Supporting Information

Photocatalytic Degradation/Adsorption of carcinogenic azo dye Disperse Red 176 by nanocage Cu_2O as a dual function catalyst on the visible-light

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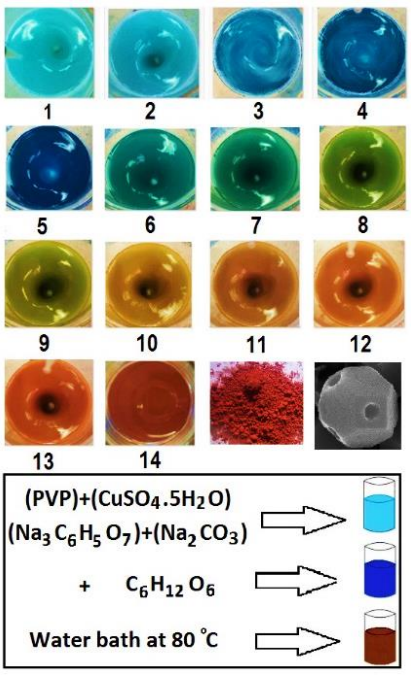

Fig. S1. The solution color changes during cage Cu_2O synthesis.

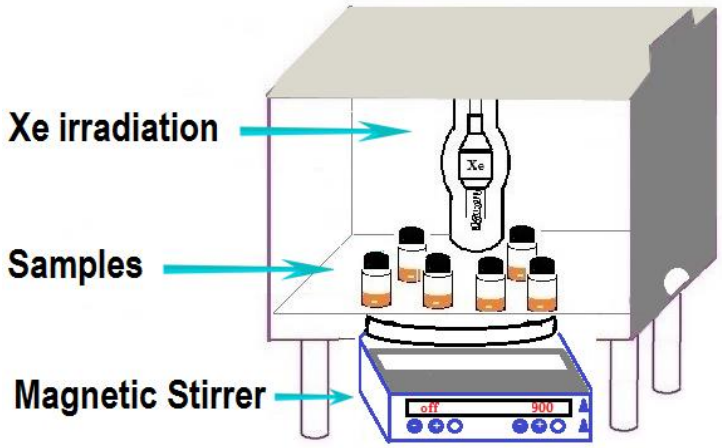

Fig. S2 The schematic view of the photoreactor.

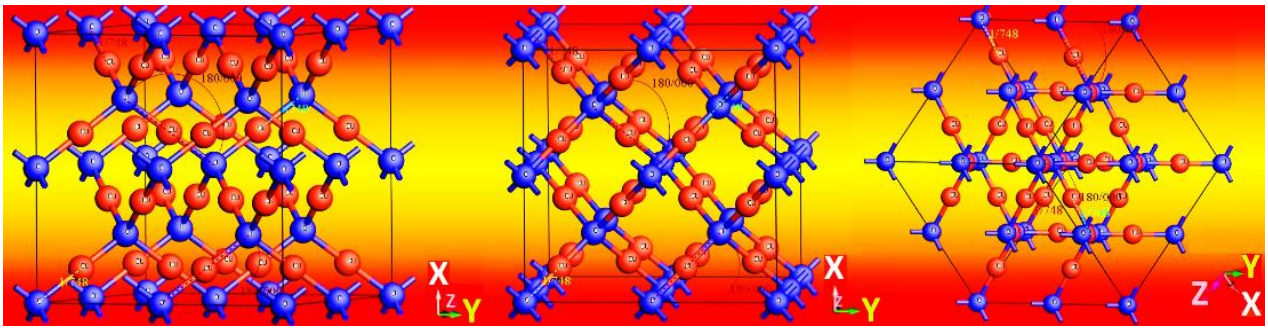

Fig. S3 Cu_2O 3D structure.

The average particle size is obtained by the Scherrer equation (Eq. S1).

$$D = \frac{K\lambda}{L\,cos\theta} \qquad \text{(S1)}$$

Where, (θ) is the angle of the highest peak in radians, (K) denotes the shape factor approximately equal to 0.9, (L) represents the full width at half maximum (FWHM) in radians, (λ) denotes the x-ray wavelength in nm, and (D) represents the average crystallite size. The average size of the crystals was estimated to be 40.8 based on the Scherrer equation. Scherrer method uses the highest peak (FWHM and 2θ) to calculate the crystallite size for symmetrical and especially spherical particles. In contrast, Williamson-Hall method use 4 to 6 significant peak to calculate the crystallite size and ε was equal to -0.0162 and is more reliable method to evaluate sized for different morphologies.

The size in FESEM to be large compare to crystallite size because theoretical methods such as Williamson-Hall use the x-ray diffraction data to calculate the crystallite size while the microscopic micrographs gives the particle size. Since a typical particle is constructed from a number of crystallites, so it is obvious that for the micrograph results to be larger than the diffraction results.

The Tauc model shows that the ability to absorb light depends on the difference between the band gap and photon energy as follows (Eq. S2).

$$[\alpha h\nu] = A(h\nu - E_g)]^n \qquad \text{(S2)}$$

A represents a constant value, (hν) is the photon energy, α shows an absorption coefficient, (Eg) is the band gap energy, and (n) denotes a constant which depends on the light passing through the sample, indicating the direct and indirect or allowed and forbidden natures of the electronic transition. n is ½ and $^3/_2$ for the allowed and forbidden direct transition while being 2 and 3 for allowed and forbidden indirect transition, respectively. In the energies greater and lower than the band gap, there was a deviation from linearity in the diagram, due to occurrence of the defect state near the band edge and increase in the available transition states, respectively. Around the band gap, the curve is linear and the band gap is obtained by extrapolation [1, 2]. The results of the direct and indirect allowed band gap shown in Fig. S4.

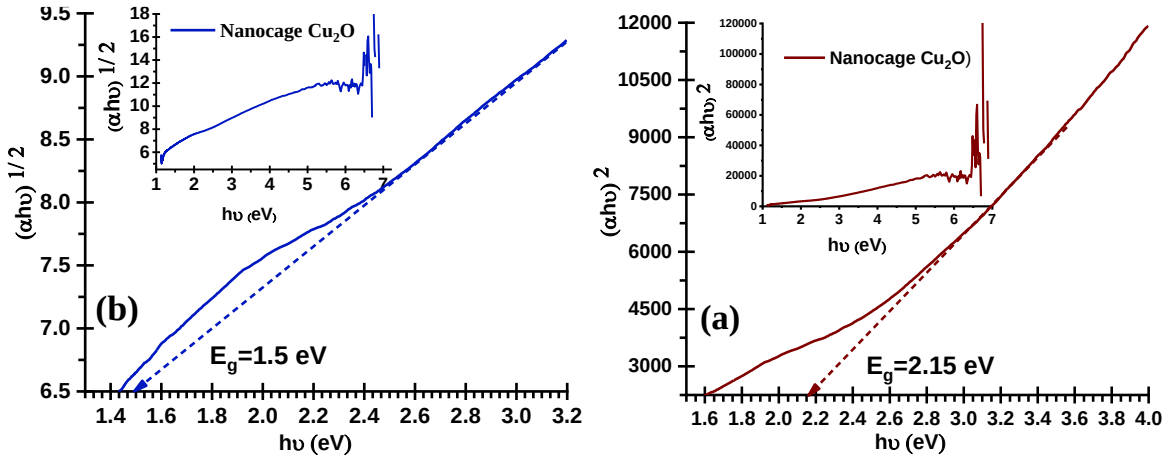

Fig S4. Allowed band gap of cage Cu_2O based on the Tauc model (a) direct (b) indirect.

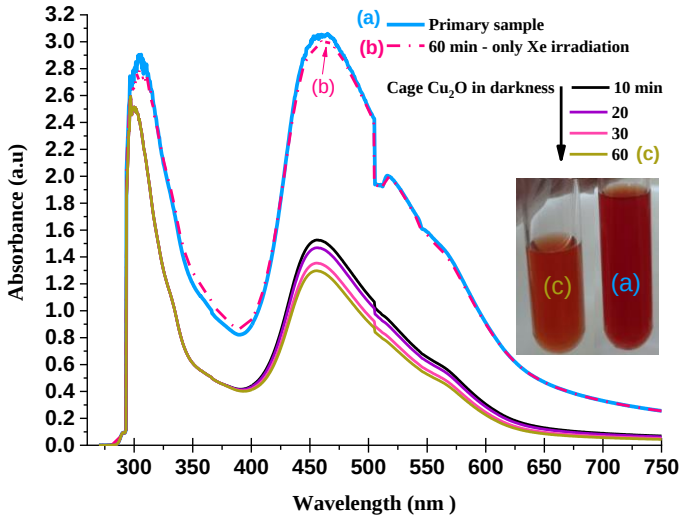

Fig S5. The process of changes in the dye concentration: (a) primary sample, (b) in the presence of synthetic copper oxide and dark environment, (c) photodissociation effect.

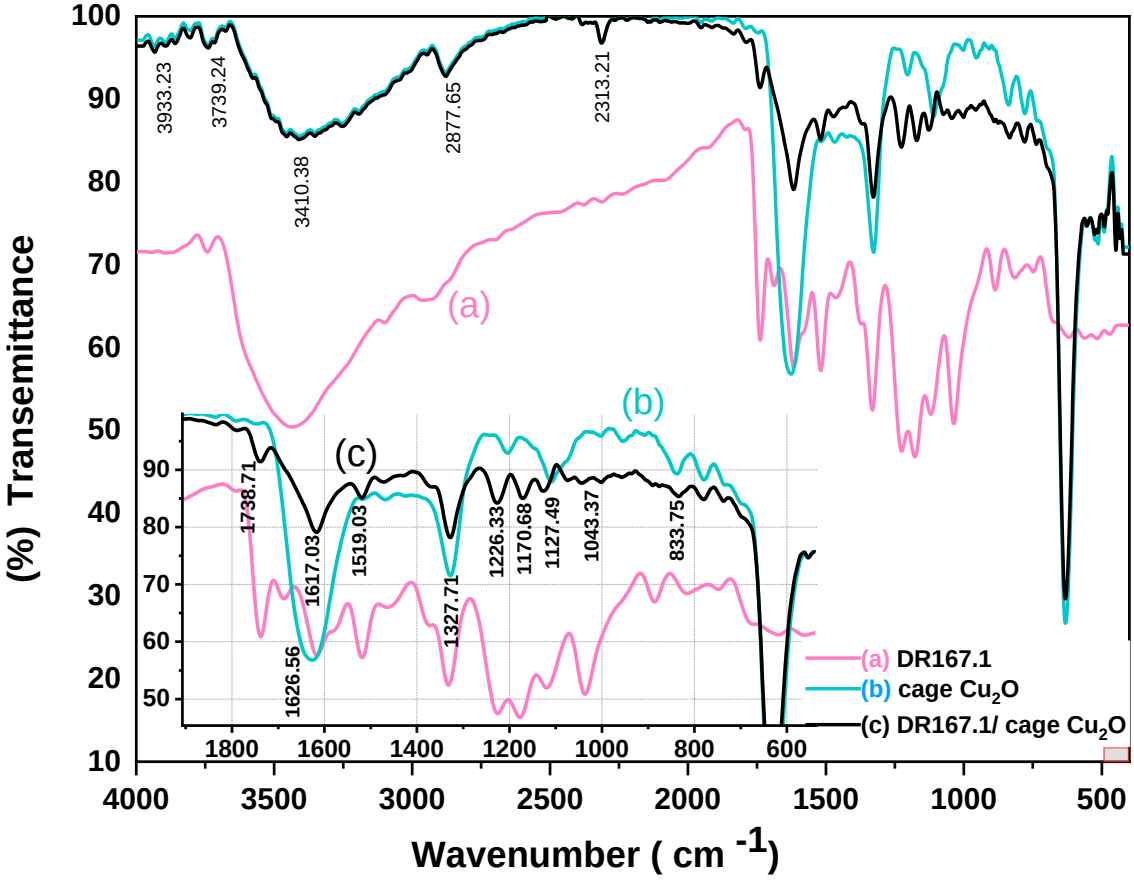

Fig. S6 . FTIR spectra of cage Cu_2O, DR 167.1 and cage Cu_2O / DR 167.1.

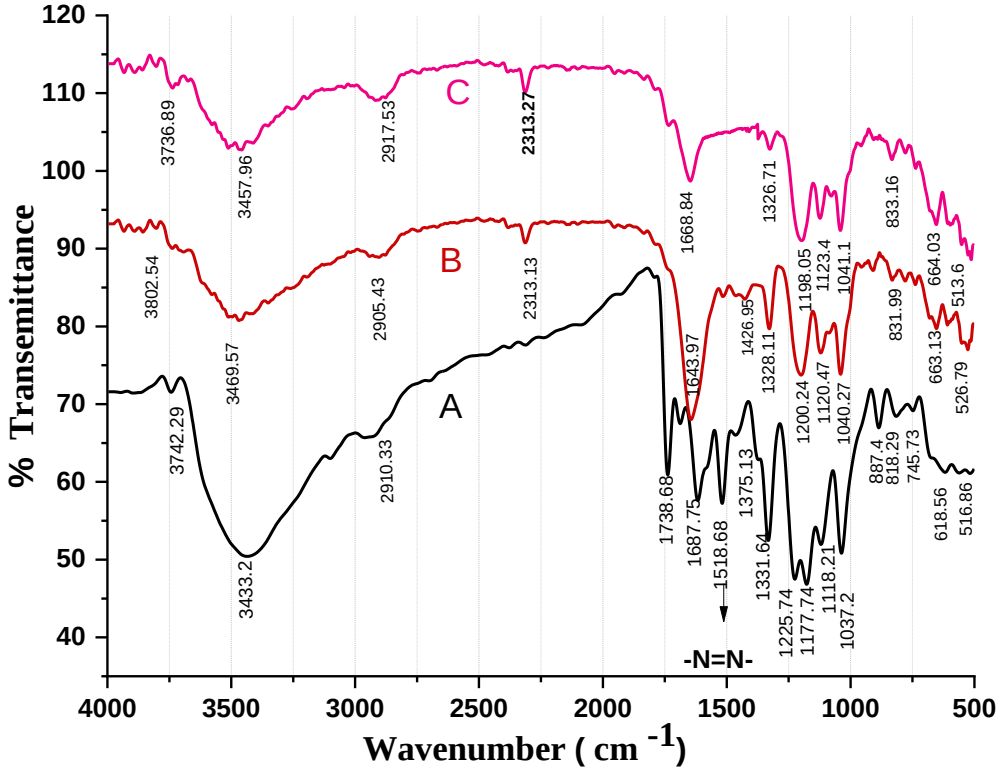

Fig. S7. FTIR spectrum of DR167.1; (A) initial condition, after (B) 2 min (C) 25 min of photodegradation

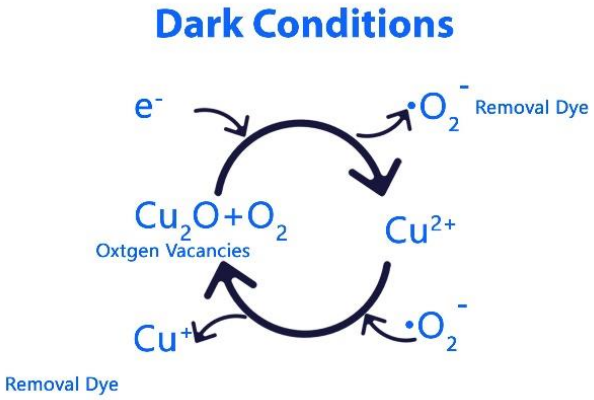

Fig S8. Removal cycle of DR 167.1 dye in dark conditions.

[1]. Ming-Dong W, Dao-Yun Z, Yi L, Lin Z, Chang-Xi Z, Zhen-Hui H, Di-Hu C, Li-Shi W. (2008) Determination of thickness and optical constants of ZnO thin films prepared by filtered cathode vacuum arc deposition. Chinese Physics Letters. 25(2):743.

[2]. Viezbicke BD, Patel S, Davis BE, Birnie III DP (2015) Evaluation of the Tauc method for optical absorption edge determination: ZnO thin films as a model system. physica status solidi (b). 252(8):1700-10. DOI: 10.1002/pssb.201552007