Supporting Information

TiO₂-multi-walled carbon nanotube nanocomposites: hydrothermal synthesis and temporally-dependent optical properties

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Figure S1. XPS wide-scan spectrum of MWCNTs.



Figure S2. FTIR spectrum of TiO₂.



Figure S3. Fluorescence spectrum of the MWCNTs.



Figure S4. HRTEM images of (a) M0.25, (b) M0.50 and (c) M1.00.



Figure S5. High-resolution XPS spectra of (a) O 1s and (b) C 1s for M1.00, and (c) the Ti 2p core level XPS spectra of TiO₂ and M1.00.

Further information regarding the chemical and bonding environment of TiO_2 and the $TiO_2/MWCNT$ nanocomposites was ascertained from XPS studies. With respect

to the XPS O 1s spectrum of M1.00 in Figure S5a, the asymmetric and broad O 1s peak is due to different oxygen bonds and environments. The four peaks at 530.1, 530.7, 531.2 and 532.6 eV from fitting the O 1s spectrum of M1.00 are ascribed to lattice oxygen, carbonyl, phenol, and carboxyl groups, respectively.¹ Similarly, the C 1s peak can be fitted to four peaks (Figure S5b) at 284.6, 285.1, 286.4, and 289.6 eV ascribed to the sp² hybridized carbon of the MWCNTs, and C-O, C=O, and O=C-O species, respectively.² With such surface functional groups, the TiO_2 may be grafted onto the MWCNTs' surfaces via C-O-Ti bonds, such structures facilitating the desired charge transfer upon light excitation.³ However, no peak was observed at 283.1 eV, strongly suggesting that the carbon atoms do not directly enter the TiO₂ lattice, presumably a result of the low synthesis temperature. Figure S5c shows the Ti core XPS spectra of TiO₂ and the M1.00 nanocomposite. The Ti core-level XPS spectrum of TiO₂ exhibits two peaks centered at 464.3 and 458.6 eV, corresponding respectively to the Ti 2p_{1/2} and Ti 2p_{3/2} photoelectrons in the Ti⁴⁺ state.⁴ For the M1.00 nanocomposite, these two peaks occur at 464.6 and 458.9 eV, respectively. In each sample, the Ti $2p_{1/2}$ and Ti $2p_{3/2}$ spin-orbit splitting is 5.7 eV, consistent with the presence of Ti^{4+} in the TiO_2 and M1.00 nanocomposite. This shift may be due to bonding between oxygen and carbon present in the MWCNTs. The O/Ti atomic ratio is ca. 2.6, which is higher than that of 2 for pure TiO₂. This may be because some oxygen is contributed from the MWCNTs. Similar results are seen for M0.25 and M0.50 as with M1.00, the results being shown in Figures S6 and S7.



Figure S6. High resolution XPS spectra of (a) O 1s and (b) C 1s for M0.25, and (c) Ti 2p core level XPS spectra of TiO₂ and M0.25.



Figure S7. High resolution XPS spectra of (a) O 1s and (b) C 1s for M0.50, and (c) Ti 2p core level XPS spectra of TiO₂ and M0.50.

References

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