

## Supplementary Information

# Photocatalytic Decolorization and Biocidal Applications of Nonmetal Doped TiO<sub>2</sub>: Isotherm, Kinetic Modeling and Insilco Molecular Docking Studies

Muhammad Saqib Khan <sup>1</sup>, Jehanzeb Ali Shah <sup>1</sup>, Muhammad Arshad <sup>2</sup>, Sobia Ahsan Halim <sup>3</sup>, Ajmal Khan <sup>3</sup>, Ahson Jabbar Shaikh <sup>4</sup>, Nadia Riaz <sup>1</sup>, Asim Jahangir Khan <sup>1</sup>, Muhammad Arfan <sup>5</sup>, Muhammad Shahid <sup>1</sup>, Arshid Pervez <sup>1</sup>, Ahmad al Harasi <sup>3\*</sup>, Muhammad Bilal <sup>1\*</sup>

<sup>1</sup> Department of Environmental Sciences, COMSATS University Islamabad, Abbottabad Campus, Abbottabad, 22060, Pakistan; [muhammadsaqib@yahoo.com](mailto:muhammadsaqib@yahoo.com) (M.S.K); [jehanzeb360@yahoo.com](mailto:jehanzeb360@yahoo.com) (JAS); [nadiariazz@gmail.com](mailto:nadiariazz@gmail.com) (N.R); [asimjk@cuiatd.edu.pk](mailto:asimjk@cuiatd.edu.pk) (A.J.K); [muhammadshahid@ciitvehari.edu.pk](mailto:muhammadshahid@ciitvehari.edu.pk) (M.S); [pervez@cuiatd.edu.pk](mailto:pervez@cuiatd.edu.pk) (A.P)

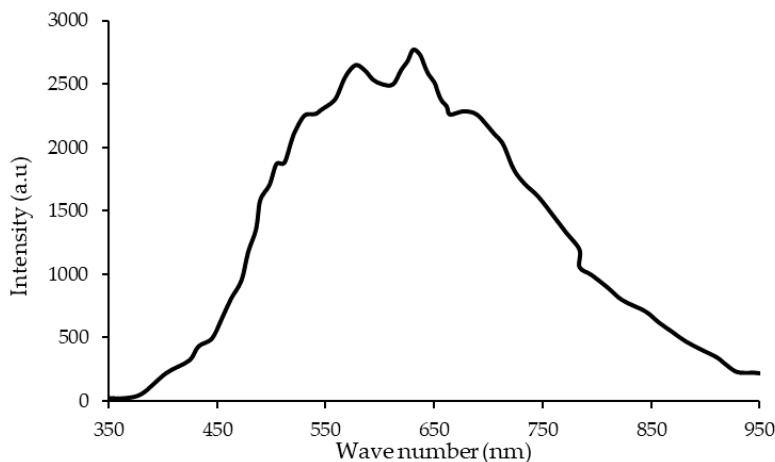
<sup>2</sup> Institute of Environmental Sciences and Engineering (IESE), SCEE, National University of Sciences and Technology, Islamabad, 44000, Pakistan; [marshad@iese.nust.edu.pk](mailto:marshad@iese.nust.edu.pk)

<sup>3</sup> Natural and Medical Sciences Research Center, University of Nizwa, P.O. Box 33, Birkat Al Mauz, Nizwa 616, Sultanate of Oman; [sobia\\_halim@unizwa.edu.om](mailto:sobia_halim@unizwa.edu.om) (S.A.H); [ajmalkhan@unizwa.edu.om](mailto:ajmalkhan@unizwa.edu.om) (A.K); [aharrasi@unizwa.edu.om](mailto:aharrasi@unizwa.edu.om) (A.A)

<sup>4</sup> Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, Abbottabad, 22060, KPK, Pakistan; [ahson@cuiatd.edu.pk](mailto:ahson@cuiatd.edu.pk)

<sup>5</sup> Department of Chemistry, SNS, National University of Sciences and Technology, Islamabad, 44000, Pakistan; [marfan@sns.nust.edu.pk](mailto:marfan@sns.nust.edu.pk)

\* Correspondence: [mbilal@cuiatd.edu.pk](mailto:mbilal@cuiatd.edu.pk) Tel.: +92-992-383591 (M.B.), [aharrasi@unizwa.edu.om](mailto:aharrasi@unizwa.edu.om) (A.a.H); Tel: +968-25446328)



**Figure S1.** Light spectrum of halogen lamp (Hi Luminar-Germany) as a light source (500 W) with a light intensity of 30798 lux.

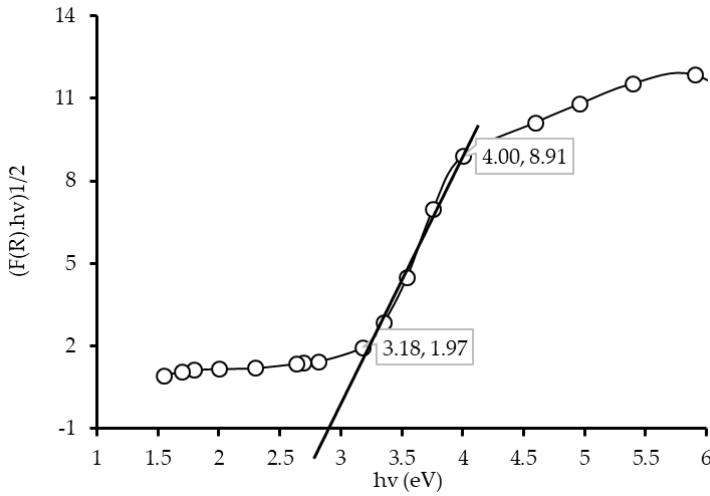


Figure S2. Bandgap estimation of 20N-TiO<sub>2</sub>-300 from DRS spectra.

The bandgap of 20N-TiO<sub>2</sub>-300 was obtained by extrapolating the tangent of the graph in the low energy range ( $h\nu$ ) axis using,

$$y = mx + c \quad (1)$$

$x_1, x_2, y_1$  and  $y_2$  were obtained from the linear curve of 20N-TiO<sub>2</sub>-300

$$x_1 = 3.18 \quad x_2 = 4.00$$

$$y_1 = 1.97 \quad y_2 = 8.91$$

To find out value of  $m$ ,

$$m = \frac{y_1 - y_2}{x_1 - x_2} \quad (2)$$

$$m = 8.4634$$

To find out value of  $c$ ,

$$-c = y - mx$$

By putting the value of  $y_2, x_2$  and  $m$ , the value of  $c$  is

$$c = -24.94$$

Therefore, inserting the value of  $m$  and  $c$  in equation 1

$$y = 8.4634x + (-24.94)$$

When  $y=0, x = 2.95$

So, the estimated bandgap for 20N-TiO<sub>2</sub>-300 is 2.95 eV