SUPPORTING INFORMATION

How to Correctly Determine the Band Gap Energy of Modified Semiconductor Photocatalysts Based on UV-Vis Spectra

Patrycja Makuła, Michał Pacia and Wojciech Macyk⁎

Faculty of Chemistry, Jagiellonian University in Kraków, ul. Gronostajowa 2, 30-387 Kraków, Poland

⁎**Corresponding Author:** macyk@chemia.uj.edu.pl

In addition to the experiment described in the paper the diffuse reflectance spectra of a ground mixture of titanium dioxide (TiO_2, anatase, AK-1, *Tronox*) with beta carotene (BC, Sigma-Aldrich) were analyzed (BC+TiO_2, 1:1 mass ratio), as well as the spectral sums of two components (BC and TiO_2, BC|TiO_2). The study also involved: i) rutile TiO_2 doped with Fe^{3+} and VO_3^- (synthesized in our laboratory); ii) catechol (Sigma-Aldrich) adsorbed at anatase TiO_2 and iii) a mixture of two semiconductors, CdS (Sigma-Aldrich) and anatase TiO_2. The spectra were recorded using a UV-Vis-NIR spectrophotometer (UV-3600 Shimadzu) equipped with a 15 cm integrating sphere in the spectral range of 250-800 nm. Barium sulfate ($BaSO_4$, *Riedel-de Haen*) was used to dilute the samples (1:100) and as a reference. The band gap energies were determined by approaches described in the paper. All determined values of E_g were collected in the Table S1 and Table S2.

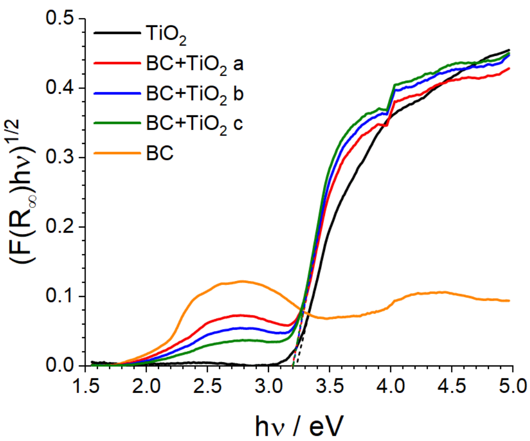

Figure S1. The Tauc plots of the BC+TiO_2 sample, bare TiO_2 and carotene. Spectra 1-3 were recorded for the same pellet differently placed in the holder. Linear fit for measurement a (red line), b (blue line) and c (green line) overlap.

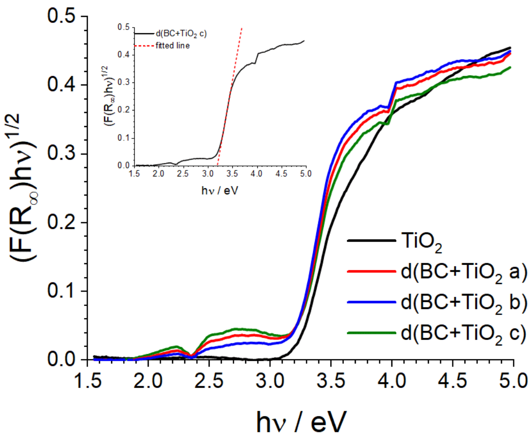

Figure S2. The Tauc plots of the differential spectra of the sample BC+TiO_2 and bare TiO_2. The determination of E_g for measurement c is shown.

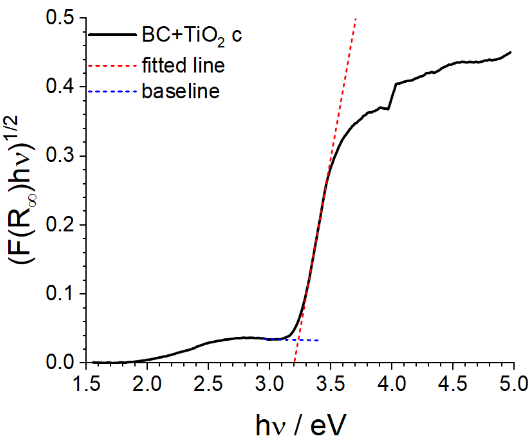

Figure S3. Transformed reflectance spectrum plot of system BC+TiO_2. The determination of E_g is shown.

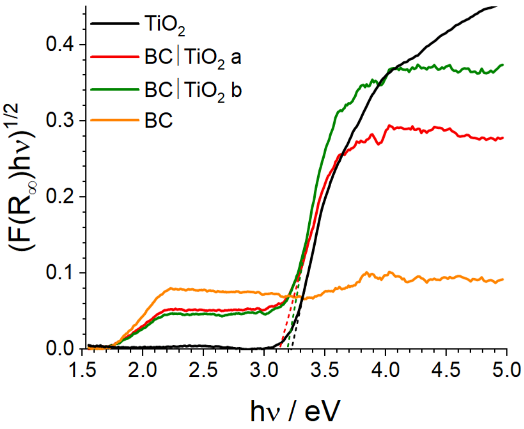

Figure S4. The Tauc plots of the BC|TiO_2 sample, bare TiO_2 and carotene. Spectra a,b were recorded for the same pellet differently placed in the holder. The inset shows schematically the BC+TiO_2 sample in the holder.

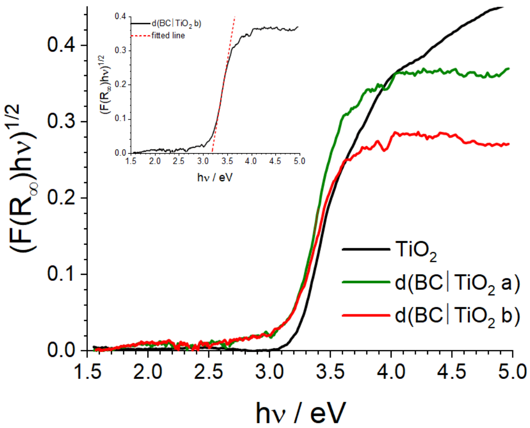

Figure S5. The Tauc plots of the differential spectra of the sample BC|TiO_2 and bare TiO_2. The determination of E_g for measurement b is shown.

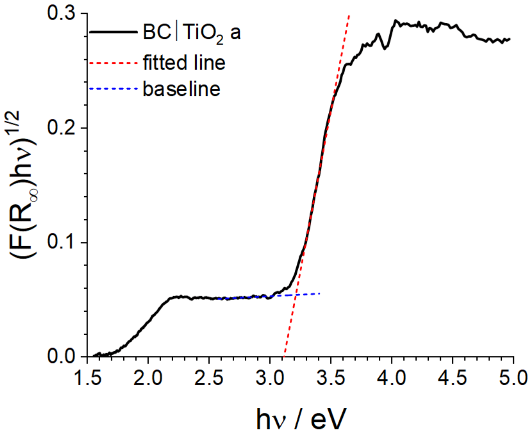

Figure S6. Transformed reflectance spectrum plot of system BC|TiO_2. The determination of E_g is shown.

Table S1. Experimental E_g values obtained with different methods.

Materials	Energy band gap $\pm$0.03 [eV]		
	Tauc plot	Differential spectra	Baseline approach
TiO_2	3.22	-	-
BC+TiO_2	3.19	3.20	3.25
	3.19	3.20	3.24
	3.19	3.20	3.23
BC|TiO_2	3.12	3.20	3.20
	3.18	3.19	3.23

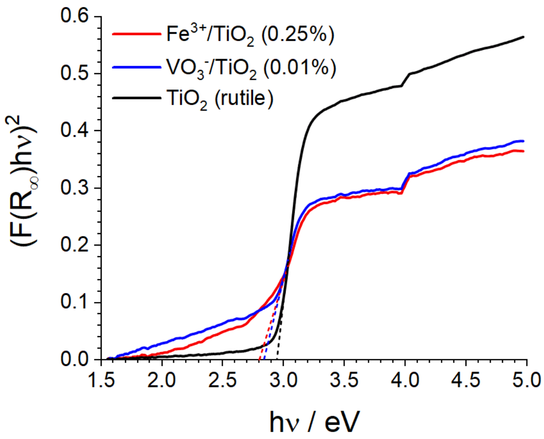

Figure S7. Tauc plots of the doped samples and bare TiO_2.

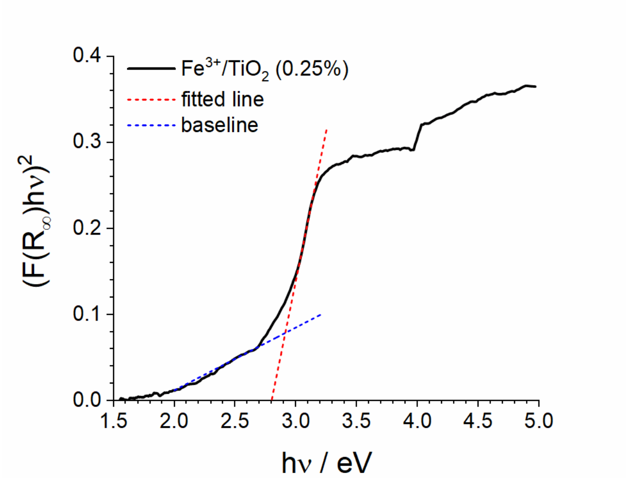

Figure S8. Transformed diffuse reflectance spectrum of Fe^{3+}/TiO_2 sample. The determination of E_g is shown.

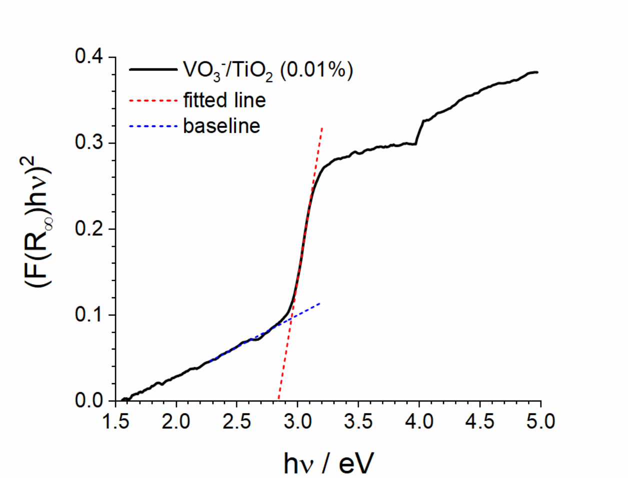

Figure S9. Transformed diffuse reflectance spectrum of VO_3^-/TiO_2 sample. The determination of E_g is shown.

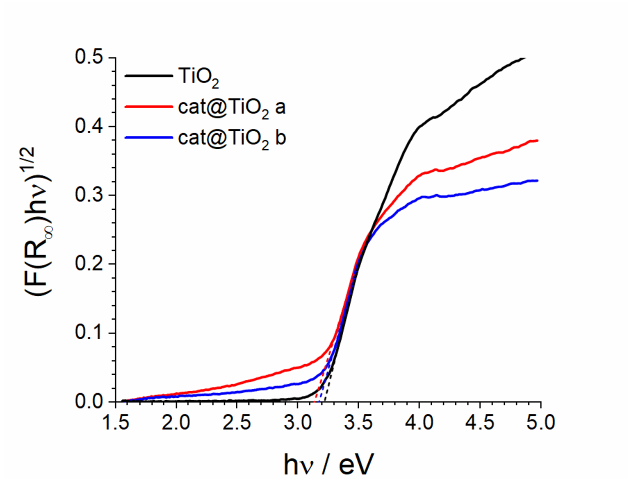

Figure S10. The Tauc plots of cat@TiO_2 samples and bare TiO_2. Spectra a, b were recorded for different concentrations of the samples.

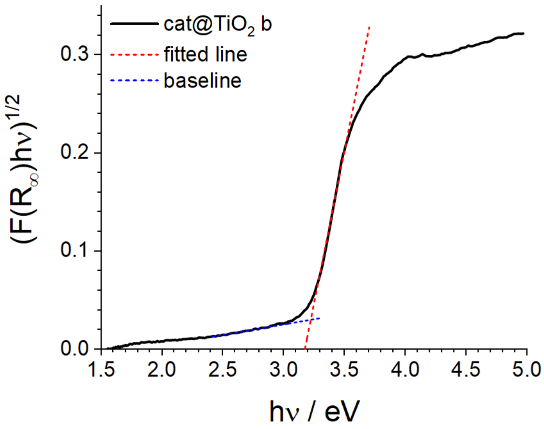

Figure S11. Transformed diffuse reflectance spectrum of cat@TiO_2. The determination of E_g is shown.

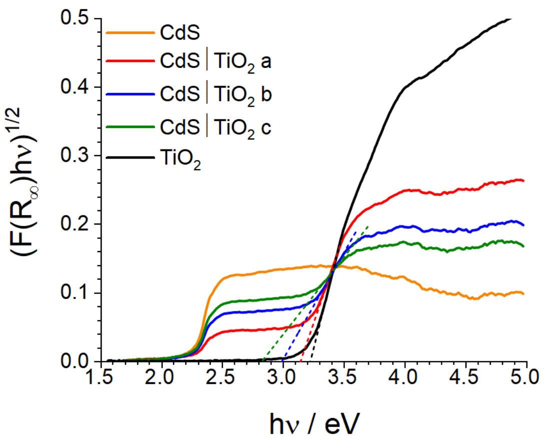

Figure S12. The Tauc plots of the CdS|TiO_2 sample and bare TiO_2. Spectra a, b were recorded for the same pellet differently placed in the holder.

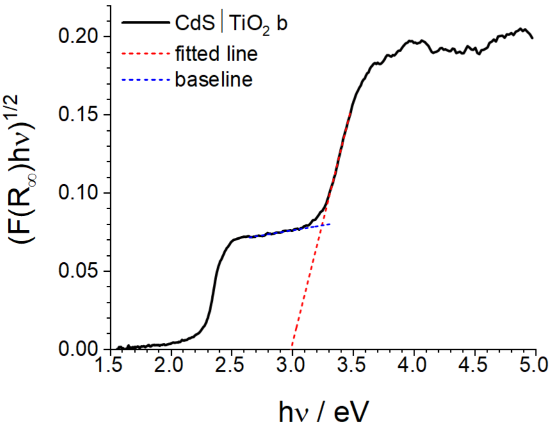

Figure S13. Transformed diffuse reflectance spectrum of CdS|TiO_2. The determination of E_g is shown.

Table S2. Experimental E_g values obtained from the application of Tauc plot and baseline approach in doped/coupled/non-interacting systems.

Materials	**Energy band gap ± 0.03 [eV]**	
	Tauc plot	Baseline approach
Rutile	2.94	-
CdS|TiO_2	3.13	3.23
	2.98	3.23
	2.81	3.23
cat@TiO_2	3.13	3.23
	3.17	3.22
Fe^{3+}/TiO_2 (rutile)	2.79	2.91
VO_3^-/TiO_2 (rutile)	2.83	2.94

The band gap energy of BC+TiO_2, MO+TiO_2, BC|TiO_2 and MO|TiO_2 systems was also determined using the Cody method, which is based on the (α /

$(E))^{-½}$ vs. $(E - E_g)$ transformation.[1] The determined values are summarized in Table S3.

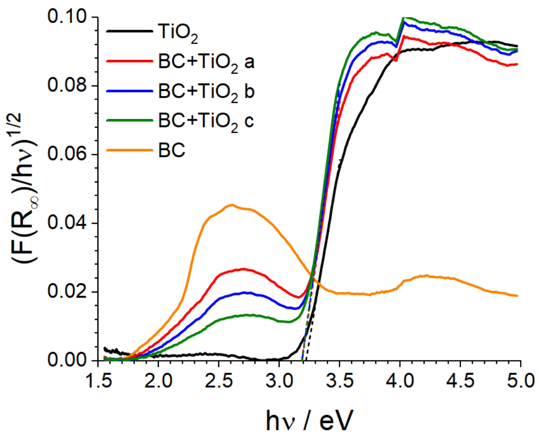

Figure S14. The Cody plots of the BC+TiO_2 sample, bare TiO_2 and carotene. Spectra a-c were recorded for the same pellet differently placed in the holder. Linear fit for measurement a (red line), b (blue line) and c (green line) overlap.

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[1] Liu, P.; Longo, P.; Zaslavsky, A.; Pacifici, D. Optical bandgap of single-and multi-layered amorphous germanium ultra-thin films. *J. Appl. Phys.* **2016,** *119*, 014304.

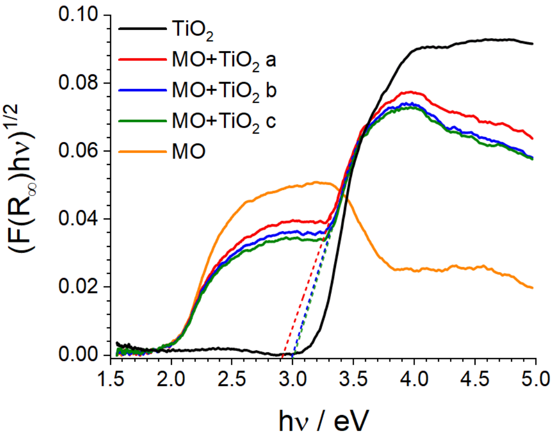

Figure S15. The Cody plots of the MO+TiO_2 sample, bare TiO_2 and carotene. Spectra a-c were recorded for the same pellet differently placed in the holder. Linear fit for measurement b (blue line) and c (green line) overlap.

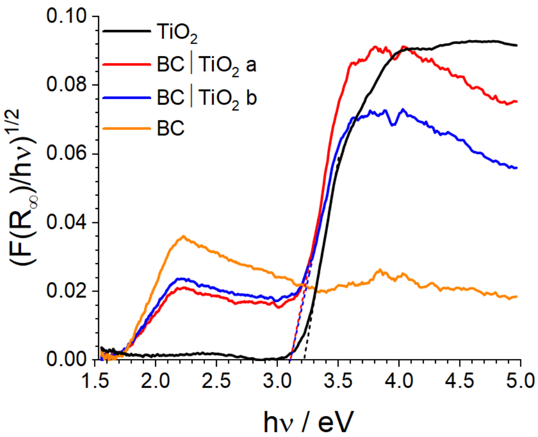

Figure S16. The Cody plots of the BC|TiO_2 sample, bare TiO_2 and carotene. Spectra a,b were recorded for the same pellet differently placed in the holder. Linear fit for measurement a (red line) and b (blue line) overlap.

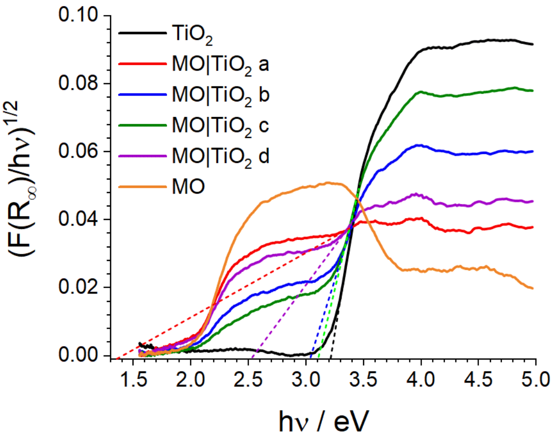

Figure S17. The Cody plots of the MO+TiO_2 sample, bare TiO_2 and carotene. Spectra a-d were recorded for the same pellet differently placed in the holder.

Table S3. Experimental E_g values obtained from the direct application of the Cody plot.

Materials	**Energy band gap ± 0.03 [eV]**
TiO_2	3.22
BC+TiO_2	3.18
	3.18
	3.18
BC|TiO_2	3.10
	3.10
MO|TiO_2	1.40
	3.04
	3.11
	2.54
MO+TiO_2	2.92
	2.99
	3.01

Analysis of the results presented in Table 3 and Figures S14-S17 shows, that also for this transformation a direct application of Cody plots leads to underestimated values of E_g. Therefore, the approaches similar to those presented in the paper should be applied here. The baseline approach can and should be applied to the Cody plots, since it subjects to the same laws as the Tauc transformation. In this case the baseline also equates the modifier absorption coefficient to 0 and the band gap energy can be obtained directly from the Cody plot.