Supporting Information

Understanding the High Photocatalytic Activity of (B, Ag)-codoped TiO_2 under Solar-light Irradiation with XPS, Solid-state NMR and DFT Calculations

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****Calculation of NMR parameters:** The isotropic chemical shift (δ_{iso}) and quadrupolar interaction parameter (P_Q) were estimated by the center of gravity of the

signal corresponding to the F1 and F2 axes (designated by δ_{F1} and δ_{F2}) observed in the 3QZ-FAM MAS NMR spectra (sheared) recorded at 9.4T in Figure 3 (see main text) using the following equations:

$$\delta_{iso} = \frac{17}{27}\delta_{F1} + \frac{10}{27}\delta_{F2}; \quad \text{Eq. (S1)}$$

$$P_Q = \upsilon_0 \times \sqrt{\frac{17}{675000} \times (\delta_{F1} - \delta_{F2})} = QCC \times \sqrt{1 + \frac{\eta^2}{3}}, \quad \text{Eq. (S2)}$$

where υ_0 denote the Larmor frequency. Accordingly, the NMR parameters, *viz.* isotropic chemical shift (δ_{iso}), quadrupolar coupling constant (QCC), and asymmetry parameter (η) corresponding to various B sites may be extracted by fitting of the second-order quadrupolar line shape obtained from slices of the ^{11}B 3QZ-FAM MAS NMR spectra (Fig.5) using the Dimfit program.[S1] In turn, these NMR parameters were adopted to simulate the 1D NMR spectra in Figure 3.

References (Supporting Information):

(S1) Massiot, D.; Fayon, M.; Capron, I.; King, S.; Le Calve', B.; Alonso, J.-O.; Durand, B.; Bujoli, Z.; Gan, Z.; Hoatson G. *Magn. Reson. Chem.* **2002**, *40*, 70.

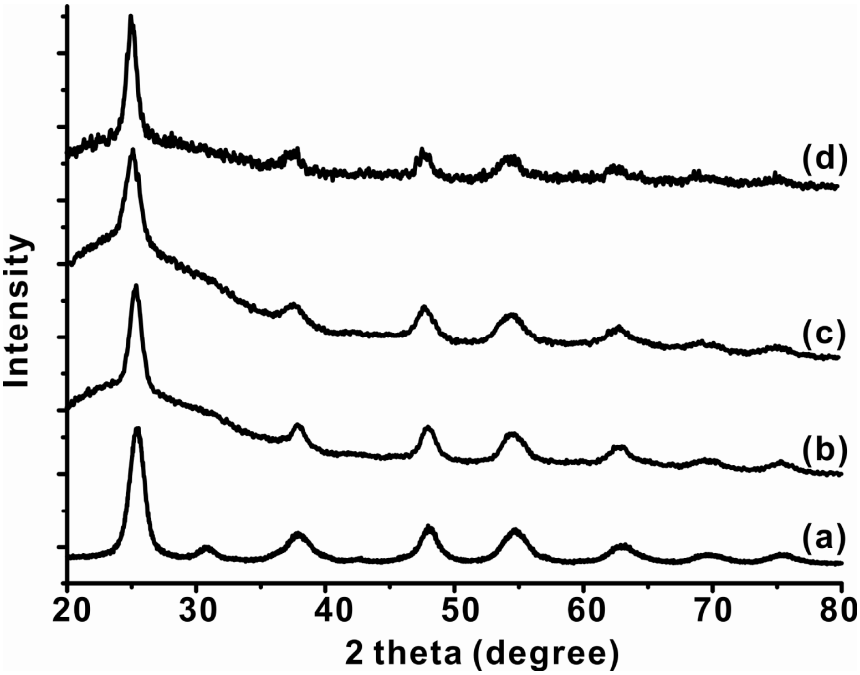

Figure S1. XRD spectra of (a) pure, (b) 3%Ag-doped, (c) 10%B-doped, and (d) (10%B, 3%Ag)-codoped TiO_2.

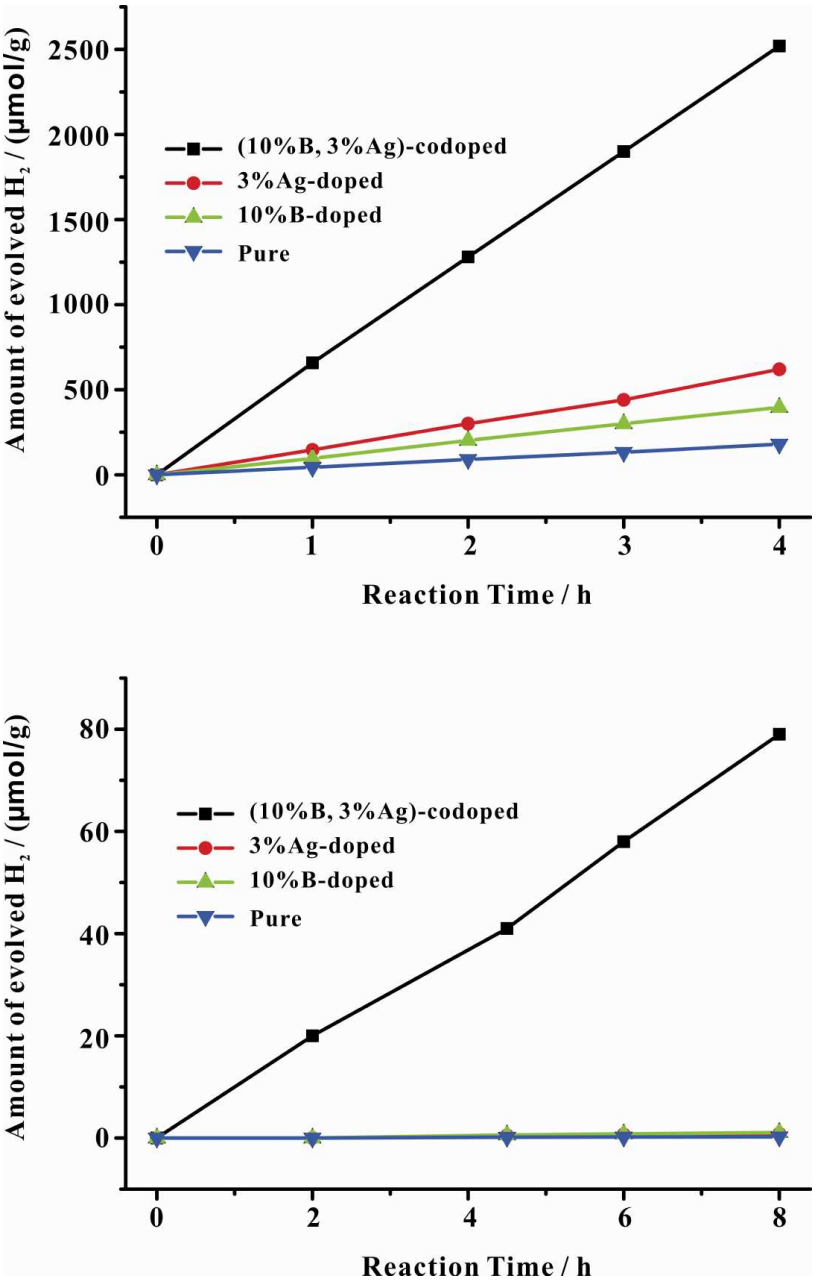

Figure S2. H_2 evolution from methanol solution (5.0 vol. %) in the suspension containing pure, B-doped, Ag-doped, and (B, Ag)-codoped TiO_2 catalysts (catalyst amount: 50 mg) under irradiation of (upper) UV-Vis light (Xe lamp, 300 W), and (bottom) visible light (Xe lamp with a 400 nm cut-on filter, λ>400 nm).

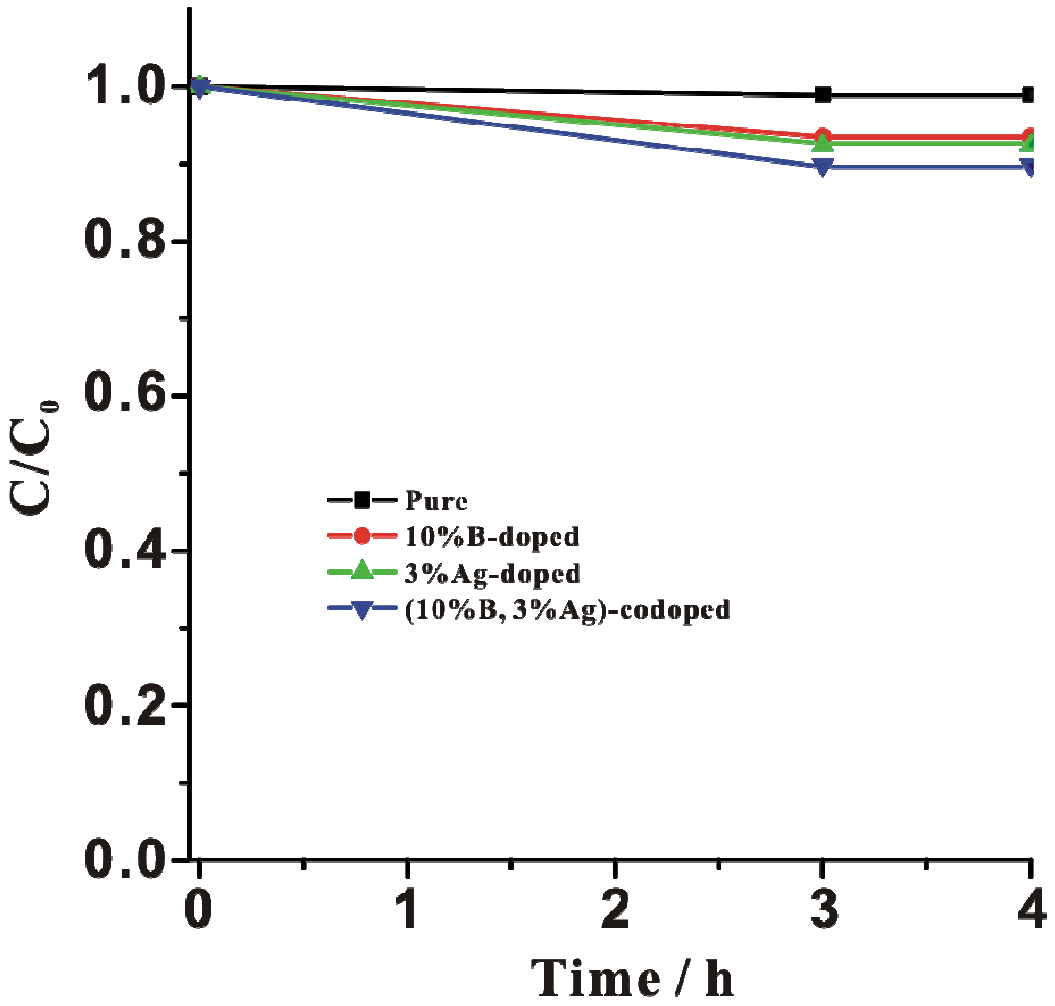

Figure S3. Adsorption curves of methylene blue on pure, 10% B-doped, 3% Ag-doped, and (10% B, 3% Ag)-codoped TiO_2 in dark. The concentrations of methylene blue were determined by the observed optical intensities at λ = 665 nm.

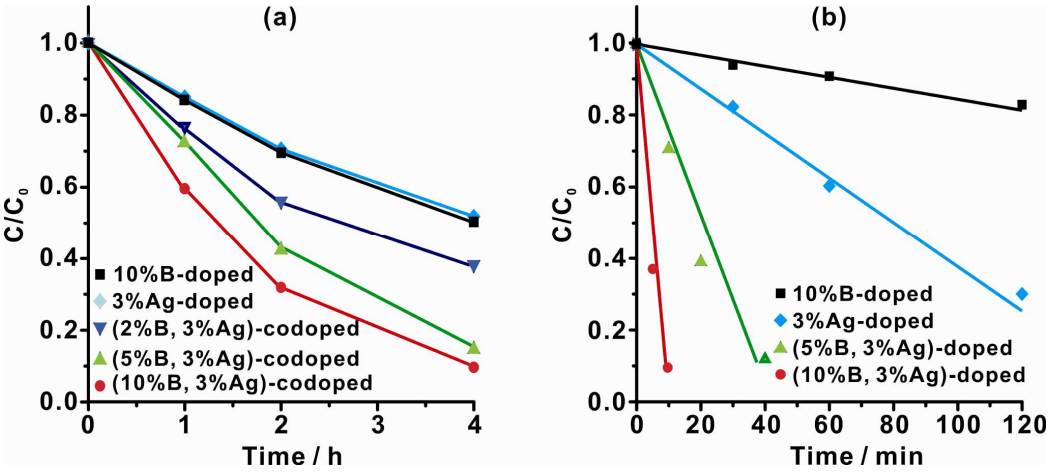

Figure S4. Photo-degradation curves of methylene blue on B-doped, Ag-doped, and (B, Ag)-codoped TiO_2 under irradiation of (a) visible-light ($\lambda > 420$ nm), and (b) solar-light. The concentrations of methylene blue were determined by the observed optical intensities at $\lambda = 665$ nm.

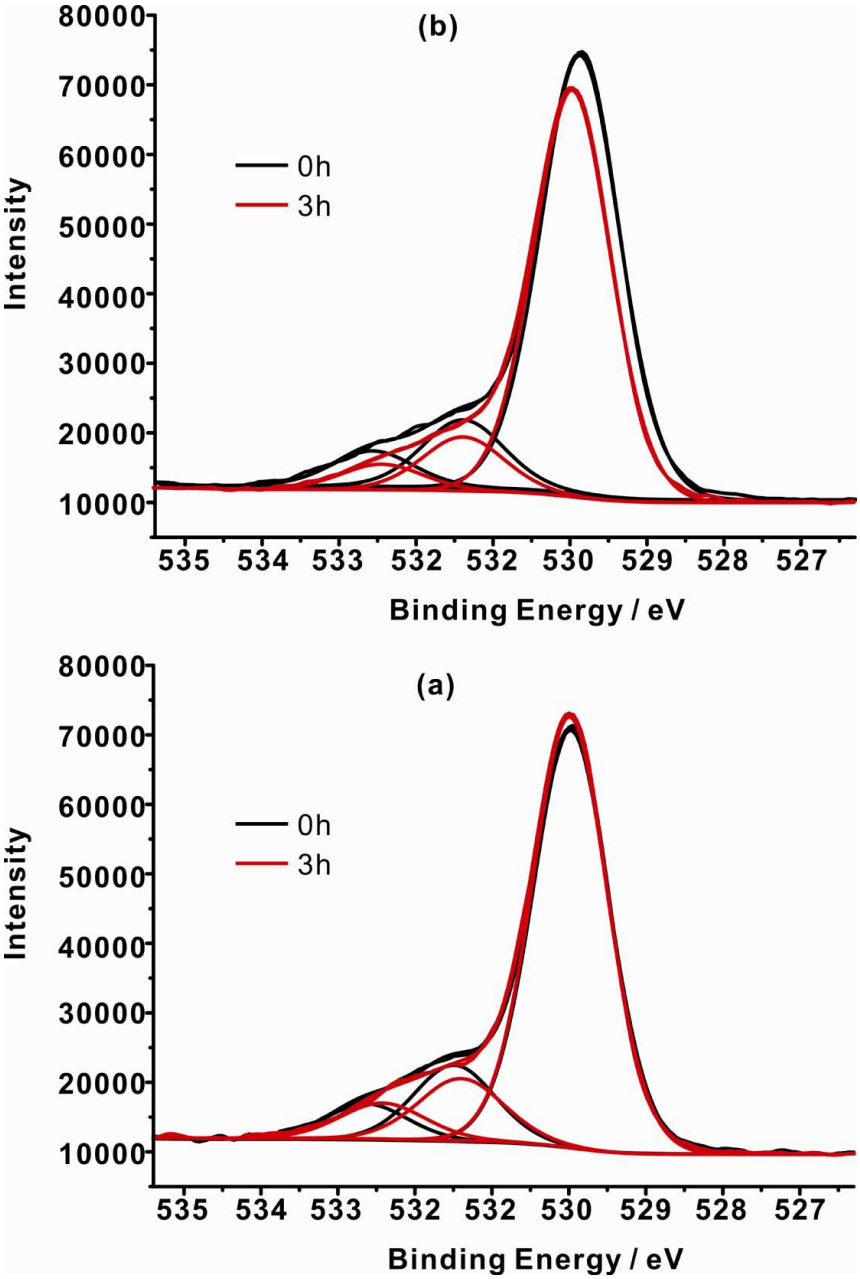

Figure S5. In-situ O 1s XPS spectra of (a) 3%Ag-doped and (b) (10%B, 3%Ag)-codoped TiO_2 samples before (black lines) and after (red lines) UV-Vis irradiation for 3 h.