

Supplementary Materials: Graphitic Layered Structures Enhancing TiNT Catalyst Photo-Electrochemical Behaviour

Rosalba Passalacqua ^{1,2,*}, Salvatore Abate ^{1,2}, Federica De Luca ¹, Siglinda Perathoner ^{1,2} and Gabriele Centi ^{1,2}

¹ Department of Chemical, Biological, Pharmaceutical and Environmental Sciences (ChiBioFarAm) University of Messina, 98166 Messina, Italy

² ERIC aisbl & INSTM CASPE (Lab. of Catalysis for Sustainable Production & Energy), University of Messina, 98166 Messina, Italy

* Correspondence: rpassalacqua@unime.it

For the estimation of the optical band gap (E_g), the relation proposed by Tauc was used:

$$(\alpha \cdot hv)^{1/n} = A(hv - E_g) \quad (1)$$

Modified as follow for diffuse reflectance spectra

$$(F(R_\infty) \cdot hv)^{1/n} = A(hv - E_g) \quad (2)$$

The Kubelka-Munk functions were modelled assuming an indirect ($n=2$) or direct ($n=1/2$) transition by plotting $(F(R_\infty) \cdot E)^{1/n}$ as a function of hv , the energy of incident photons. The intercept on the abscissa of the $(F(R_\infty) \cdot E)^{1/n}$ vs. E gave the optical absorption edge energy value.

Citation: Passalacqua, R.; Abate, S.; De Luca, F.; Perathoner, S.; Centi, G. Graphitic Layered Structures Enhancing TiNT Catalyst Photo-Electrochemical Behaviour. *Coatings* **2023**, *13*, 358. <https://doi.org/10.3390/coatings13020358>

Academic Editor: Emerson Coy

Received: 24 December 2022

Revised: 24 January 2023

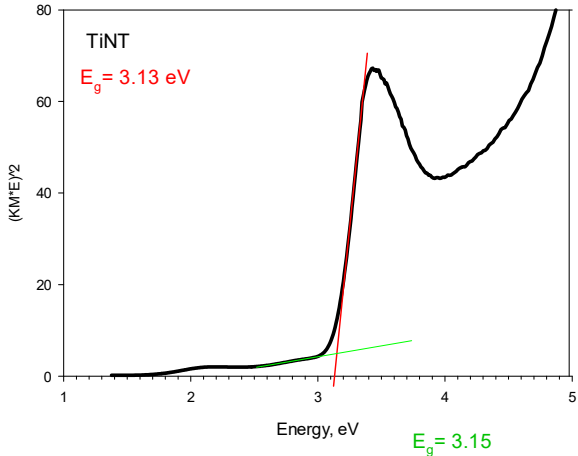
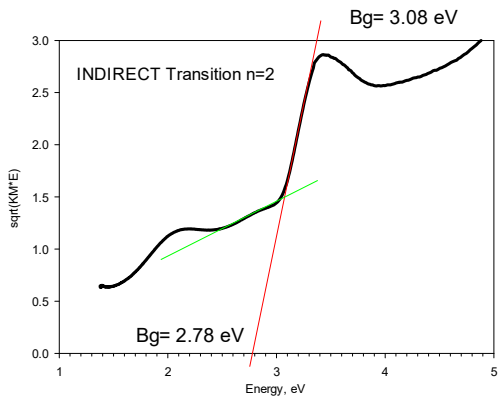
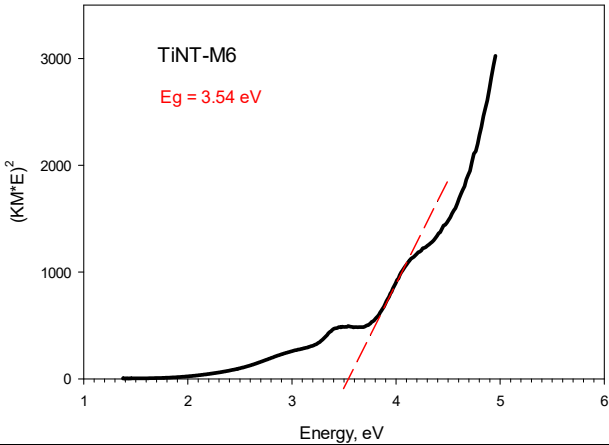
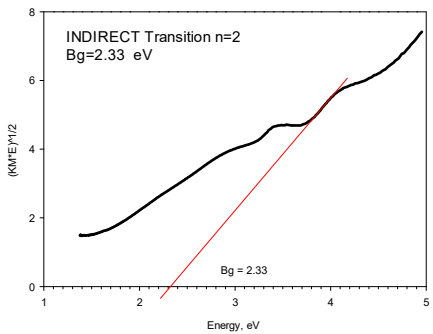
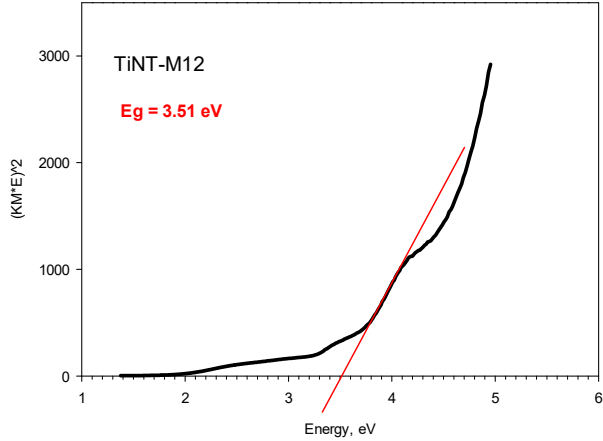
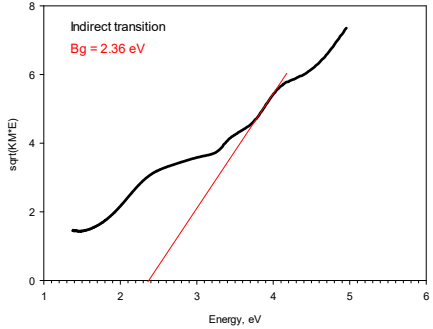
Accepted: 1 February 2023

Published: 4 February 2023

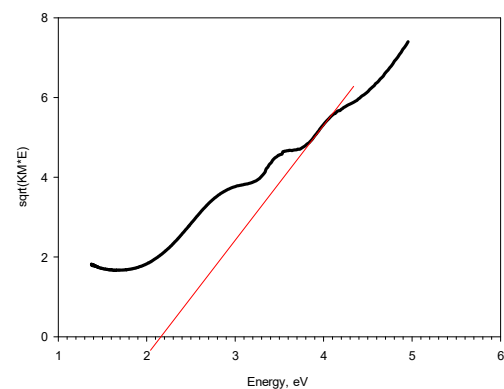
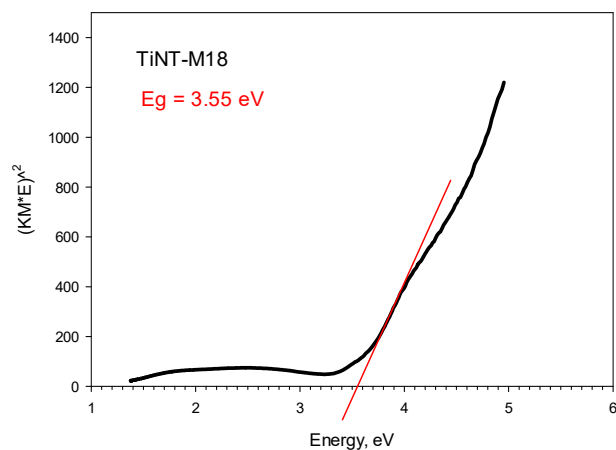


Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

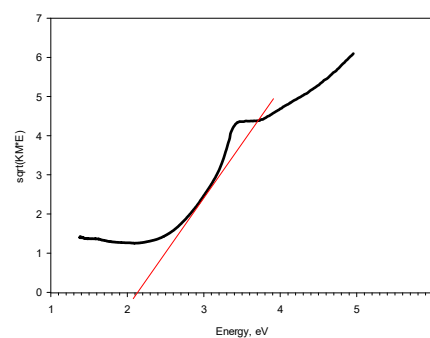
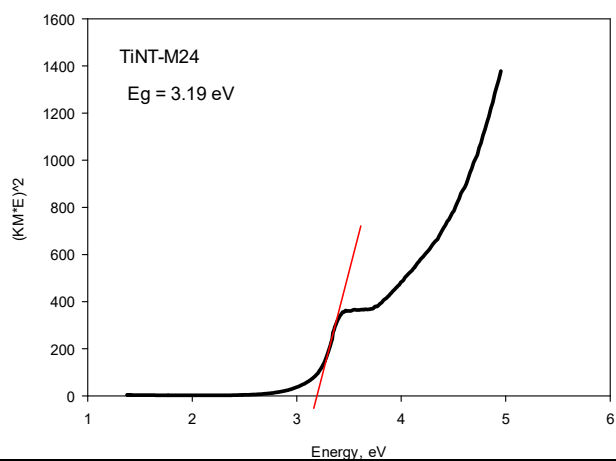
Table S1. Estimation of E_g with Tauc's plot for the investigated composites, TiNT substrate, and the M24 and MU24 powders. The fitting of the data according to a direct or indirect transition is reported.

Sample	Direct Transition $n=1/2$	Indirect $n=2$
TiNT		
TiNT-M6		
TiNT-M12		

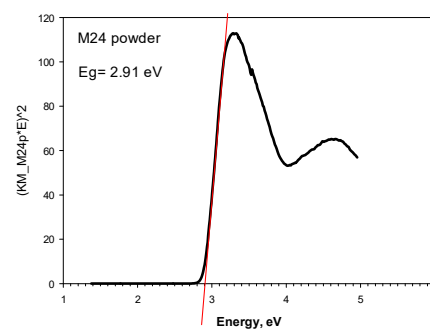
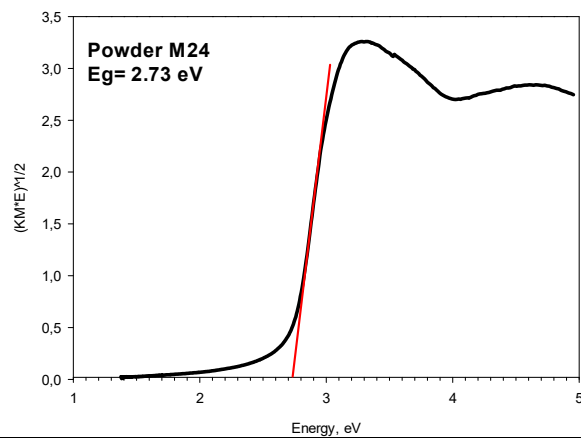
TiNT-M18



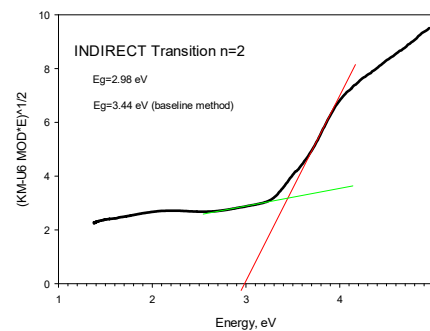
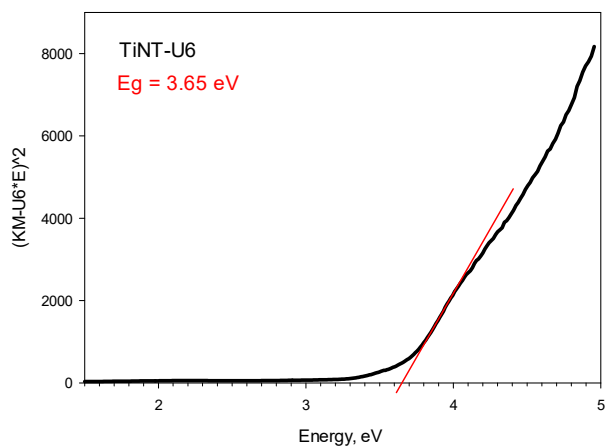
TiNT-M24



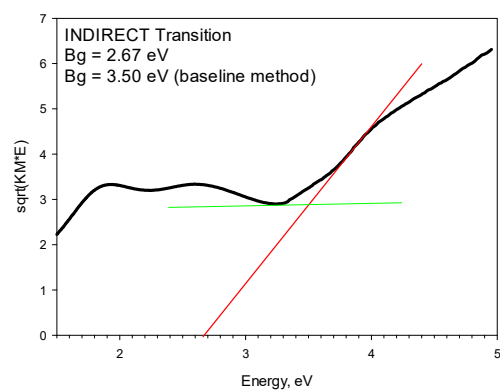
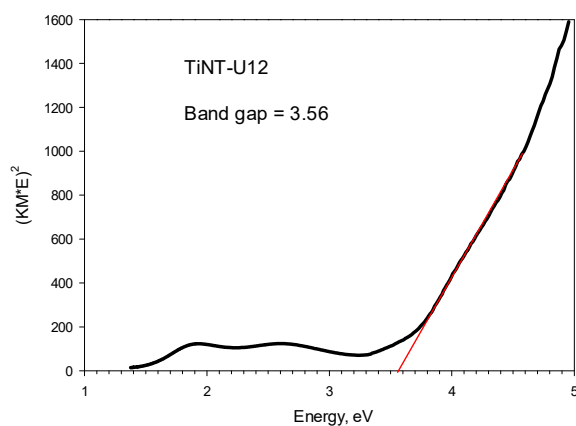
M24



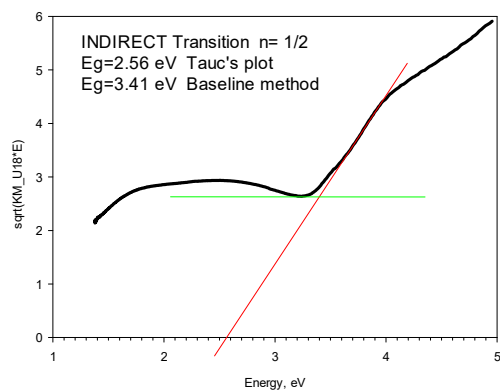
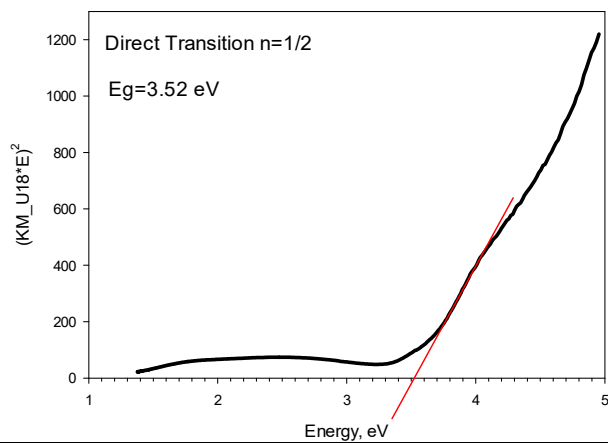
TiNT-U6



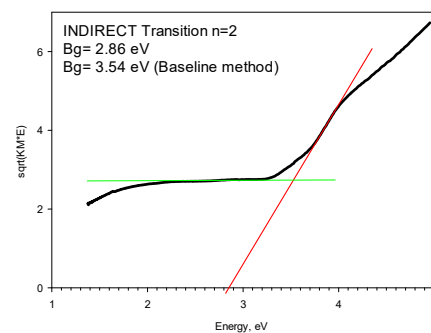
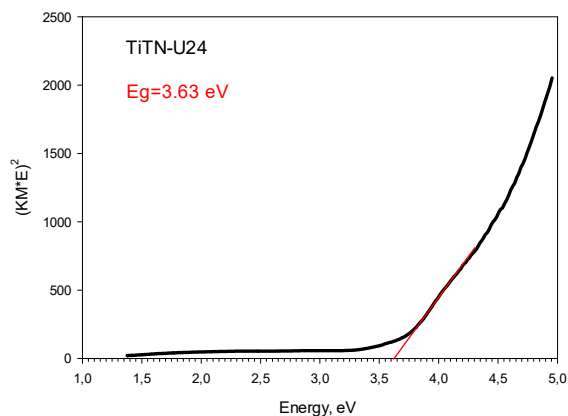
TiNT-U12



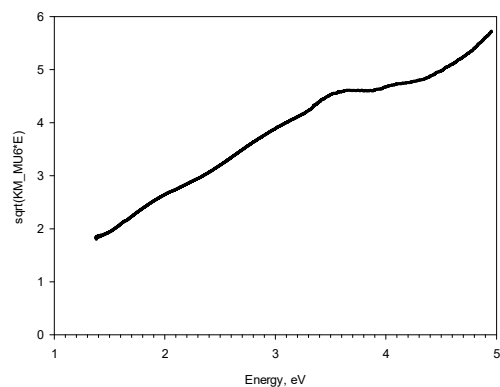
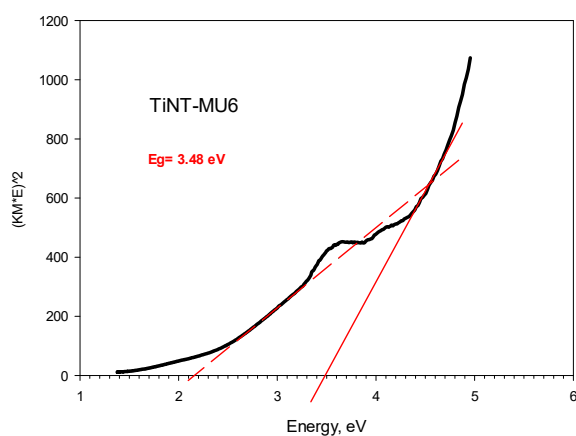
TiNT-U18



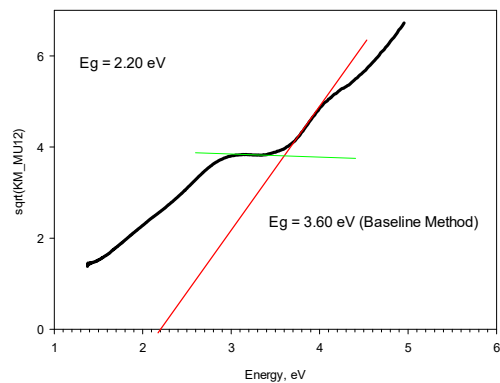
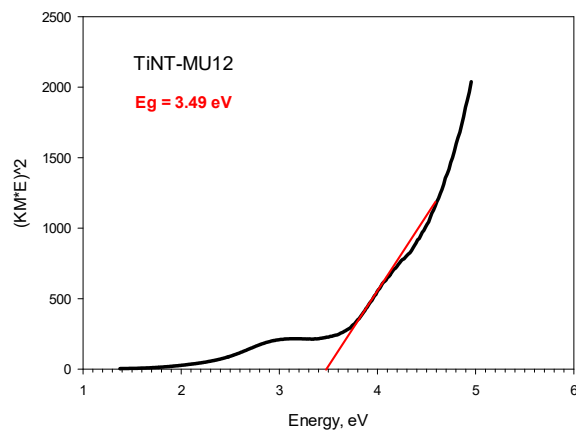
TiNT-U24



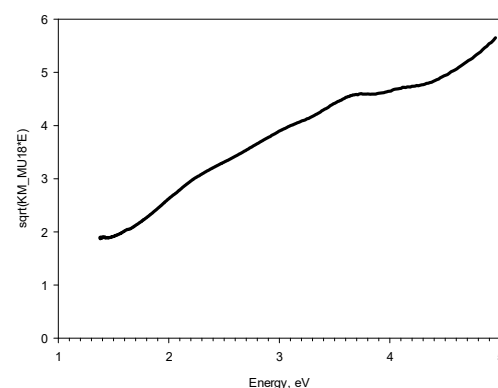
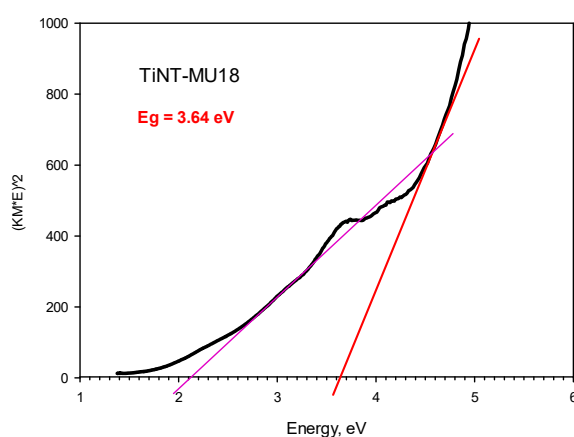
TiNT-MU6



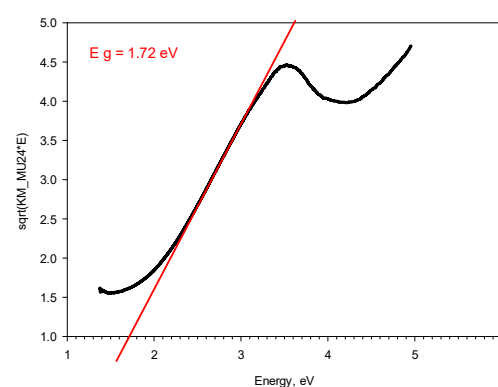
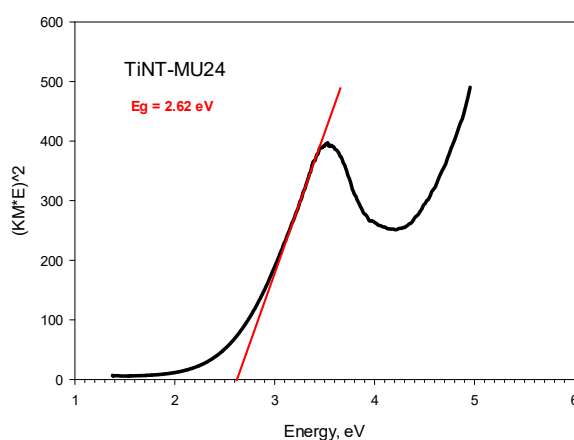
TiNT-MU12



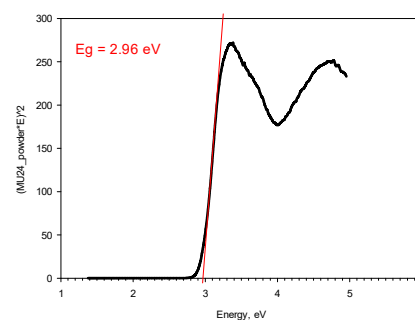
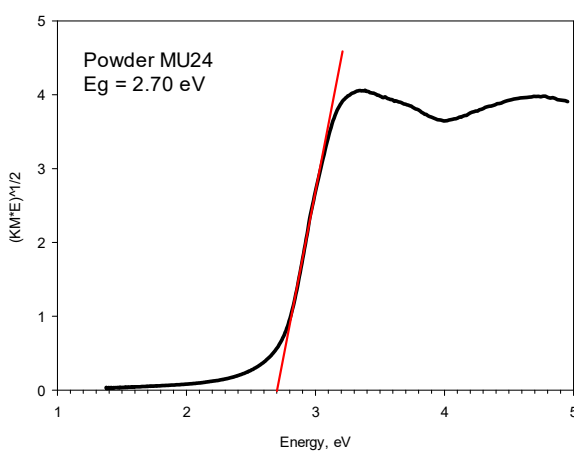
TiNT-MU18



TiNT-MU24



MU24



References

1. Tauc, J.; Grigorovici, R.; Vancu, A. Optical Properties And Electronic Structure of Amorphous Germanium. *Phys. Status Solidi B* **1966**, *15*, 627–637. <https://doi.org/10.1002/pssb.19660150224>
2. Małucha, P.; Pacia, M.; Macyk, W. How To Correctly Determine the Band Gap Energy of Modified Semiconductor Photocatalysts Based on UV–Vis Spectra. *J. Phys. Chem. Lett.* **2018**, *9*, 6814–6817. <https://dx.doi.org/10.1021/acs.jpcllett.8b02892>