Supporting Information

Minimization of electrical energy consumption in the photocatalytic reduction of Cr(VI) by using immobilized Mg, Ag co–impregnated TiO_2 nanoparticles

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Text S1.

3.1. Model analysis

The mathematical relationship of the response on these variables can be approximated by second–order polynomial equation as shown below:

$$Y = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_1x_2 + b_{13}x_1x_3 + b_{23}x_2x_3 + b_{11}x_1^2 + b_{22}x_2^2 + b_{33}x_3^2 \quad (1)$$

where Y is a predicted response of photocatalytic reduction efficiency, b_0 is the constant, b_1, b_2, and b_3 are the regression coefficients for linear effects, b_{12}, b_{13}, and b_{23} are the regression coefficients for interaction effects, b_1^2, b_2^2, and b_3^2 are the regression coefficients for squared effects and x_i is coded experimental levels of the Mg, Ag co–impregnated TiO_2 synthesis variables. Based on the results in Table 1, an empirical relationship between the response (Y) and independent synthesis variables (x_1, x_2, x_3, see Table S1) was attained as shown in Eq. (2):

$$Y = 67.47 - 6.78x_1 + 7.79x_2 + 4.49x_3 - 2.41x_1x_2 - 6.65x_1x_3 - 3.80x_2x_3 - 3.35x_1^2 - 8.33x_2^2 - 9.68x_3^2 \quad (2)$$

Equation (2) is used to predict the photocatalytic reduction of Cr(VI) by the Mg, Ag co–impregnated TiO_2 nanoparticles in a fixed–bed system with varied synthesis variables within the selected experimental ranges. By using resulted second–order polynomial equation (Eq. (2)), the predicted values of photocatalytic reduction of Cr(VI) is plotted versus corresponding experimental results in Figure S1. The results confirm that the predicted photocatalytic reduction rate from the model is in good agreement with the experimental results.

Analysis of variance (ANOVA) of the quadratic response surface model is a statistical procedure to test the significance and adequacy of the model.[1] Table S2 shows the ANOVA results for quadratic response surface model. According to the ANOVA results, the regression model present a high correlation coefficient ($R^2 = 0.9635$) for the photocatalytic reduction of Cr(VI). The value

of R^2 implies a satisfactory representation of photocatalytic reduction process by the model. Adjusted R^2 is also used to measure the goodness of fit between model and experimental data. Adjusted R^2 value (0.9027) was close to the corresponding R^2 value. The *F*–value, is the ratio between the mean square of the model and the residual error, and indicates the significance of each controlled factor on the tested model.[2] The *F*–value for the model is 13.22 and the corresponding *p*–value is <0.0001. These results indicated that the model was statistically significant and there is only a 0.01% chance that the "model *F*–value" could occur due to noise.

References:

1 H. L. Liu and Y. R. Chiou, *Chem. Eng. J.* 2005, **112**, 173–179.

2 F. Francis, A. Sabu, K. M. Nampoothiri, S. Ramachandran, S. Ghosh, G. Szakacs and A. Pandey, *Biochem. Eng. J.* 2003, **15**, 107–115.

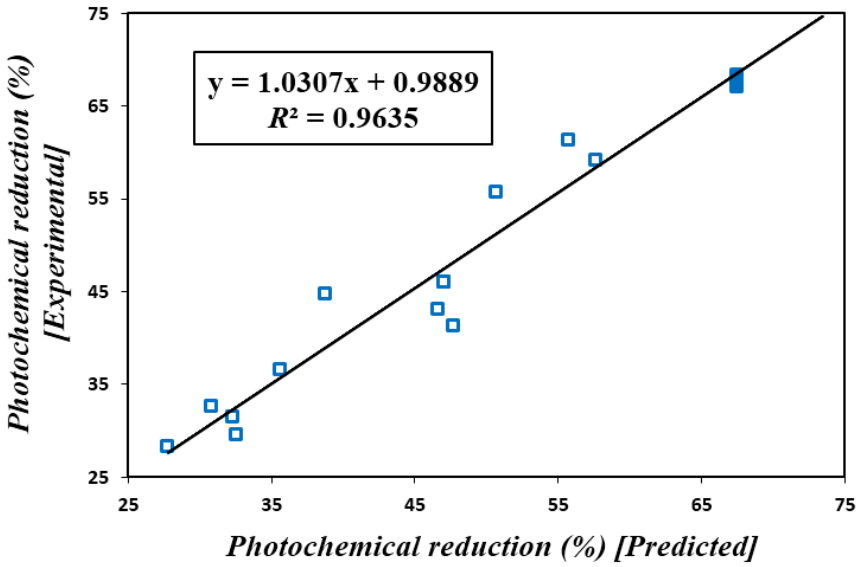

Figure S1. Comparison between predicted and experimental reduction rate of Cr(VI) by Mg, Ag co–impregnated TiO_2 nanoparticles.

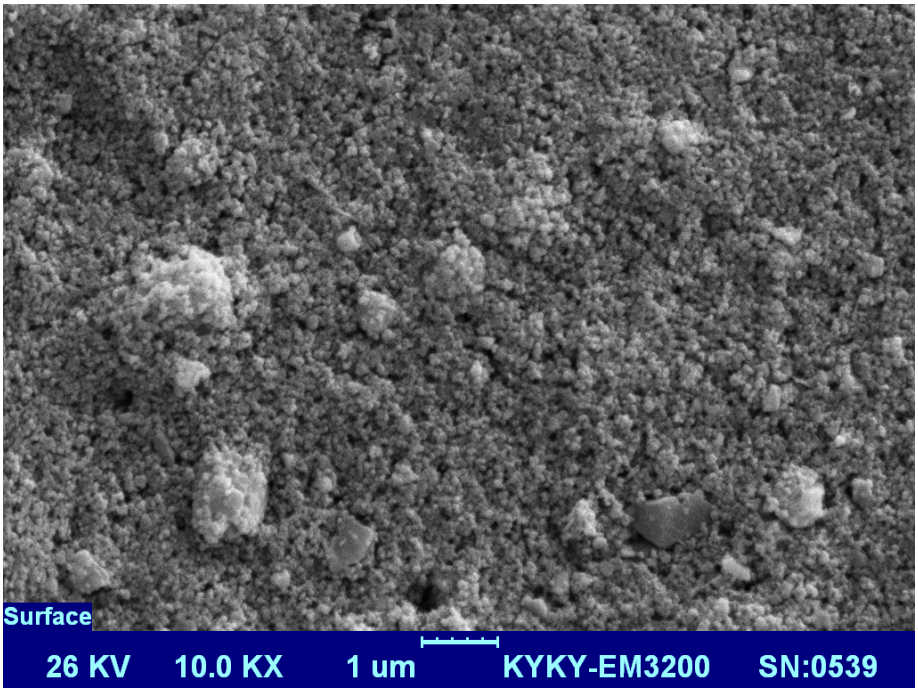

Figure S2. SEM micrograph of Mg, Ag co–impregnated TiO_2 nanoparticles immobilized nanoparticles on the glass plate, picture from the surface.

Table S1. Experimental ranges and levels of the synthesis variables.

Synthesis variables	Symbol	Ranges and levels				
	x_i	–2	–1	0	+1	+2
Mg concentration (wt%)	x_1	0	0.8	2	3.2	4
Ag concentration (wt%)	x_2	0	0.8	2	3.2	4
Calcination temperature (°C)	x_3	282	350	450	550	618

Table S2. ANOVA results of the response surface quadratic model for the photocatalytic reduction of Cr(VI).

Source of variations	Sum of squares	Degree of freedom	Mean square	*F*–Value	*p*–Value
Regression	4431.84	9	492.43	13.22	< 0.0001
Residual	372.41	10	37.24		
Total	4804.25	19			

R^2 = 0.9635, adjusted R^2 = 0.9027.