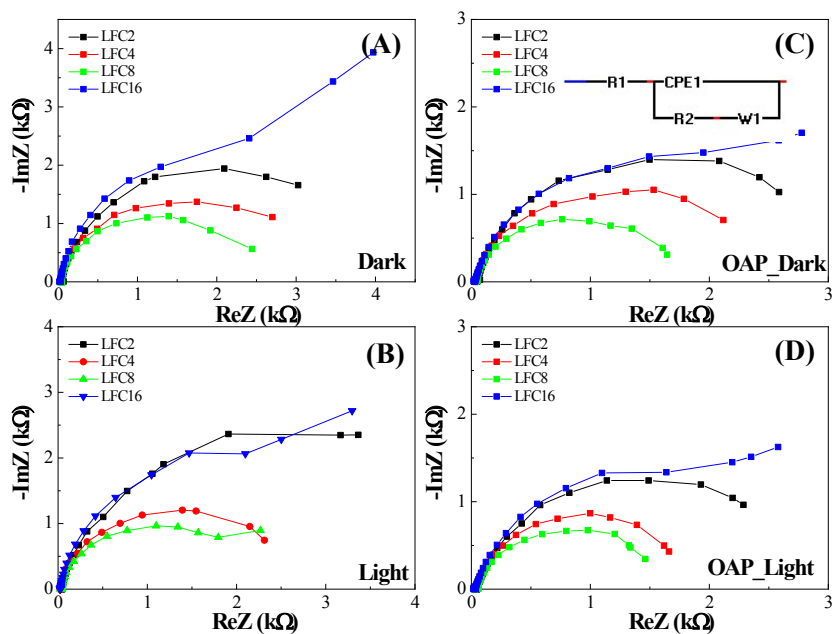


Figure S8. Nyquist plot of LaFeO₃ in (A, and B) absence and (C, and D) presence of 0.5 mM OAP in 0.1 M Na₂SO₄ at E_{DC} = 0.5 V vs. Ag/AgCl, E_{AC} = 10 mV (peak to peak) and frequency range of 100 kHz to 3 Hz.

Table S8. Electrochemical impedance analysis of LaFeO₃ samples.

	LFC2				LFC4				LFC8				LFC16			
	Dark	Light	OAP Dark	OAP Light	Dark	Light	OAP Dark	OAP Light	Dark	Light	OAP Dark	OAP Light	Dark	Light	OAP Dark	OAP Light
R1 (Ω)	28	30	40	35	24	23	23	21	26	28	33	40	20	24	23	20
R2 (kΩ)	4	4	3.1	2.75	3.1	2.6	2.1	1.85	2.45	2.1	1.6	1.5	3.2	4.4	2.7	2.6
W (Ωs ⁻¹)	17	80	3	22	17	9	25	20	13	9	13	8	185	60	70	60
P1 (μF)	0.02	0.01	0.016	0.07, .013	0.02	0.018	0.02	0.02	0.02	0.018	0.014	0.018	0.013	0.02	0.012	0.012
n1	0.93	0.9	0.93	0.88	0.93	0.93	0.91	0.89	0.93	0.93	0.9	0.89	0.97	0.93	0.91	0.9

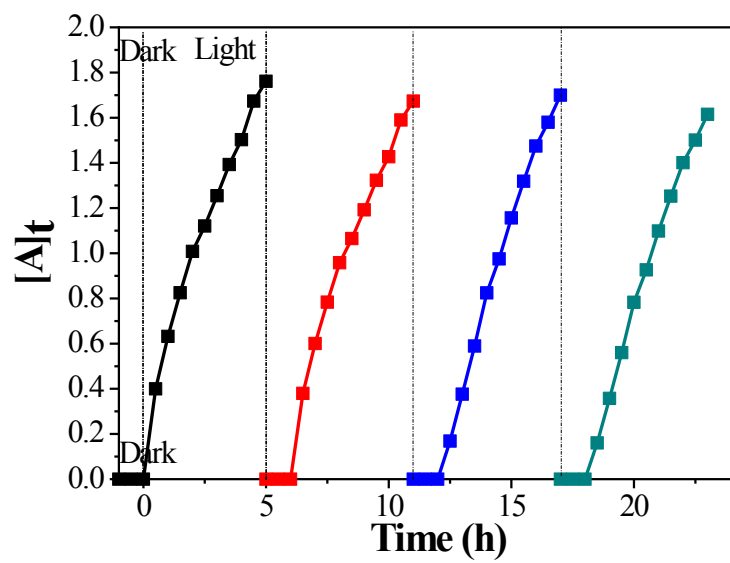


Figure S9. Reusability of LFC4 for photocatalytic conversion of OAP in acetonitrile/water under nitrogen atmosphere.