Supplementary Information

Uncapped SnO_2 Quantum Dots for selective adsorption, separation and photocatalytic degradation of mixture of dyes

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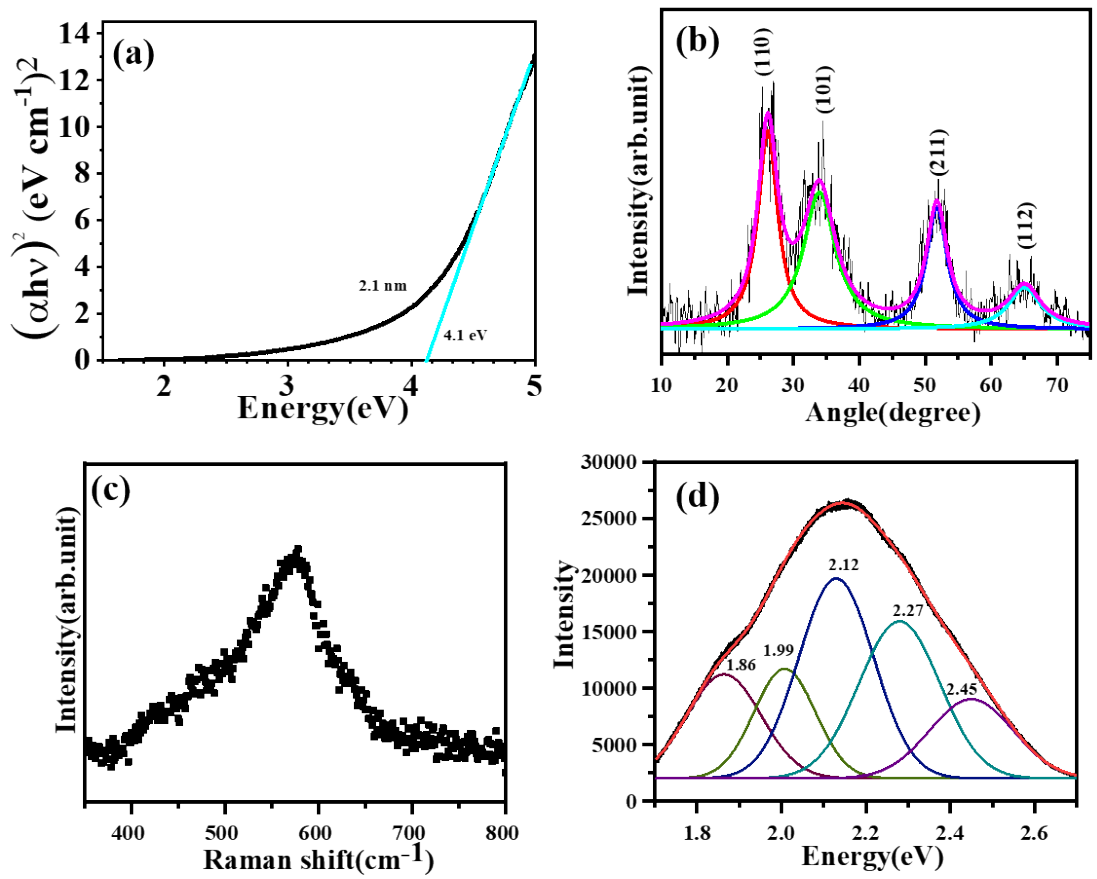

Figure S1. Tauc's plot (a), XRD (b), Raman (c) and PL spectrum (d) of SnO_2 QD 1

Detailed characterization of QD 1 which was prepared in similar way to QD 2 but dried at a relatively higher temperature of 100 ^{o}C was also done. Fig S1.a shows the Tauc's plot of the SnO_2 QD 1.The deduced band gap is found to be around 4.1 ±0.1 eV, which is also shifted from the bulk value of 3.67 eV due to the quantum confinement size effect. Fig S1**.** b depicts the XRD patterns of QD1. Broad peaks at 2θ values of 26.3˚, 33.9˚, 51.7˚, and 64.65˚ corresponding to (110), (101), (211), and (112) planes confirm the rutile tetragonal structure of SnO_2 (ICDD No. 41-1445).The deduced average crystallite size is found to be 2.3 ± 0.2 nm. Fig S1**.** c displays the Raman spectrum of QD 1 which shows a broad feature at 575 cm^{-1} similar to QD 2. Similarly, Fig S1 d shows the PL spectrum of QD 1. The broad feature around 2.1 eV as observed due to the presence of various oxygen vacancies is also similar to QD 2. The PL spectrum was also deconvoluted with six Guassian peaks that were centered at 1.86, 1.99, 2.12, 2.27, 2.45 eV. The peaks at 1.86, 1.99, and 2.12 eV corresponded to the bridging oxygen vacancy (V_B), and the peaks at 2.27 eV and 2.45eV were mainly from in-plane oxygen vacancies (V_P)[1]. Thus, there is little dissimilarlity between two QDs. The most srticking difference is huge surface charge in QD 2 as revealed by Zeta potential value(~50 mV). Thus, subtle change in synthesis process allows creation of two different surfaces without affecting SnO_2 structure and morphology significantly.

Table S1. Various Raman modes of MB.[2].

Peak position(cm^{-1})	**Assignment**
450	α(C-N-C)$_{AMG}$ (in-plane bending)
481	Observance of new peak(Monomer formation)
500	(C-N-C)$_{AMG}$ (in –plane bending)
669	(C-C-C) $_{ring}$ (in –plane bending)
772	(C-N)$_{AMG}$ (stretching)
1035	(C-S) $_{ring}$(stretching)
1147	(C-H) (in –plane bending)
1300	(C-N) $_{ring}$(stretching)
1390	(C-N)$_{ring}$(stretching)
1625	(C-C)/(C-N) $_{ring}$(stretching)

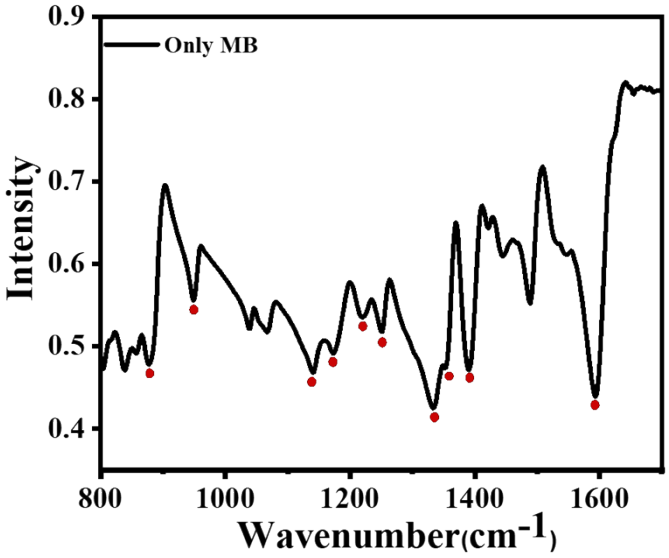

Figure S2. The FTIR spectrum of MB

Various vibrational modes recorded using by FTIR can be assigned and they are tabulated below. The characteristic frequencies of the FTIR bands of MB molecule are given below [3].

Table S2. The characteristic frequencies of the FTIR bands of MB molecule.

Peak position	Assignment
1602 cm^{-1}	$(C=C)_{ring}/(C=N)_{ring}$ stretching
1395 cm^{-1}	(C-H) in-plane bending
1357 cm^{-1}	$(C=S^{+})_{ring}$ stretching
1336 cm^{-1}	(C-N) stretching vibration
1249 cm^{-1}	(C-H) in-plane bending and out of plane bending vibration
1223 cm^{-1}	$(C-C)_{ring}$ stretching vibration
1143 cm^{-1}	$(C-N)_{ring}$ in-plane bending
1178 cm^{-1}	$(C-H)_{ring}$ in-plane bending

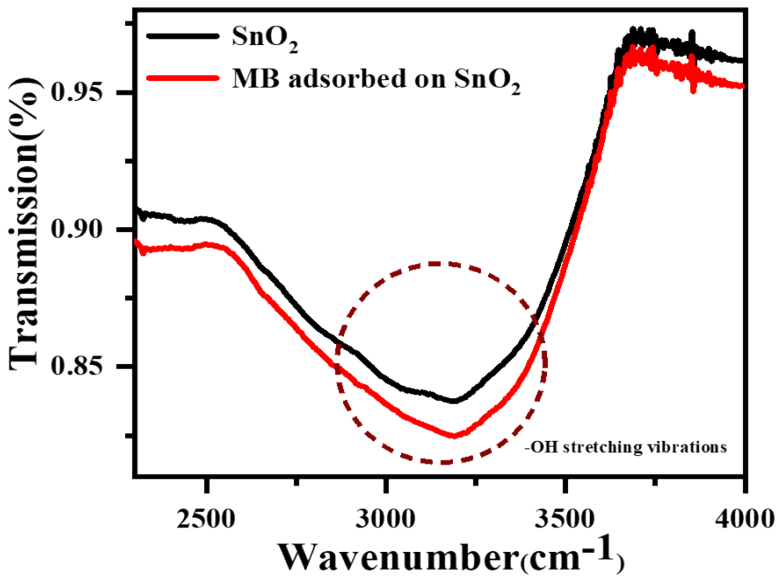

Figure S3 . The FTIR spectra of SnO_2 QD 2 before and after adsorption (Hydroxyl group region)

Figure S3 displays the FTIR spectra of SnO_2 QD 2 before and after adsorption (hydroxyl group region). The FTIR spectra of SnO_2 and the MB adsorbed SnO_2 show significant change in the stretching vibration of the hydroxyl group. The FTIR spectrum of SnO_2 QD 2 has a stretching mode of –OH group around 3000- 3400 cm^{-1}which is affected due to adsorption of MB. This change indicates prevailed interaction between MB and OH group of the SnO_2 QD 2.

The un-adsorbed MO is degraded photocatalytically by irradiating with UV light. The Schematic diagram is given in Fig. S4. Electron–hole pairs are generated by the absorption of UV light by SnO_2 QD 2. The electrons react with dissolved oxygen to form superoxide radical and the holes reacts with H_2O to form hydroxyl radical. These hydroxyl and superoxide radicals reacts with MO into form CO_2 and H_2O[4].

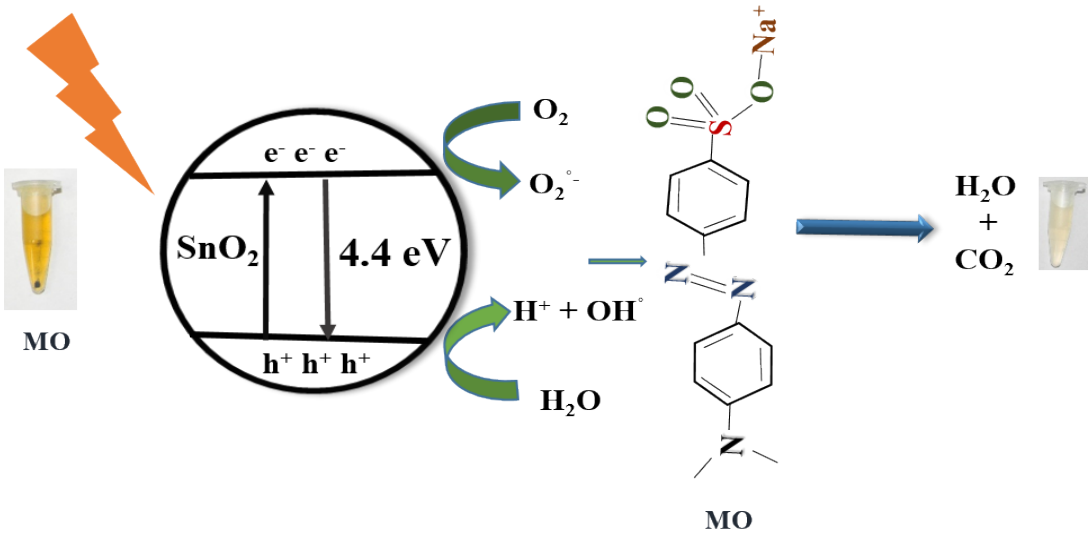

Figure S4 . The schematic diagram of photocatalytic degradation of MO by QD 2 under irradiation with UV light.

References

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2. S. Dutta Roy, M. Ghosh and J. Chowdhury, *Journal of Raman Spectroscopy*, 2015, **46**, 451-461.
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