

Supplementary Material

N-Doped Graphene Quantum Dots/Titanium Dioxide Nanocomposites: A Study of ROS-Forming Mechanisms, Cytotoxicity and Photodynamic Therapy

Pravena Ramachandran ¹, Boon-Keat Khor ², Chong Yew Lee ², Ruey-An Doong ³, Chern Ein Oon ⁴, Nguyen Thi Kim Thanh ^{5,6,*} and Hooi Ling Lee ^{1,7,*}

¹ Nanomaterials Research Group, School of Chemical Sciences, Universiti Sains Malaysia, USM, Penang 11800, Malaysia; pravena@ioioleo.com

² School of Pharmaceutical Sciences, Universiti Sains Malaysia, USM, Penang 11800, Malaysia; khorboonkeat@student.usm.my (B.-K.K.); chongyew@usm.my (C.Y.L.)

³ Institute of Analytical and Environmental Sciences, National Tsing Hua University, Hsinchu 30013, Taiwan; radoong@mx.nthu.edu.tw

⁴ Institute for Research in Molecular Medicine (INFORMM), Universiti Sains Malaysia, USM, Penang 11800, Malaysia; chern.oon@usm.my

⁵ Biophysics Group, Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

⁶ UCL Healthcare Biomagnetics and Nanomaterials Laboratories, 21 Albemarle Street, London W1S 4BS, UK

⁷ School of Chemistry, The University of Sydney, Sydney, NSW 2006, Australia

* Correspondence: ntk.thanh@ucl.ac.uk (N.T.K.T.); hllee@usm.my (H.L.L.)

Table S1. Crystallite size, lattice parameters and lattice strain of TiO₂ NPs and N-GQDs/TiO₂ NCs.

Nanomaterial	Crystallite size (nm)	Lattice parameter, a (Å)	Lattice parameter, c (Å)	Lattice strain
TiO ₂ NPs	12.2	3.782	9.514	0.0008
N-GQDs/ TiO ₂ NCs	11.2	3.794	9.523	0.0014

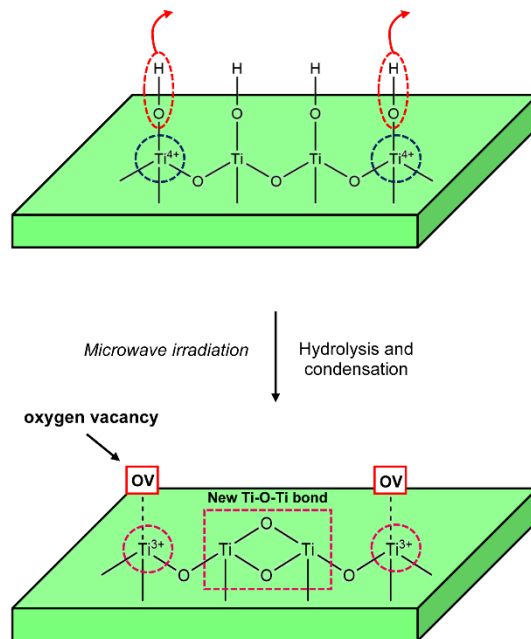


Figure S1 The possible formation mechanism of oxygen vacancies and Ti^{3+} ions.

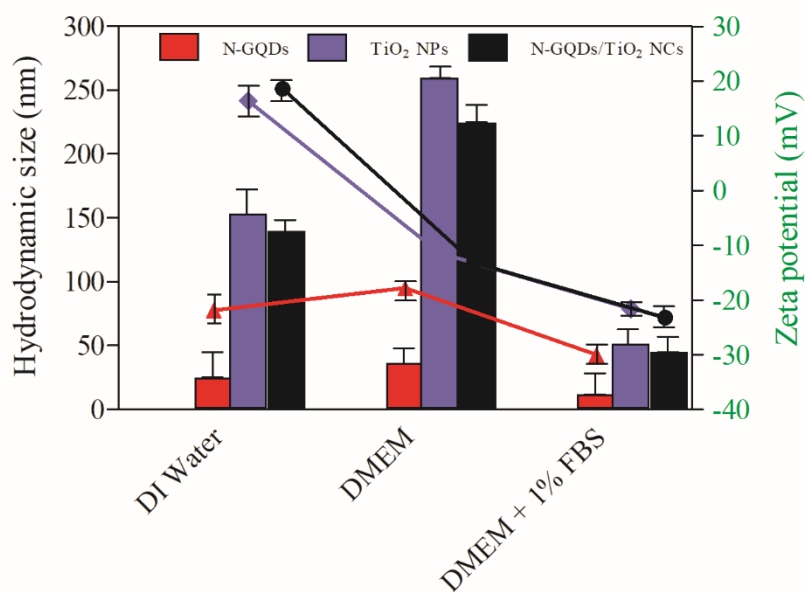


Figure S2 Hydrodynamic size and zeta potential of N-GQDs, TiO_2 NPs, N-GQDs/ TiO_2 NCs in cell culture medium (mean \pm SD, $n=3$). The nanomaterials were dispersed in water or medium with or without FBS (1%, v/v), then sonicated, vortexed and hydrodynamic size and zeta

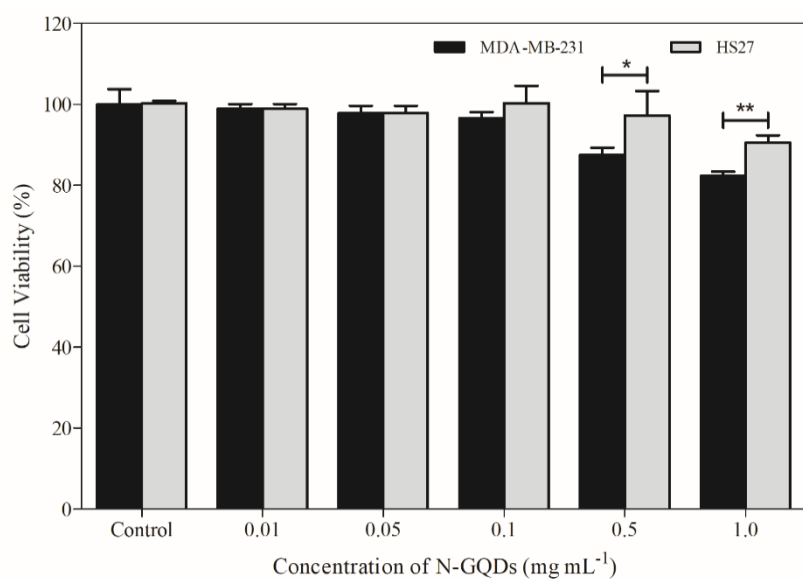


Figure S3 Cell viability of MDA-MB-231 and HS27 cells after 24 h post-treatment. Data are presented as the mean \pm SD of two independent experiments made in three replicates ($n = 6$) and normalized to control. Significant difference was tested using two-way ANOVA followed by Bonferroni post-hoc test as compared to control *($p < 0.05$) and **($p < 0.01$).