SUPPLEMENTARY MATERIAL

# Mesoporous $TiO_2$ implanted ZnO QDs for the photodegradation of tetracycline: Material Design, Structural Characterization and Photodegradation Mechanism

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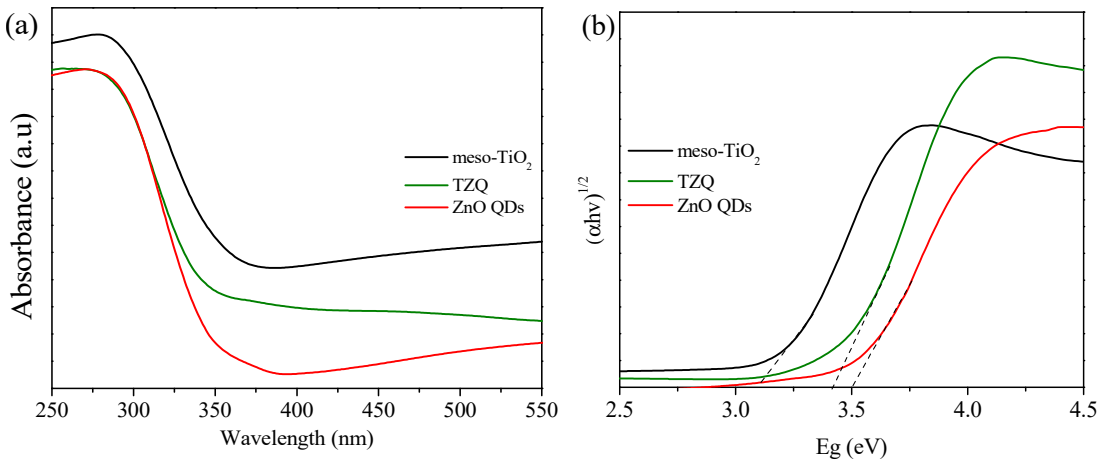



**Figure S1.** UV-Vis absorbance spectra (a) and (b) the corresponding Tauc's plot of $(\alpha h\nu)^{1/2}$ versus E (eV) of meso-$TiO_2$, TZQ and ZnO QDs.

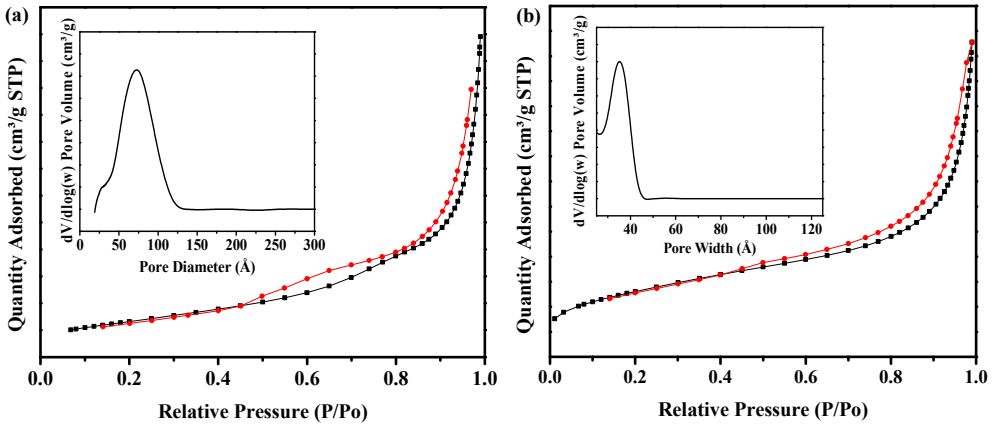
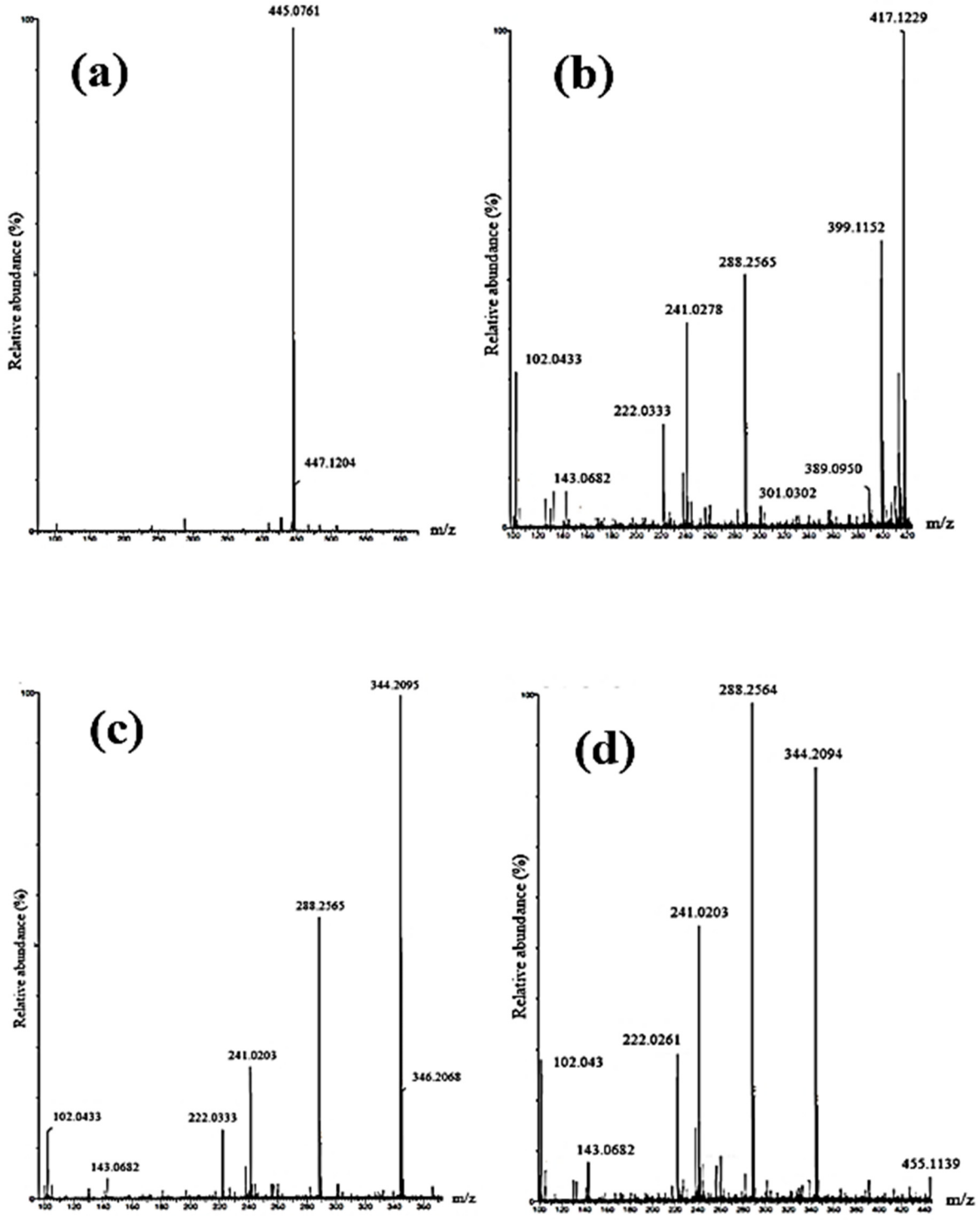



**Figure S2.** $N_2$ sorption isotherms and (inset: BJH pore size distribution) of (a) meso-$TiO_2$ and (b) TZQ.


(a)
445.0761
447.1204
Relative abundance (%)
m/z
(b)
417.1229
399.1152
288.2565
241.0278
102.0433
222.0333
143.0682
389.0950
301.0302
Relative abundance (%)
m/z
(c)
344.2095
288.2565
241.0203
346.2068
102.0433
222.0333
143.0682
Relative abundance (%)
m/z
(d)
288.2564
344.2094
241.0203
222.0261
102.043
143.0682
455.1139
Relative abundance (%)
m/z

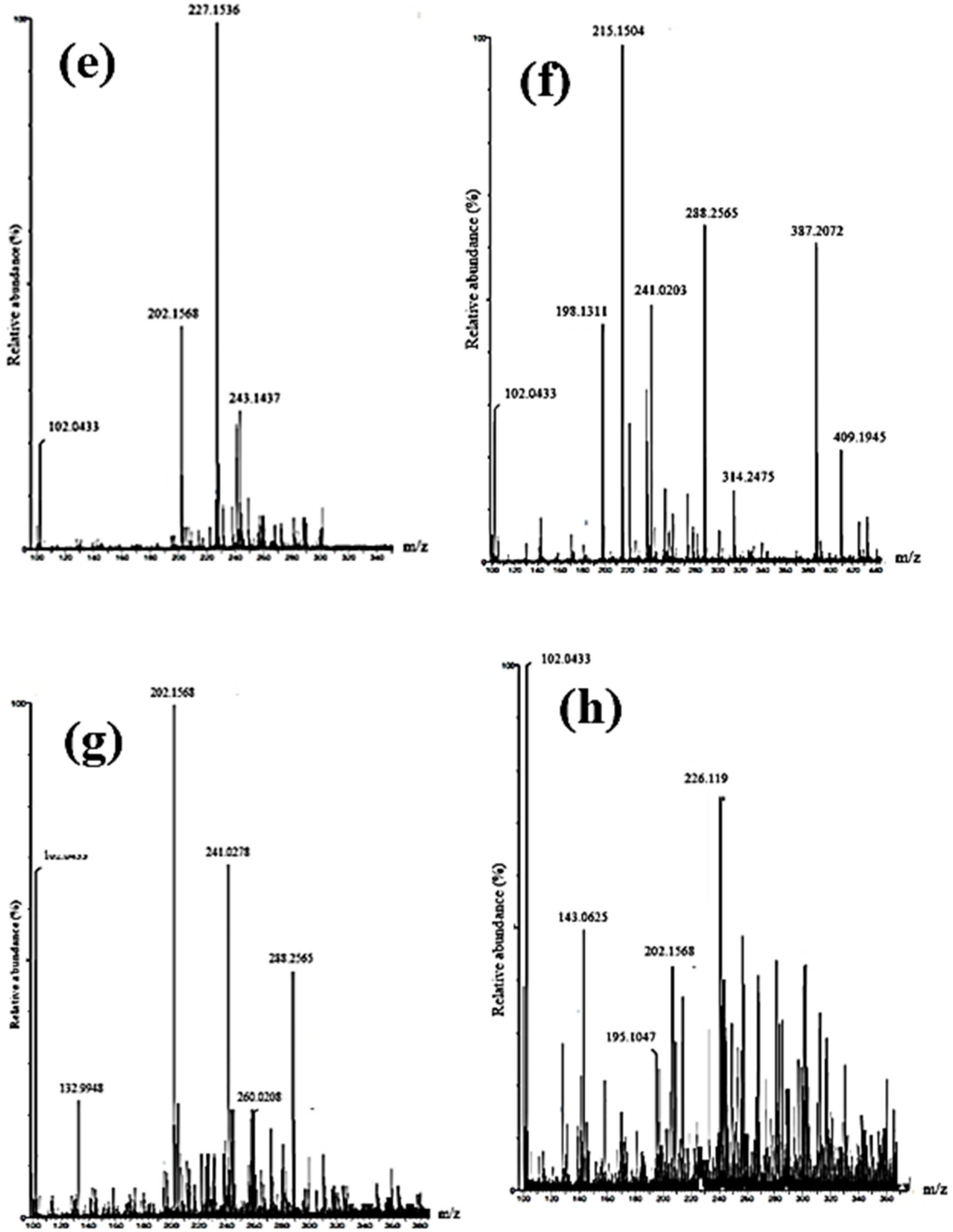



**Figure S3.** (a) Mass spectra of TC (a) and its intermediates during photodegradation in the presence of TZQ (b-h).

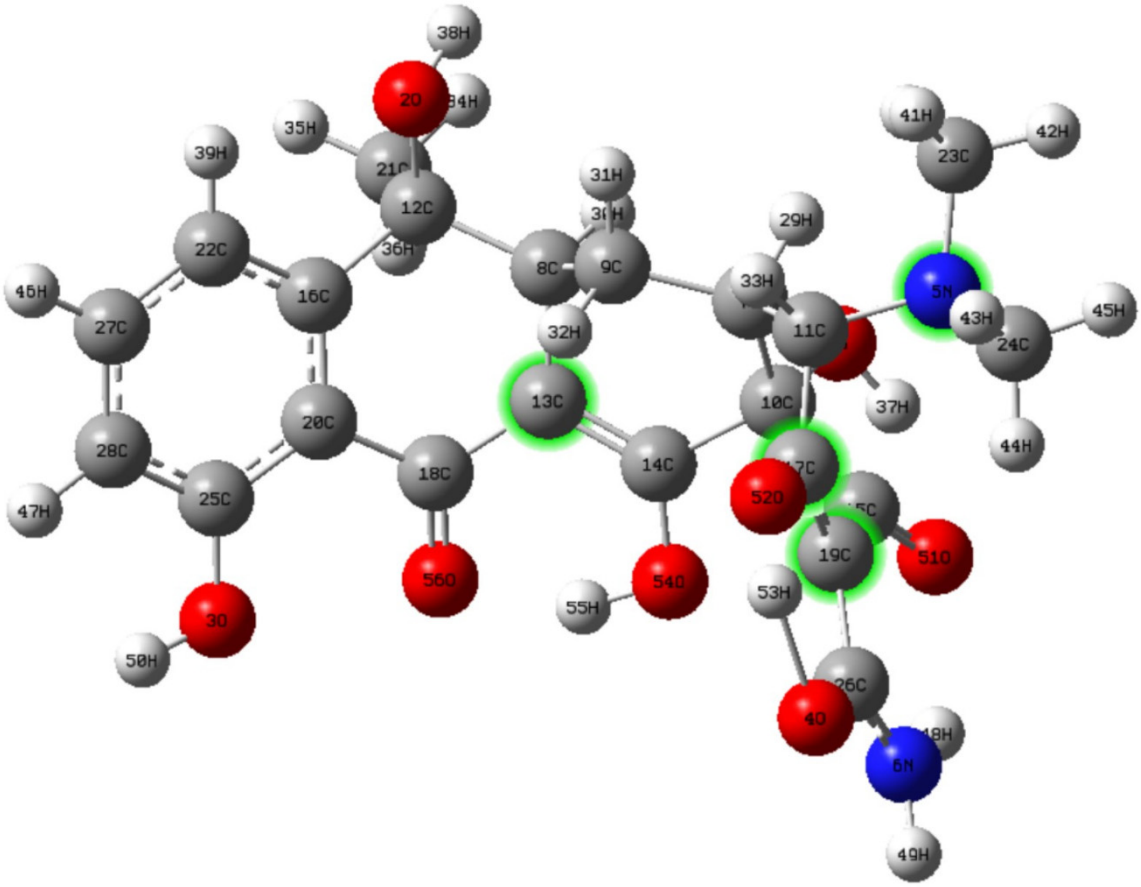



**Figure S4.** The chemical structure of TC and its distribution of Fukui index ($fk^0$) for the radical attack.

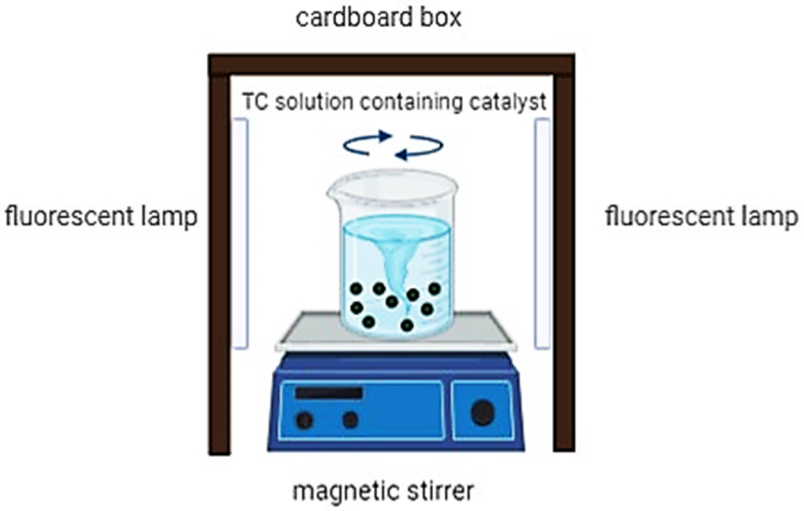



**Figure S5.** Schematic diagram of the photocatalytic degradation reaction system under fluorescent light irradiation.

**Table S1:** Fukui index of TC atoms.

| Atom | No | $fk^+$ | $fk^-$ | $fk^0$ |
|---|---|---|---|---|
| O | 1 | 0.01302 | 0.03504 | 0.01101 |
| O | 2 | 0.00005 | -0.00011 | -0.00008 |
| O | 3 | 0.00699 | 0.07101 | 0.03201 |
| O | 4 | 0.00283 | 0.00251 | -0.00016 |
| N | 5 | 0.00646 | 0.22230 | **0.10792** |
| N | 6 | -0.00307 | -0.00020 | 0.00143 |
| C | 7 | -0.00878 | -0.00623 | 0.00127 |
| C | 8 | 0.09551 | -0.06458 | -0.08004 |
| C | 9 | -0.02203 | 0.09046 | 0.05624 |
| C | 10 | 0.06009 | -0.01911 | -0.03960 |
| C | 11 | -0.02839 | -0.00259 | 0.01290 |
| C | 12 | 0.00466 | -0.00528 | -0.00497 |
| C | 13 | -0.10071 | 0.29559 | **0.19815** |
| C | 14 | 0.18165 | 0.03418 | -0.07374 |
| C | 15 | 0.03719 | 0.05134 | 0.00707 |
| C | 16 | 0.06391 | -0.04382 | -0.05387 |
| C | 17 | 0.21385 | 0.02030 | **-0.09678** |
| C | 18 | -0.08307 | -0.04606 | 0.01850 |
| C | 19 | 0.12869 | -0.04619 | **-0.08744** |
| C | 20 | 0.00606 | 0.08430 | 0.03912 |
| C | 21 | -0.00731 | 0.00315 | 0.00523 |
| C | 22 | -0.06442 | 0.09605 | 0.08023 |
| C | 23 | 0.00095 | -0.01374 | -0.00734 |
| C | 24 | 0.00362 | -0.02318 | -0.01340 |
| C | 25 | 0.09278 | 0.06958 | -0.01160 |
| C | 26 | 0.03859 | -0.01387 | -0.02623 |
| C | 27 | 0.16741 | 0.01530 | -0.07606 |
| C | 28 | -0.03195 | 0.00262 | 0.01729 |
| H | 29 | 0.00786 | -0.00457 | -0.00622 |
| H | 30 | -0.00344 | 0.01414 | 0.00879 |
| H | 31 | -0.00057 | 0.00583 | 0.00320 |
| H | 32 | 0.00082 | -0.00196 | -0.00139 |
| H | 33 | 0.00263 | 0.02741 | 0.01239 |

| | | | | |
|---|---|---|---|---|
| H | 34 | 0.00075 | -0.00066 | -0.00070 |
| H | 35 | -0.00109 | -0.00001 | 0.00054 |
| H | 36 | 0.00210 | -0.00064 | -0.00137 |
| H | 37 | -0.00099 | -0.00062 | 0.00018 |
| H | 38 | 0.00274 | 0.00001 | -0.00137 |
| H | 39 | 0.00395 | -0.00484 | -0.00439 |
| H | 40 | -0.00043 | 0.00281 | 0.00162 |
| H | 41 | 0.00042 | 0.02207 | 0.01083 |
| H | 42 | 0.00164 | 0.00222 | 0.00029 |
| H | 43 | 0.00013 | 0.02373 | 0.01180 |
| H | 44 | -0.00115 | 0.00322 | 0.00218 |
| H | 45 | 0.00104 | 0.00078 | -0.00013 |
| H | 46 | -0.01024 | -0.00143 | 0.00440 |
| H | 47 | 0.00113 | -0.00113 | -0.00113 |
| H | 48 | 0.00029 | 0.00017 | -0.00006 |
| H | 49 | 0.00460 | -0.00004 | -0.00232 |
| H | 50 | 0.00060 | -0.00245 | -0.00152 |
| O | 51 | 0.04504 | -0.00142 | -0.02323 |
| O | 52 | 0.02985 | 0.00278 | -0.01354 |
| H | 53 | -0.00101 | -0.00035 | 0.00033 |
| O | 54 | 0.04033 | 0.09192 | 0.02580 |
| H | 55 | -0.00328 | -0.00270 | 0.00029 |
| O | 56 | 0.10738 | 0.01699 | -0.04520 |