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Effect of UV irradiation on the Structural Variation of Metal Oxide-Silica Nanocomposites for Enhanced Removal of Erythromycin at Neutral pH

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ERY degradation kinetics can be calculated by the pseudo-first-order kinetic model($\mathrm{Ln}(C_0/C_t)=k_{app}t$), where C_0 and C_t are the ERY concentration at $t = 0$ and t, respectively. The K_{app} is the apparent rate constant (min^{-1}). The $\ln(C_0/C_t)$ versus t plots for heterogeneous photo-Fenton systems have been shown in Supplementary Figure 1a. The kinetic parameters (K_{app}), and linear regression value (R^2) were estimated 1.13 min^{-1} and 0.98, respectively.

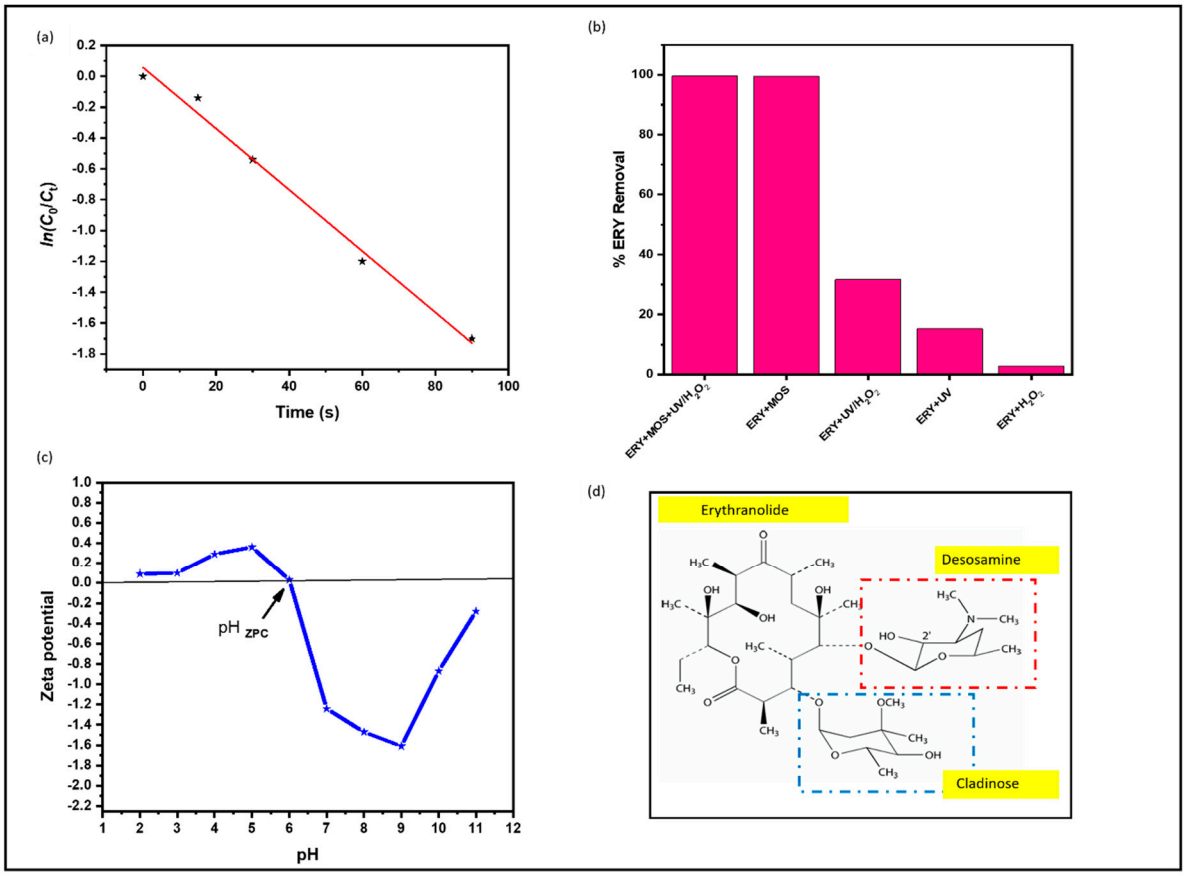

Figure S1. (a) Degradation kinetic modeling of ERY under UV/H_2O_2/MOS system, (b) Removal of ERY using pristine nanocomposite, (c) Zeta potential of MOS, (d) Chemical structure of ERY

Possible mechanisms for degradation of ERY:

Scavenger studies: To identify the main active species responsible for ERYdegradation, the radical scavenging test was performed using EDTA as quenching agent for the holes (h^+), $K_2Cr_2O_7$ for the electrons (e^-), p-benzoquinone for superoxides ($^{\bullet}O_2^-$), tert-butanol for hydroxyl radical ($^{\bullet}OH$), and, KI for surface-bound $^{\bullet}OH$ ($^{\bullet}OH_{surf}$). The experiments were performed at the same conditions as mentioned in the main manuscript, but 2 mg L^{-1} of scavengers were added to the solution in this experiment. The results have been shown in Supplementary Figure 2. As shown in the figure, only 15.8% and 18.53 % of ERY were removed after adding

of KI and tert-butanol to the solution, but more than 70% ERY degradation was observed in the presence of other scavengers. These results indicate that both $^{\bullet}OH$ radicals and ($^{\bullet}OH_{surf}$) played an essential role in the degradation and other scavengers had a less important role . All the possible reactions involved in degradation are as follows:

$$Fe_2O_3 + h\nu \rightarrow Fe_2O_3^*(e_{CB}^- + h_{VB}^+) \quad (1)$$

$$Mn_2O_3 + h\nu \rightarrow Mn_2O_3^*(e_{CB}^- + h_{VB}^+) \quad (2)$$

$$e_{CB}^-(Fe_2O_3) \rightarrow e_{CB}^-(Mn_2O_3) \quad (3)$$

$$h_{VB}^+(Fe_2O_3) \rightarrow h_{VB}^+(Mn_2O_3) \quad (4)$$

$$Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + {}^{\bullet}OH + HO^- \quad (5)$$

$$Fe^{3+} + e_{CB}^- \rightarrow Fe^{2+} \quad (6)$$

$$Mn^{2+} + H_2O_2 \rightarrow Mn^{3+} + {}^{\bullet}OH + HO^- \quad (7)$$

$$Mn^{3+} + e_{CB}^- \rightarrow Mn^{2+} \quad (8)$$

$$H_2O_2 + e_{CB}^- \rightarrow {}^{\bullet}OH + HO^- \quad (9)$$

$$h_{VB}^+ + ERY \rightarrow [ERY^+]^* \rightarrow \text{degradation by} - \text{products} \quad (10)$$

$$H_2O + h_{VB}^+ \rightarrow {}^{\bullet}OH + H^+ \quad (11)$$

$$Mn_2O_3/Fe_2O_3(e^-) \rightarrow SiO_2((e_{CB}^-) \quad (12)$$

$$SiO_2((e_{CB}^-) + O_2 \rightarrow \bullet O_2^- \quad (13)$$

$$\bullet O_2^- + H_2O \rightarrow {}^{\bullet}OH + H^+ \quad (14)$$

$$O_2^{0-} + H^+ \rightarrow HO_2^0 \quad (15)$$

$$2HO_2^0 \rightarrow H_2O_2 + O_2 \quad (16)$$

$$H_2O_2 + e^- \rightarrow {}^{\bullet}OH + OH^- \quad (17)$$

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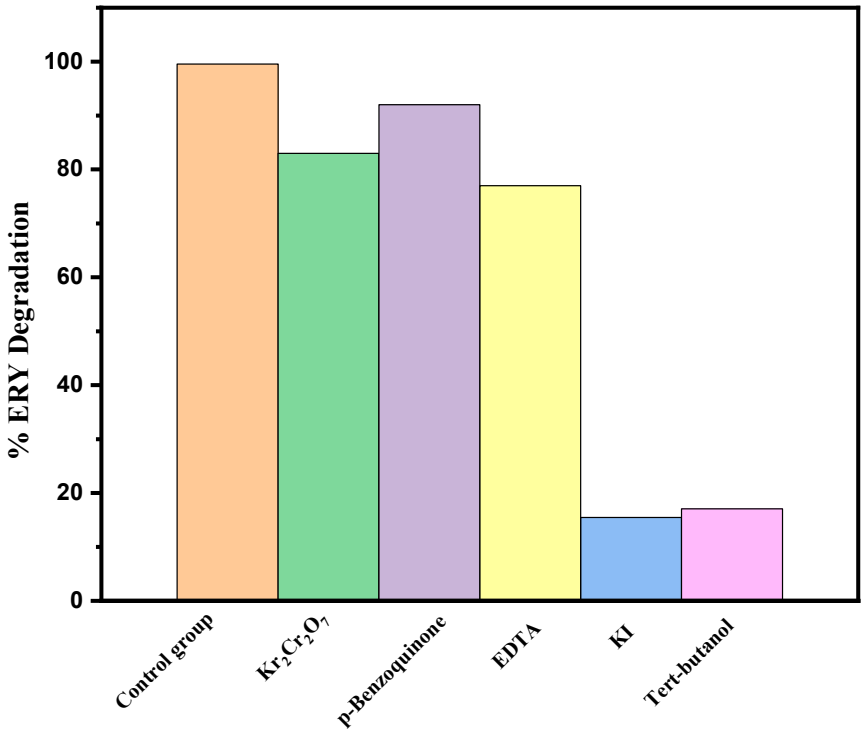

Figure S2. Radical scavenger experiment

Table S1. Detailed methodology for ERY analysis using LC/MS/MS

Instrument	Thermo Vanquish
Ion Source Type	H-ESI
Spray Voltage	Static
Positive Ion (V)	3500
Negative Ion (V)	2500

Sheath Gas (Arb)	50
Aux Gas (Arb)	10
Sweep Gas (Arb)	1
Ion Transfer Tube Temp (°C)	325
Vaporizer Temp (°C)	350
Column	Waters Cortects C18 (2.1x100, 1.6um)
Column Temp (°C)	45
Mobile phase A	0.1% Fumic acid in Distilled Water
Mobile phase B	0.1% Fumic acid in acetonitrile
Flow (ml/min)	0.5
Retention time (min)	3.38