Supplementary data

Improved Adsorption and Photocatalytic Degradation of Methyl Orange by Onion-like Nanocarbon/TiO_2 Nanocomposites

Themba D. Ntuli [1,2], Ludwe L. Sikeyi [2], Faria Dziike [3], Neil J. Coville [1,2], Edward N. Nxumalo [4] and Manoko S. Maubane-Nkadimeng [1,2,5,*]

[1] DSI-NRF Centre of Excellence in Strong Materials, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg 2050, South Africa
[2] The Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg 2050, South Africa
[3] Technology Transfer and Innovation Directorate, Steve Biko Campus, Durban University of Technology, Durban 4000, South Africa
[4] Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Private Bag X6, Florida 1709, South Africa
[5] Microscopy and Microanalysis Unit, University of the Witwatersrand, Private Bag 3, Johannesburg 2050, South Africa
* Correspondence: manoko.maubane@wits.ac.za

Powder X-ray diffraction spectroscopy

The powder X-ray diffraction (PXRD) peaks of all the materials are shown in Figure S1. Only the TiO_2 peaks are seen as the carbon is amorphous and in a low concentration. The diffraction peaks for all the nanocomposites showed peaks at the correct 2θ degree values for the expected planes of the anatase phase of TiO_2 (JCPDS Card No. 78-2486). Similar patterns have been reported in the literature for OLNCs/TiO_2 nanocomposites [1].

Figure S1 has been shown in the format given to indicate that only anatase TiO_2 was made. Note (i) the peaks have been shifted to remove overlap (they all occur at the same position) and (ii) The intensities have been scaled for viewing purposes. No internal standard was used to determine the peak sizes or locations.

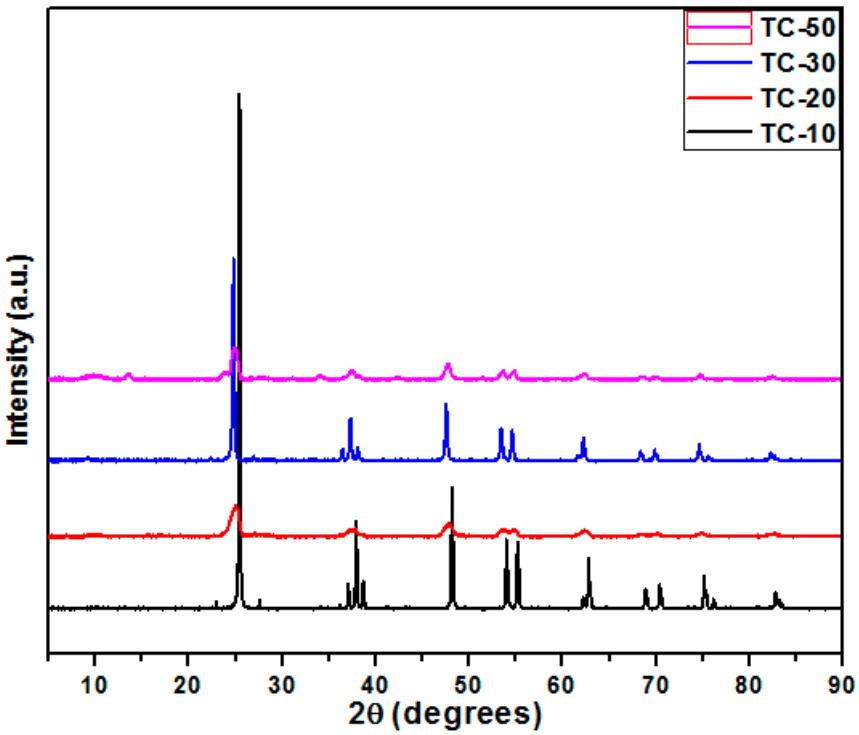

Figure S1: PXRD patterns of anatase TiO_2 phase for TC-10, TC-20, TC-30, and TC-50

X-ray photoelectron spectroscopy

To supplement what we have discussed in the paper regarding the synthesized TiO_2-OLNC nanocomposites, the TC-10 catalyst was selected for XPS analysis and the data is presented in Figure S2 and Table S1. The XPS survey spectra show all the characteristic peaks of a TiO_2-carbon composites material with peaks at 284.7 eV (C1s), 531.1 eV (O1s) and 458.9 eV (Ti_{2p}) (Figure S2a). This indicated that the elemental composition of the photocatalyst was mainly C, O and Ti [2].

The XPS data were deconvoluted and the Ti, C and O spectra are shown in Figure S2b, S2c and S2d respectively. The deconvoluted peak positions and intensities are given in Table S2. The Ti peak occurs at 458.9, corresponding to Ti in oxidation state 4^+ typical of a Ti-O bond. No indication of Ti-C bonding was observed (or expected). The C peak region showed the presence of C=C (13.9%), C-C (32.8%) and C-O/C=O (9.8%) bonds. The

XPS O spectral region showed that O was in different environments typical of C=O (6.3%), (C-O) (6.7%) and TiO_2 (8.3%Ti; 17.3% O)).

These results were in agreement with those of Raman and PXRD, consistent with the synthesis of a TiO_2-OLNC composite.

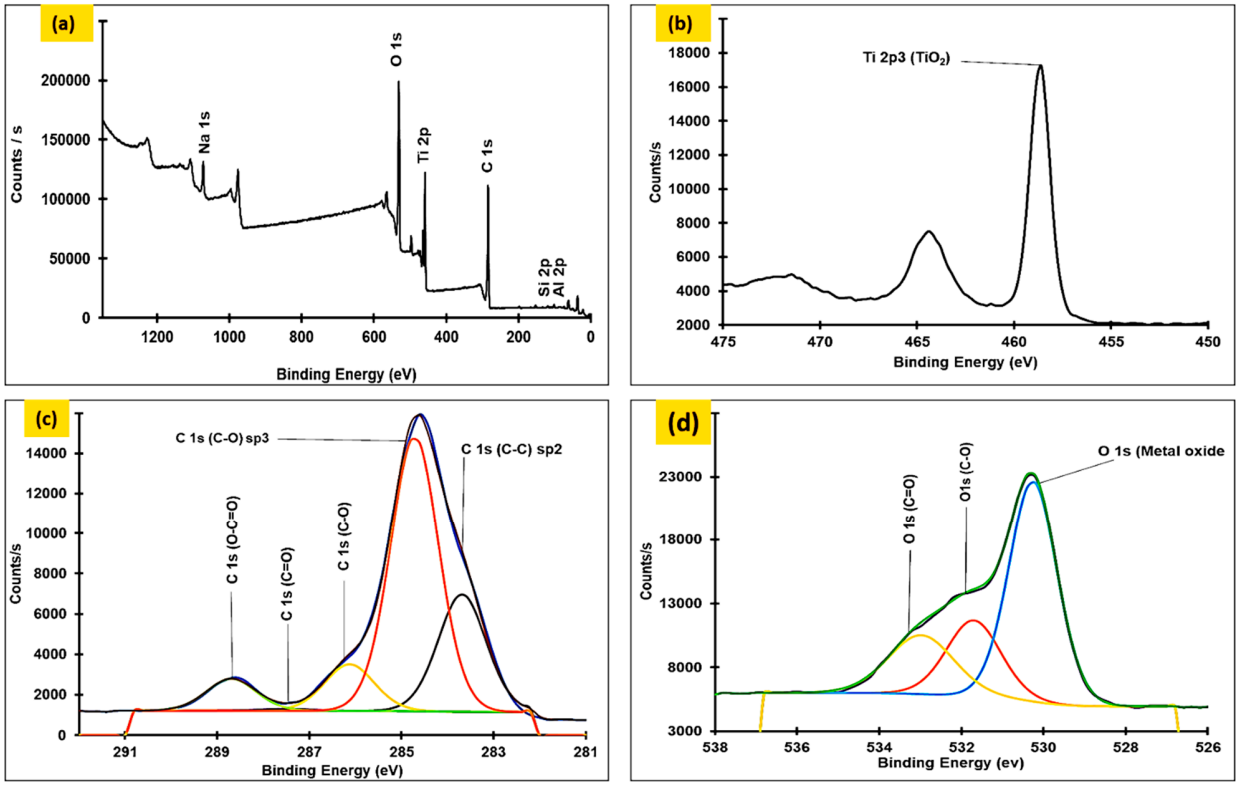

Figure S2: XPS survey spectra of TC-10 photocatalyst (a), deconvoluted spectra for Ti (b), C (c) and O (d) respectively.

Table S1: Elemental identification and quantification

Name	Peak BE	FWHM (eV)	Atomic %
Al 2p	74.2	2.6	1.1
C 1s	284.7	3.3	55.6
Na1s (~19% area is Ti LM2)	1072.1	3.7	3.2
O 1s (~5% area is Na KL2)	531.1	3.7	30.4
Si 2p	102.1	2.8	1.1
Ti 2p	458.9	2.8	8.7

Table S2: Data from the deconvoluted XPS spectra

Name	Peak BE	FWHM eV	Atomic %
C1s (C-C) sp2	283.7	1.2	13.9
C1s (C-C) sp3	284.7	1.2	32.8
C1s (C-O)	286.1	1.3	5.7
C1s (C=O)	287.5	1.3	0.2
C1s (O-C=O)	288.7	1.3	3.9
O1s (C-O)	531.7	1.6	6.7
O1s (C=O)	533	1.9	6.3
O1s (Metal Oxide)	530.3	1.4	17.3
Ti2p3 (TiO2)	458.7	1.2	8.3

Table S3: Adsorption capacity of all the photocatalysts

Catalyst	Co (mg/L)	Ce (mg/L)	qe (mg/g)
TiO_2	10	9.9	1
Tc-10	10	8.4	16
TC-20	10	8	20
TC-30	10	7.6	24
TC-50	10	7.3	27

Equations

$$q_e = \left(\frac{C_O - C_e}{m}\right)V \quad \text{S1}$$

$$\frac{C_e}{q_e} = \left(\frac{1}{Q^o_{max}}\right)C_e + \frac{1}{Q^o_{max}K_L} \quad \text{S2}$$

$$Log\ q_e = n\ Log\ C_e + Log\ K_F \quad \text{S3}$$

where C_O (mg/L) and C_e (mg/L) are the initial and equilibrium concentrations of the dye, m is the mass (g) of the catalyst, V is the volume (L) of the dye q_e (mg/g) is the adsorption capacity at equilibrium and Q^O_{max} (mg/g) is the maximum adsorption capacity. K_L (L/mg) is a constant that is related to the affinity between the catalyst and the dye. K_F (mg/g)/(mg/L)^n is the Freundlich constant, and n is the Freundlich intensity parameter and is dimensionless.

Adsorption isotherms and intra-particle diffusion

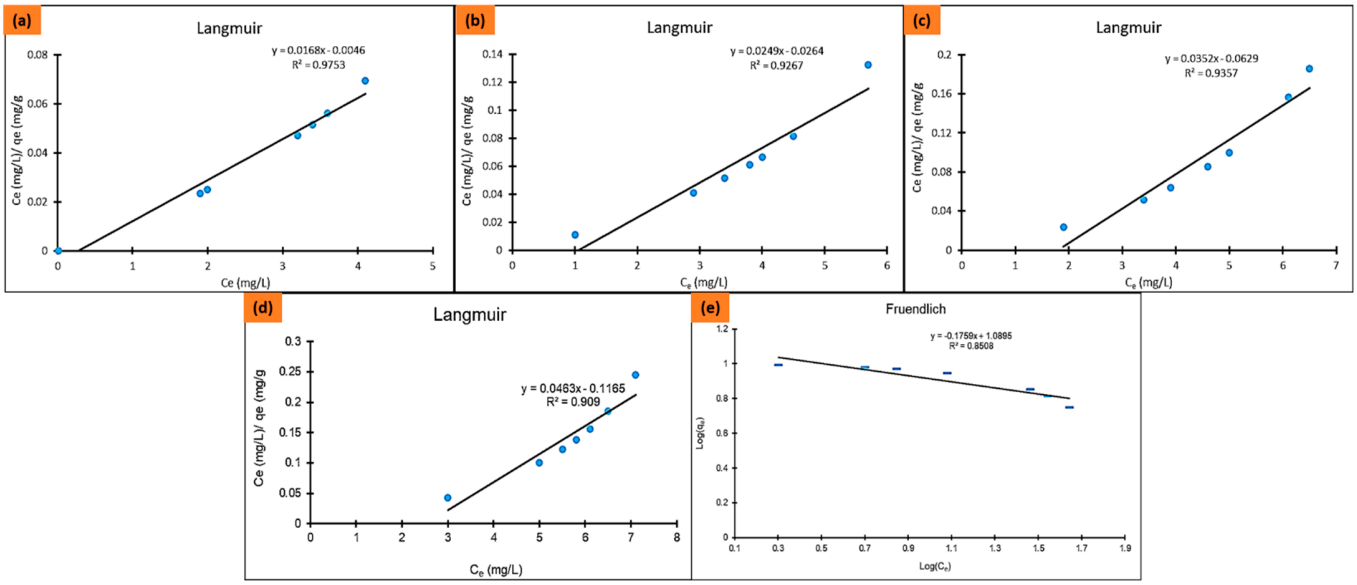

Figure S3: Linear plots for Langmuir isotherm TC-10 (a), TC-20 (b), TC-30 (c), TC-50 (d) and the Fruendlich isotherm TiO_2 (e).

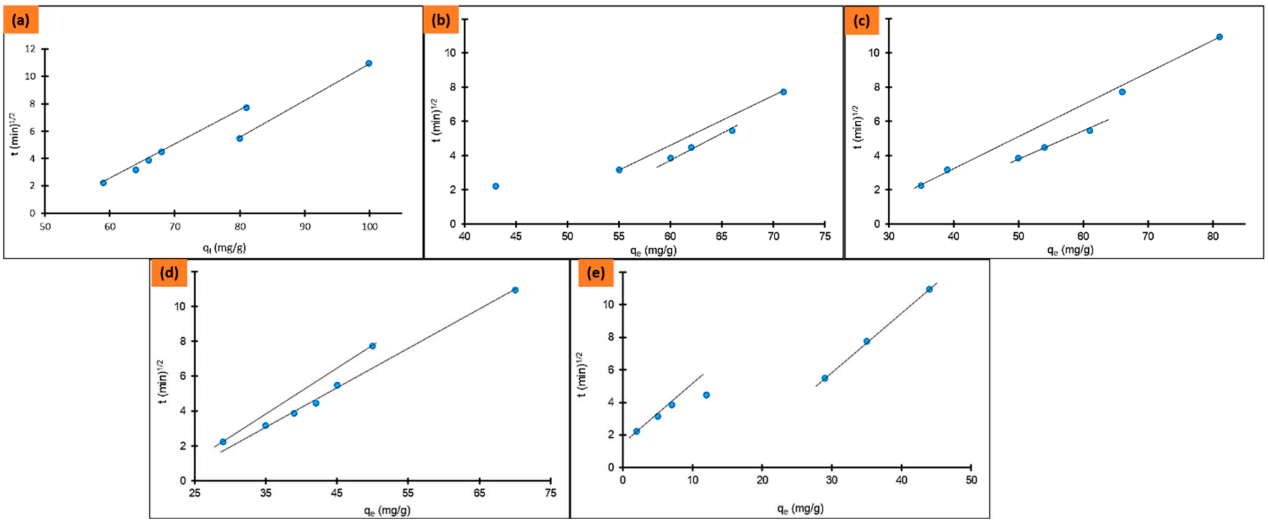

Figure S4: Intra-particle diffusion plots for all the catalysts TC-10 (a), TC-20 (b), TC-30 (c), TC-50 (d) and TiO_2 (e).

References

[1] A.K. John, S. Palaty, S.S. Sharma, Greener approach towards the synthesis of titanium dioxide nanostructures with exposed {001} facets for enhanced visible light photodegradation of organic pollutants, J. Mater. Sci. Mater. Electron. 31 (2020) 20868–20882. https://doi.org/10.1007/s10854-020-04602-1.

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