

Enhancement of Photocatalytic Activity and Microstructural Growth of Cobalt-Substituted $\text{Ba}_{1-x}\text{Co}_x\text{TiO}_3$ $\{x = 0, \dots, 1\}$ Heterostructure

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*****supplementary materials *****

1. Experimental Process

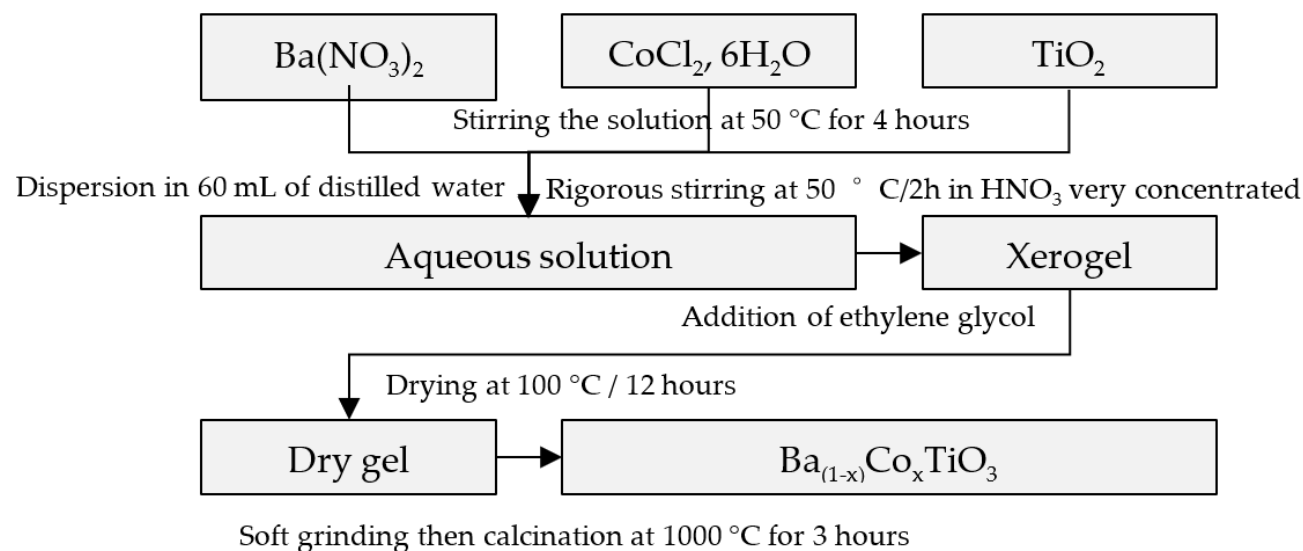


Figure S1. Flow chart of the sol-gel processing of $(x = \{0, \dots, 1\})$ powder ceramics.

2. Materials and Methods: Photocatalytic Application

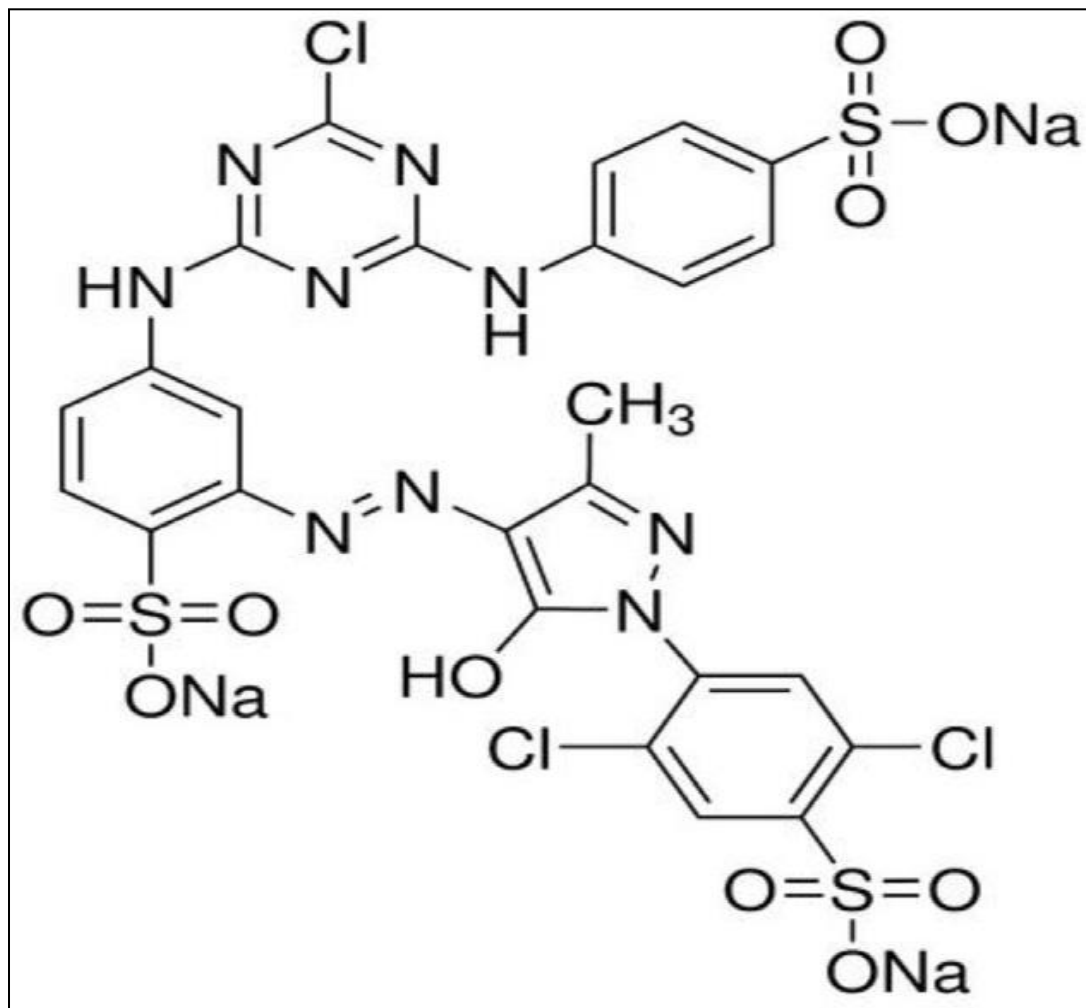


Figure S2. Characteristics and chemical formula of Cibacron Brilliant Yellow 3G-P (Y).

3. Qualitative PXRD analysis

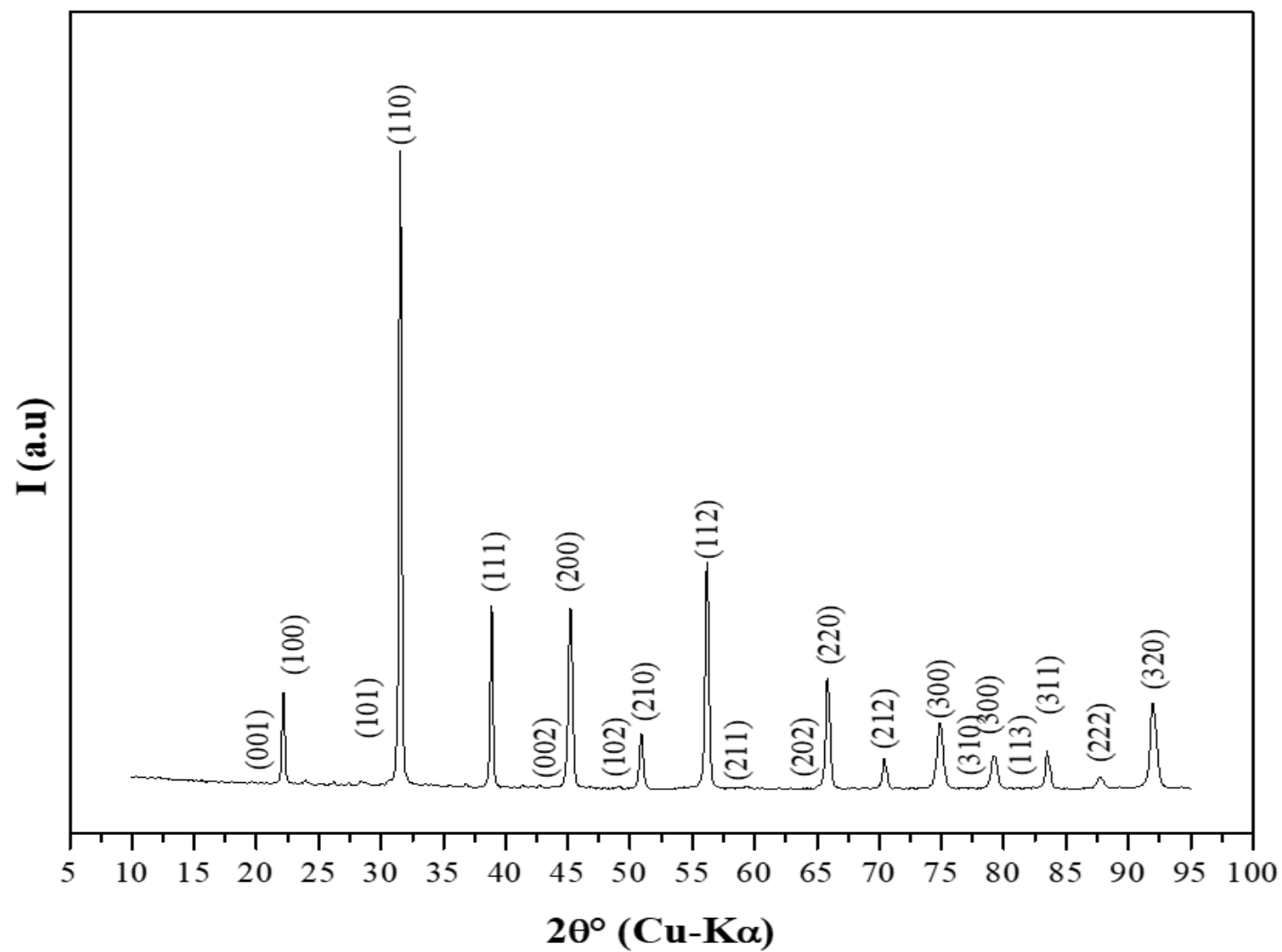


Figure S3. Powder x-ray diffraction pattern of synthesized pure BT nanoparticles heated at 1000 °C.

Quantitative PXRD analysis

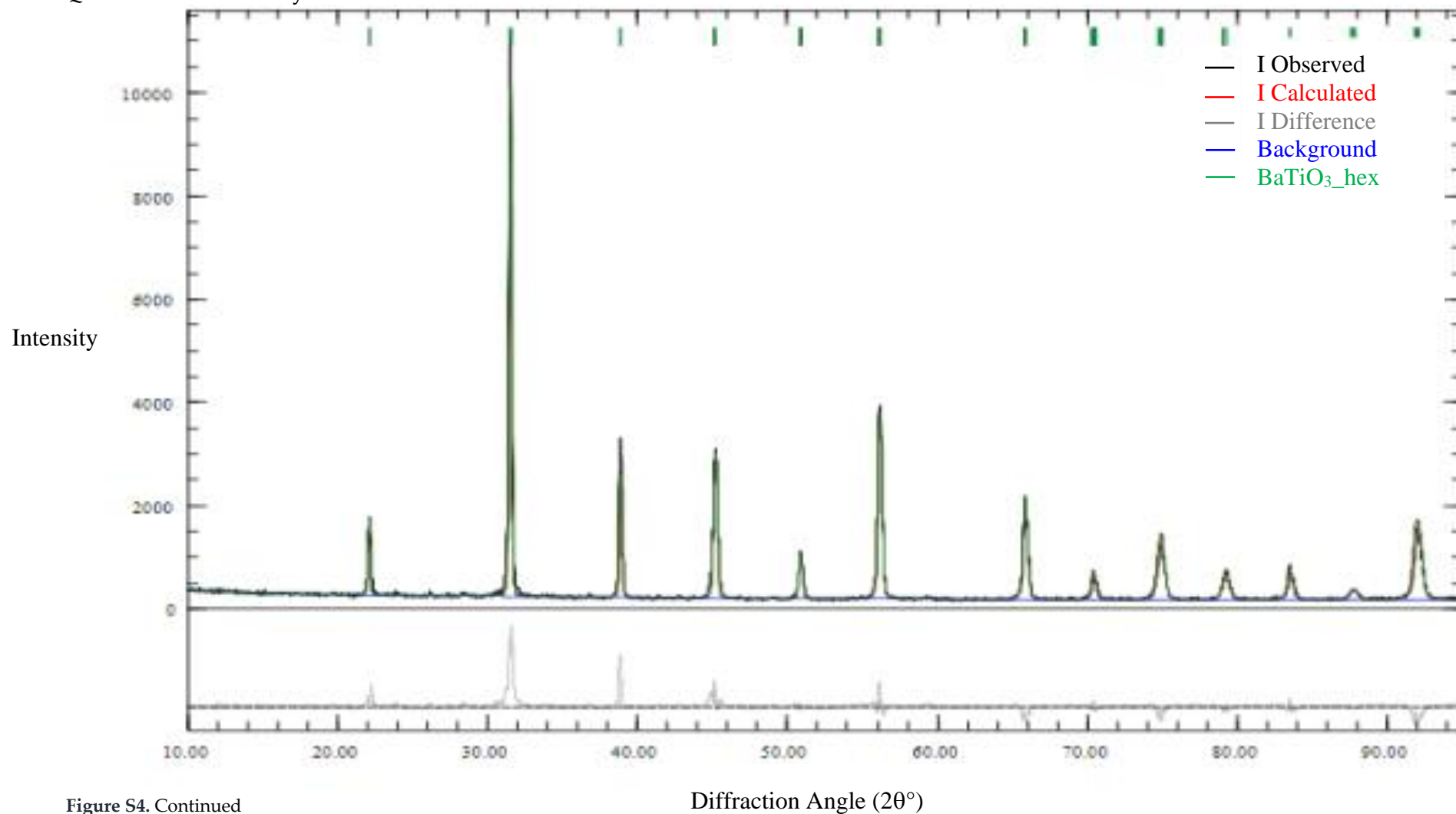


Figure S4. Continued

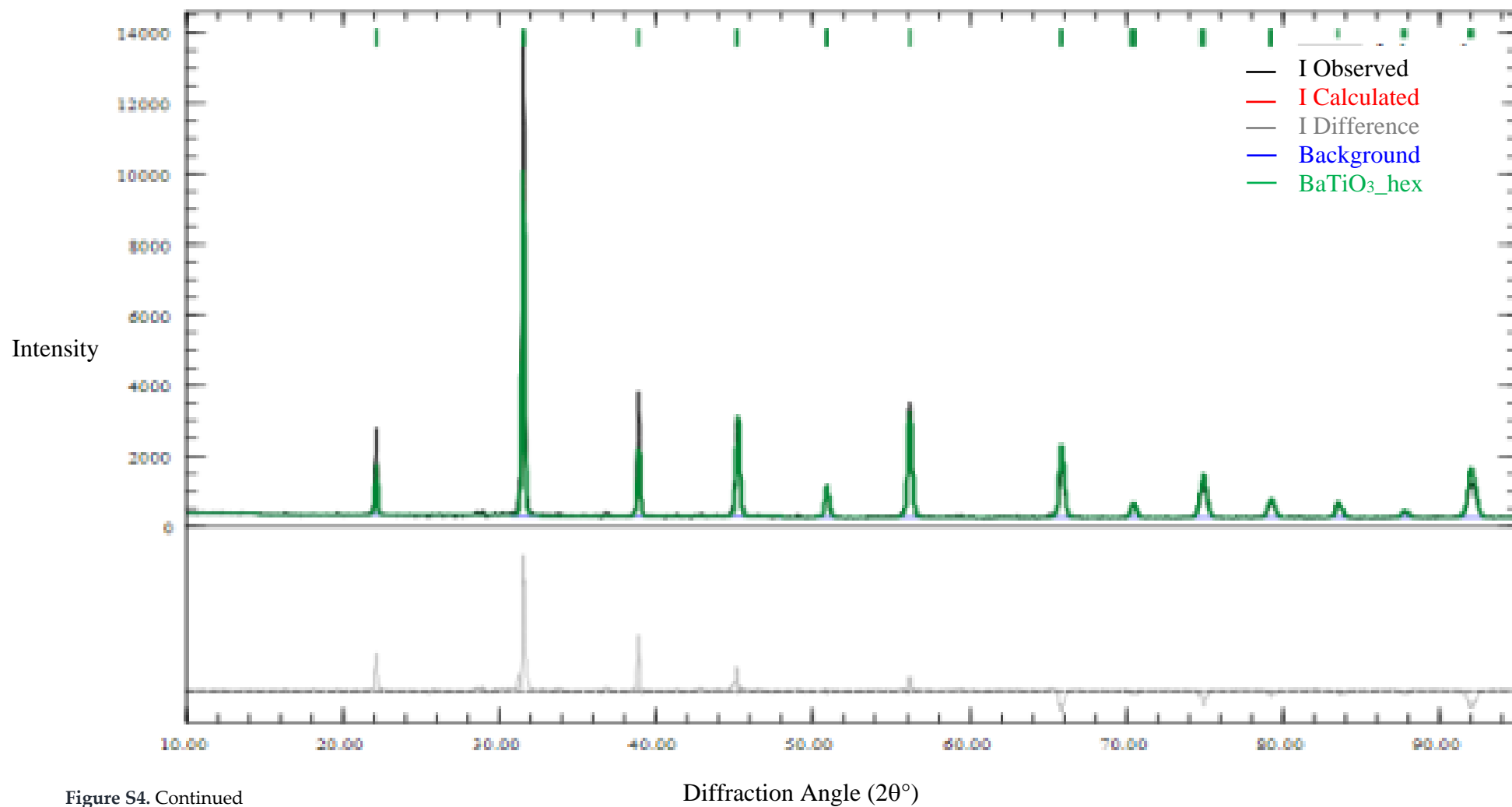


Figure S4. Continued

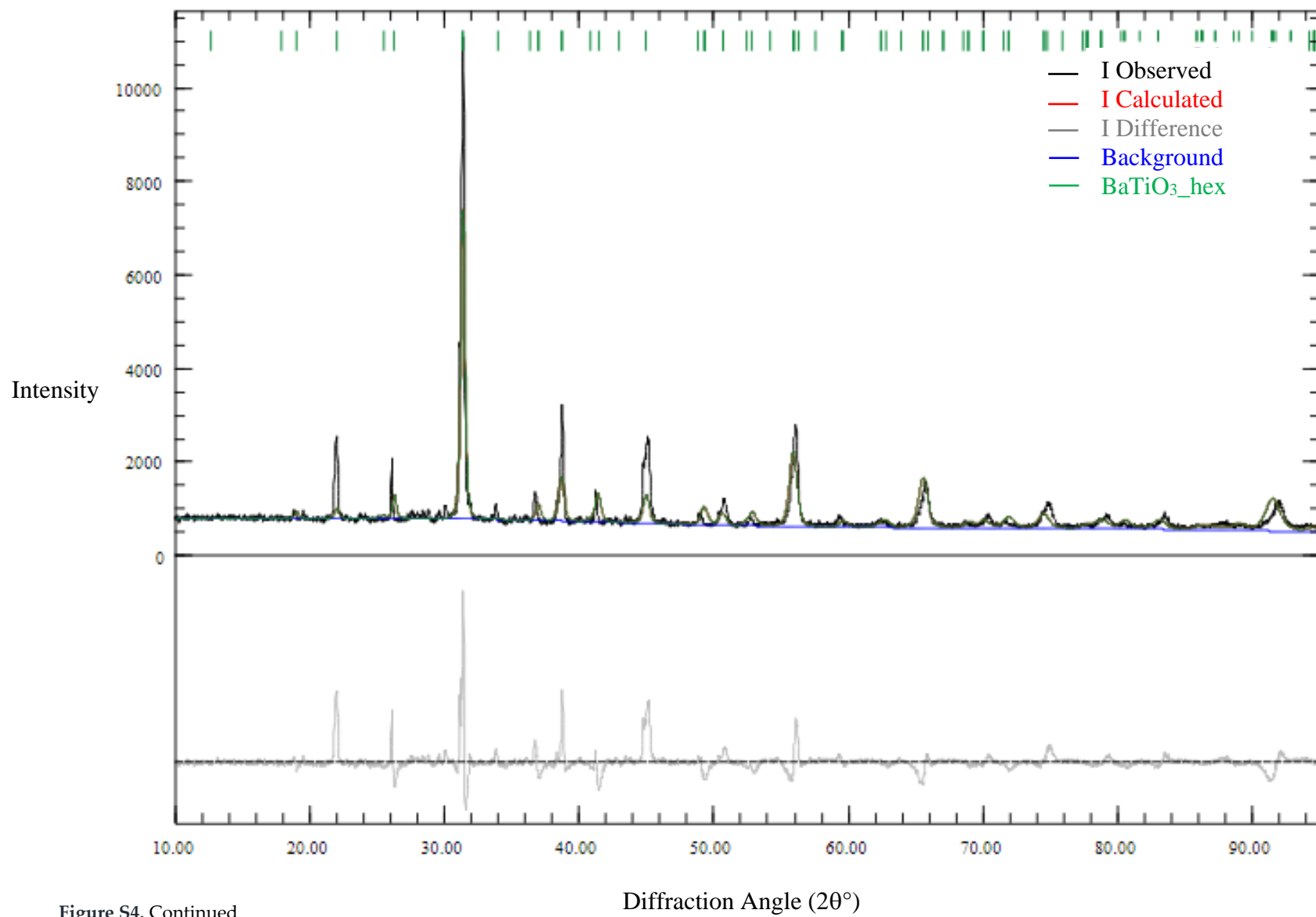


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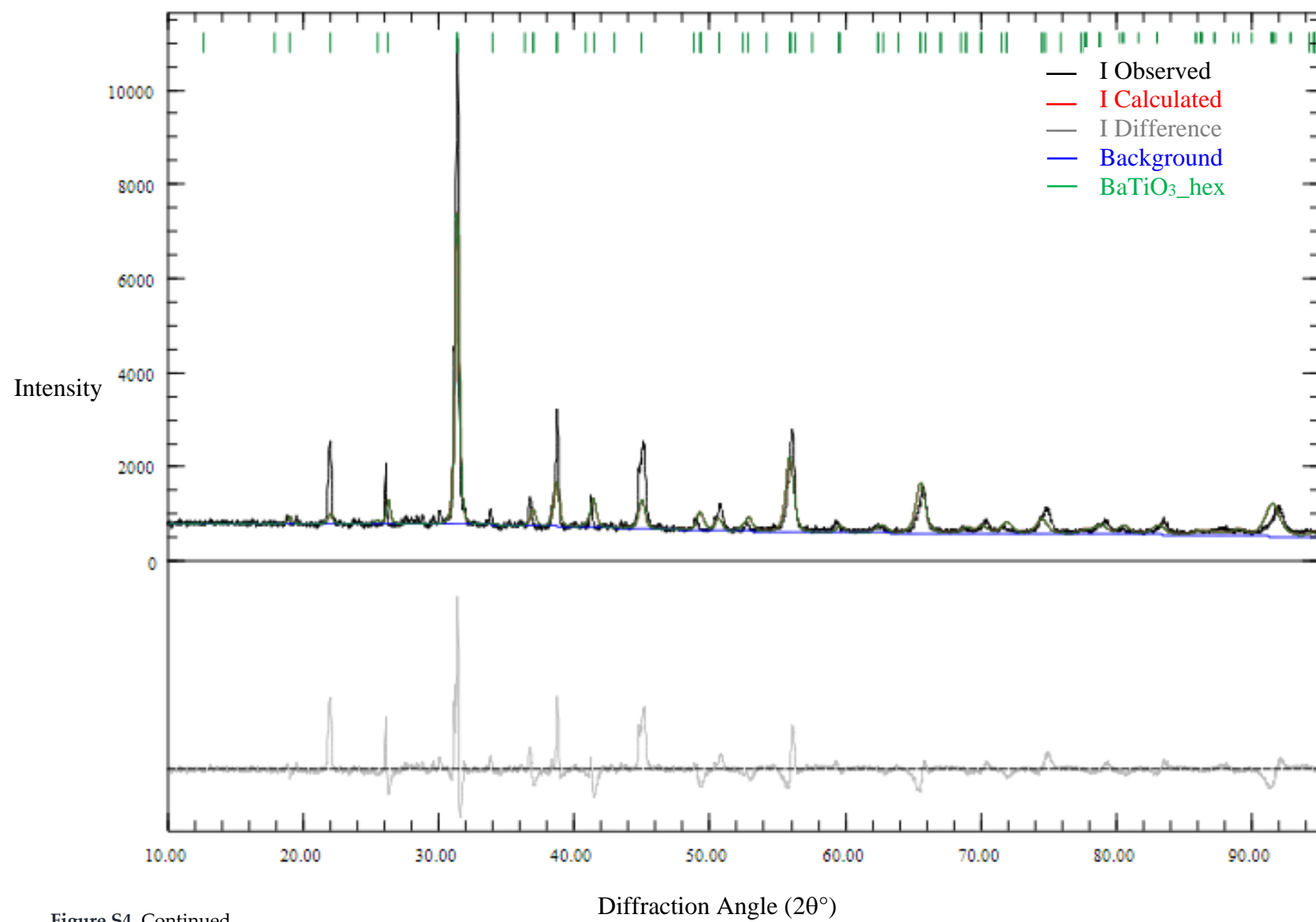


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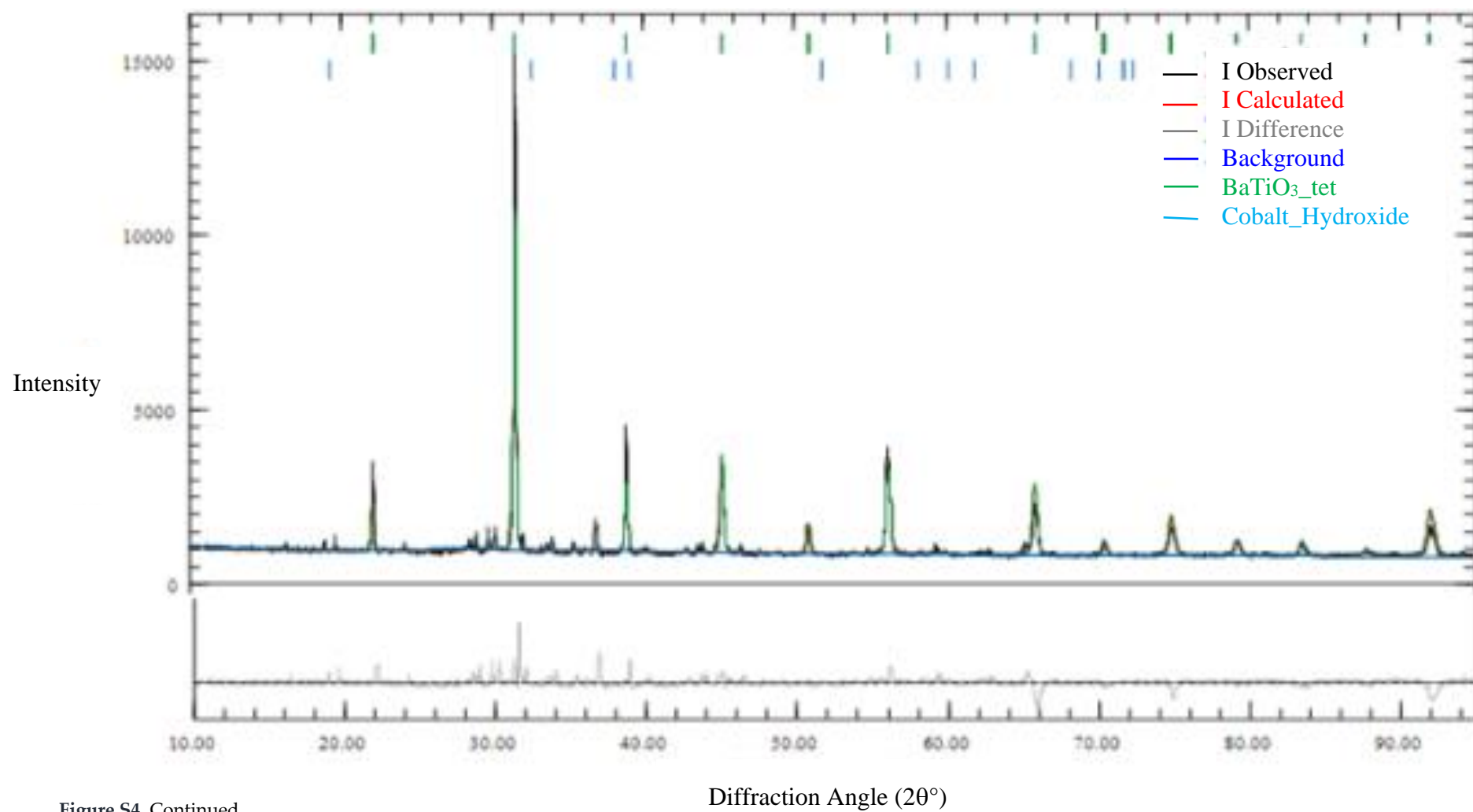


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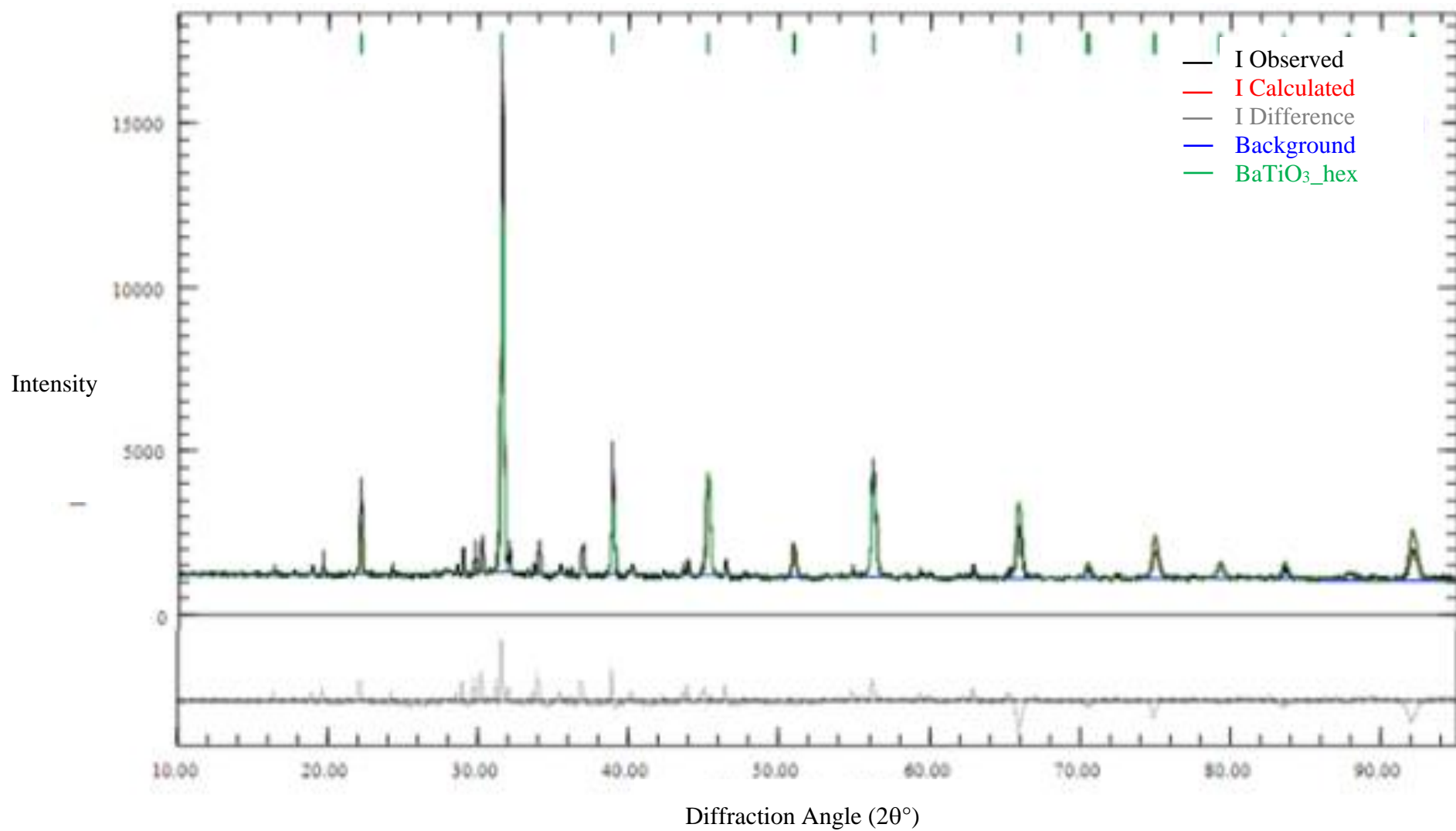


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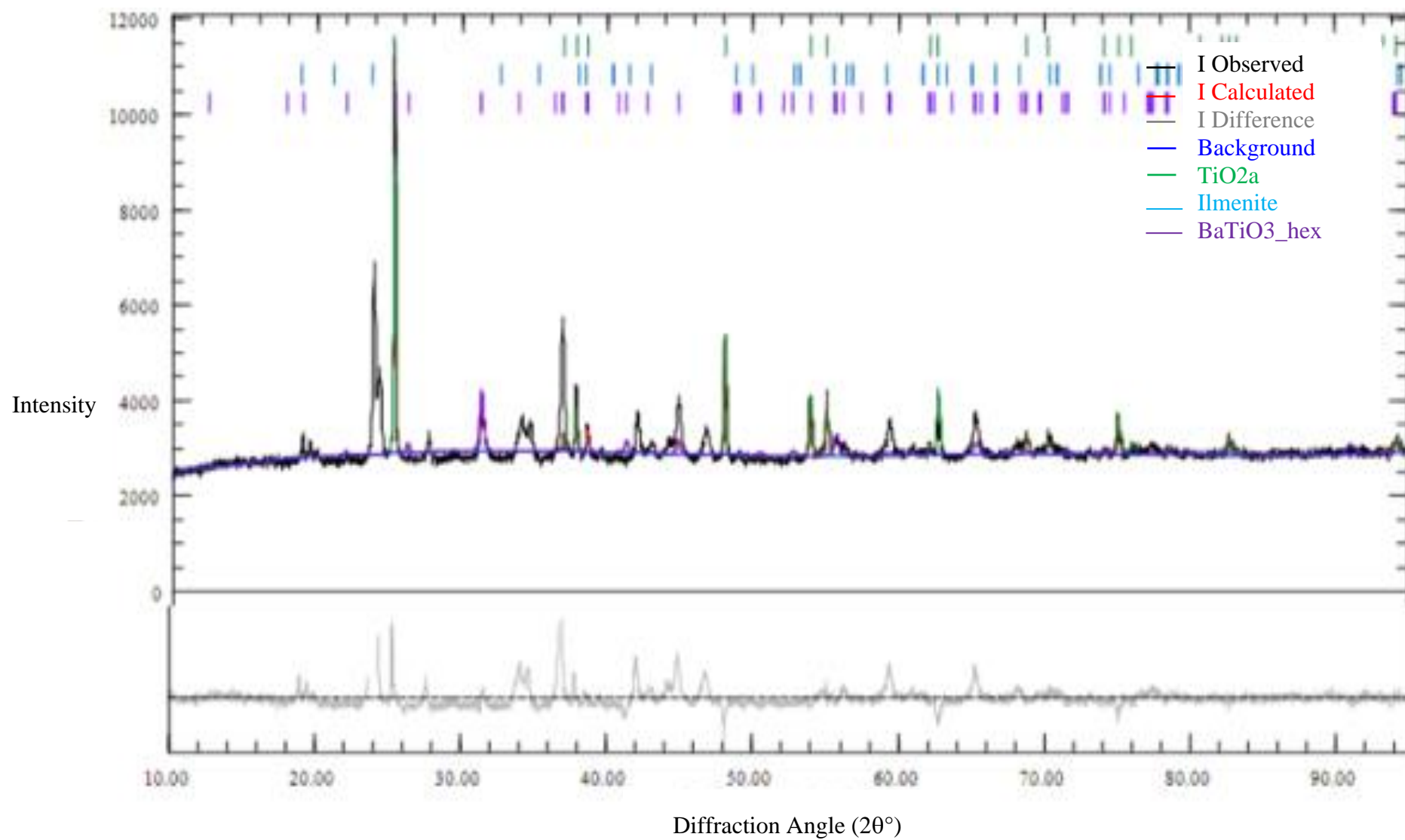


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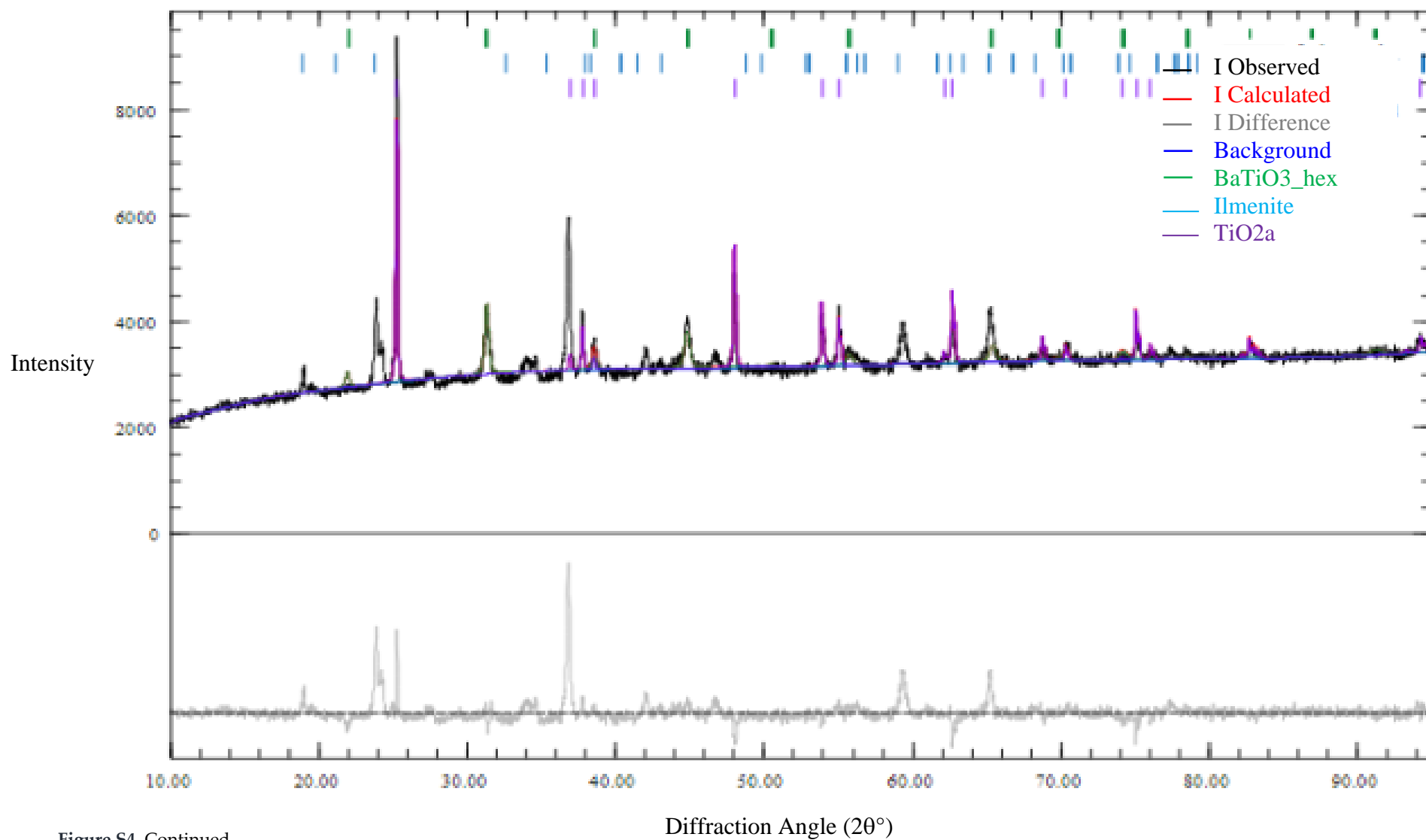


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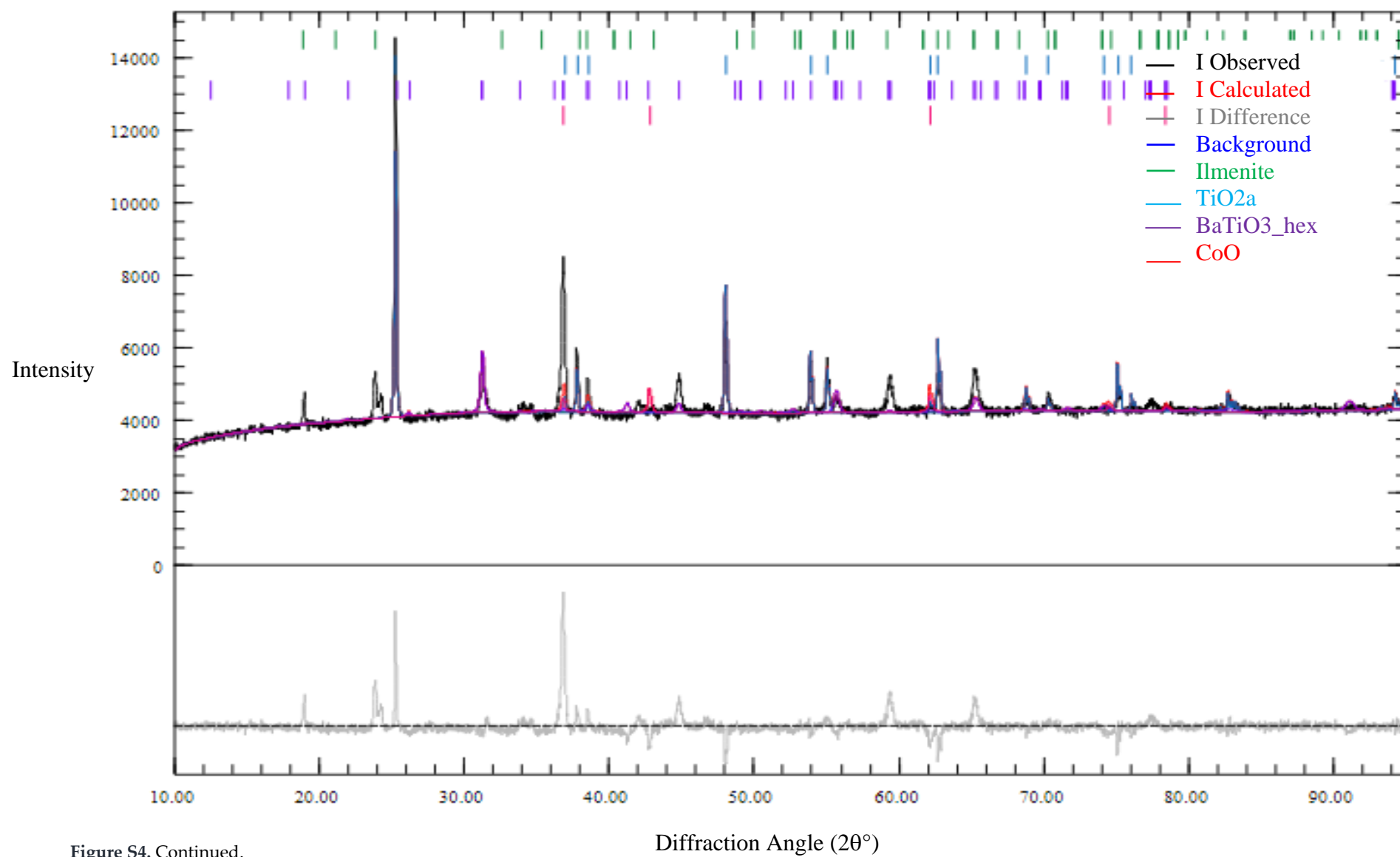


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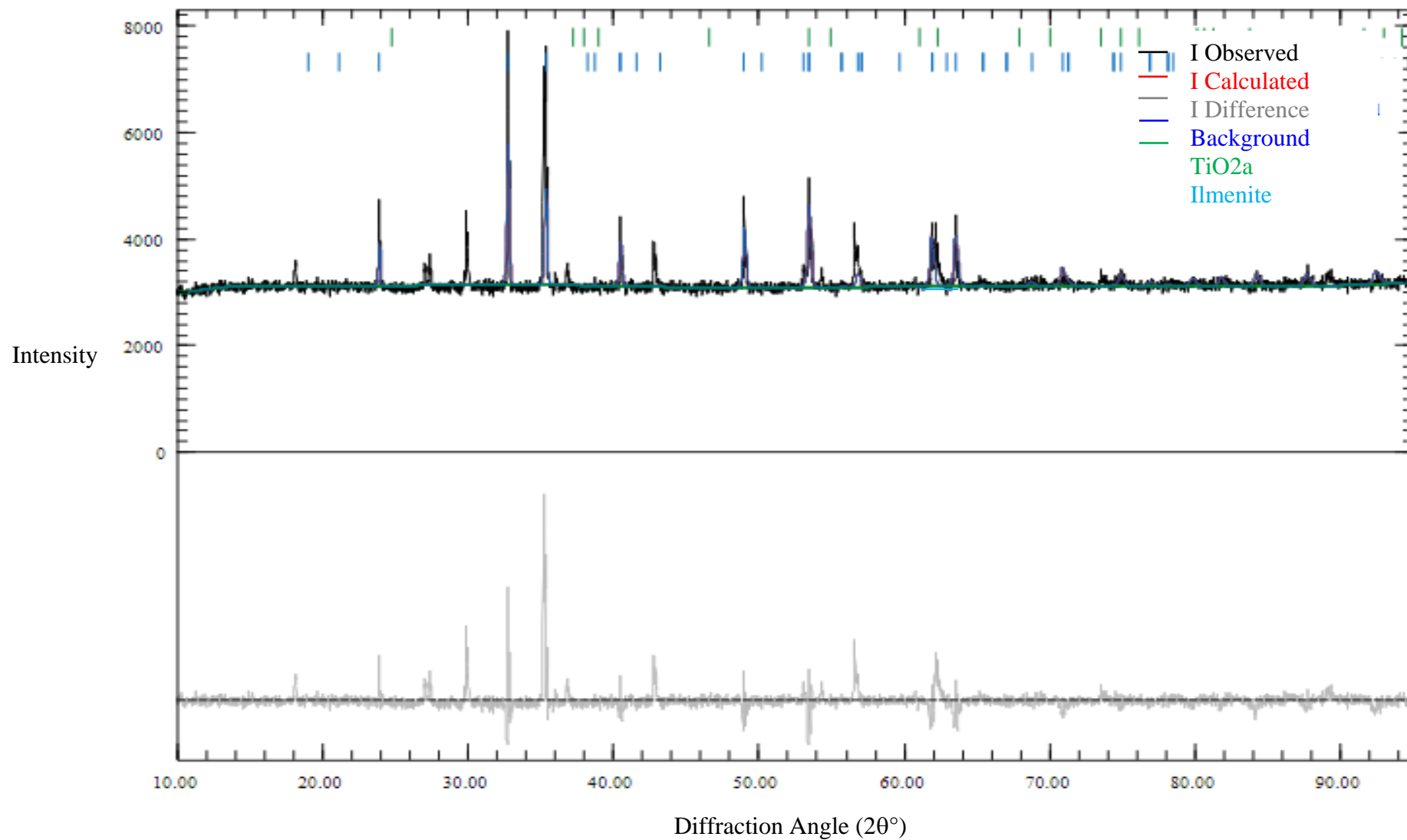


Figure S4. Rietveld refinement of synthesized (a) Ba_{0.9}Co_{0.1}TiO₃, (b) Ba_{0.8}Co_{0.2}TiO₃, (c) Ba_{0.7}Co_{0.3}TiO₃, (d) Ba_{0.6}Co_{0.4}TiO₃, (e) Ba_{0.5}Co_{0.5}TiO₃, (f) Ba_{0.4}Co_{0.6}TiO₃, (g) Ba_{0.3}Co_{0.7}TiO₃, (h) Ba_{0.2}Co_{0.8}TiO₃, (i) Ba_{0.1}Co_{0.9}TiO₃, and (j) CoTiO₃ structure using Profex BGMN software.

4. TEM

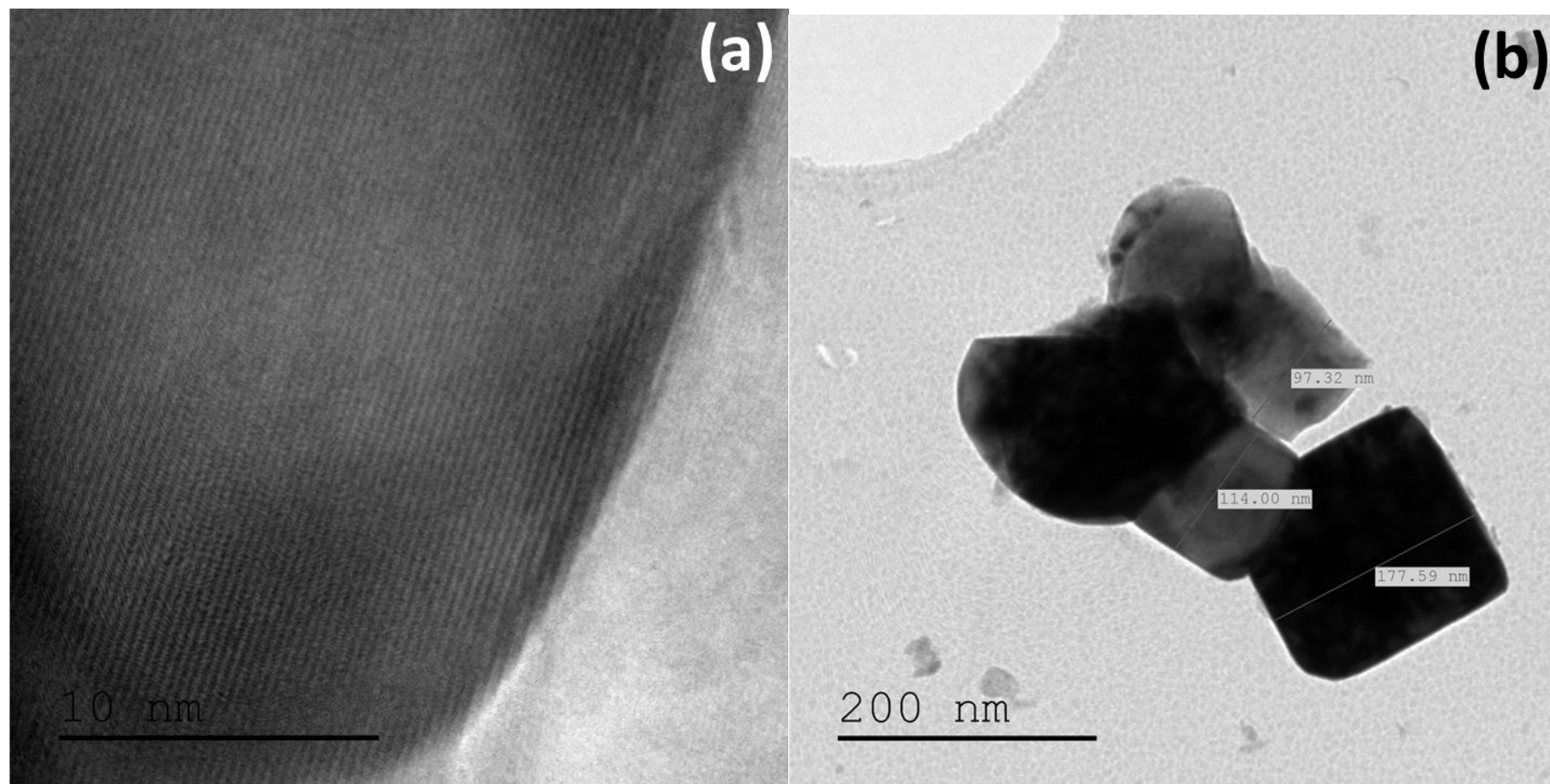


Figure S5. Continued.

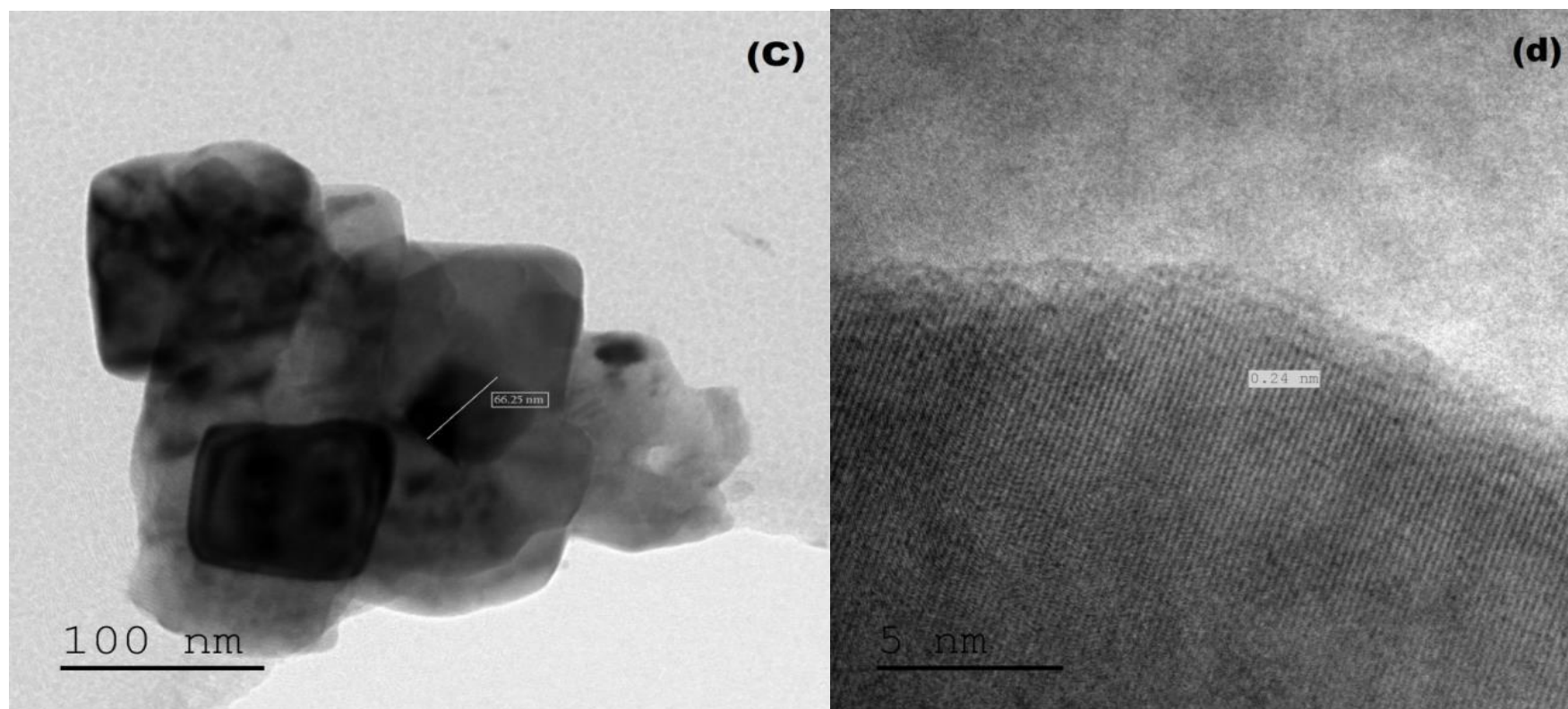


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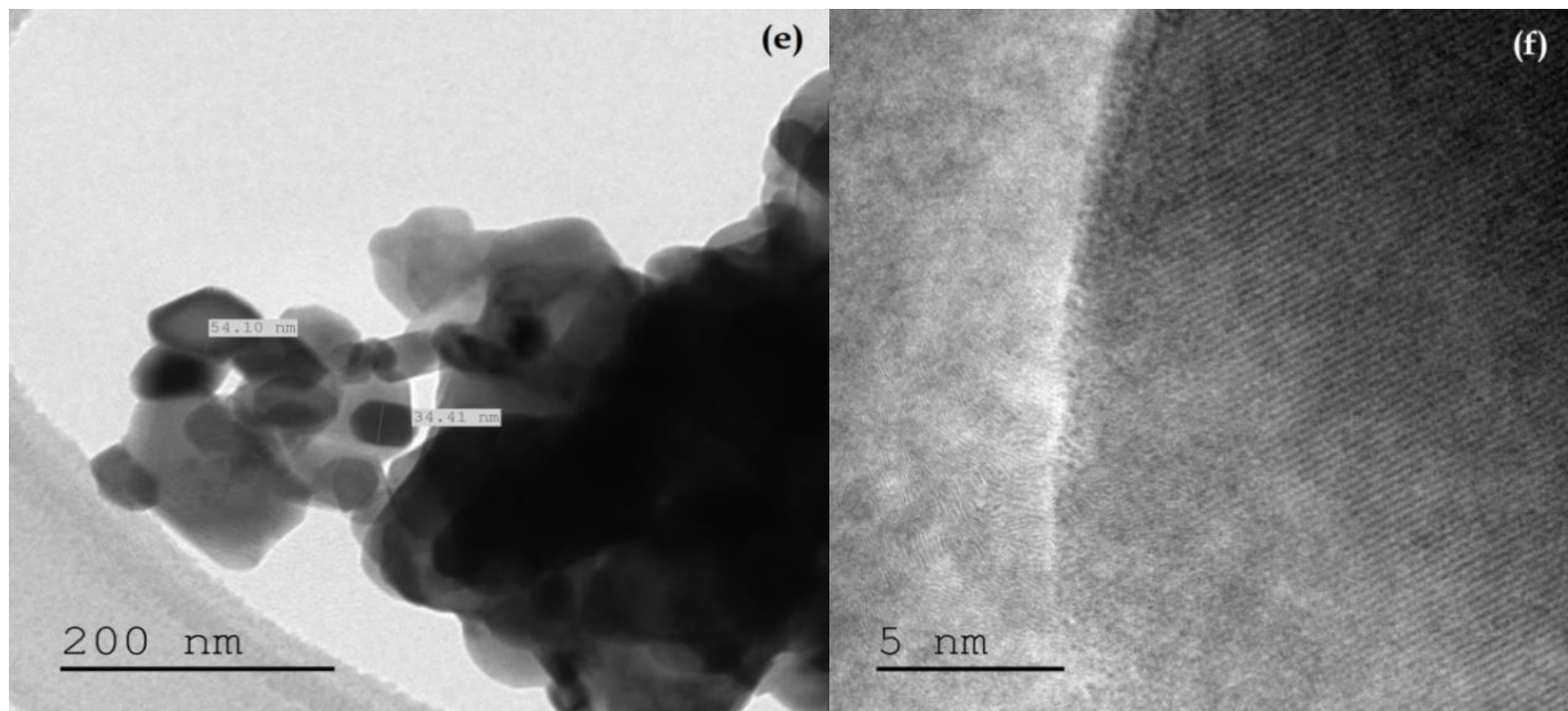


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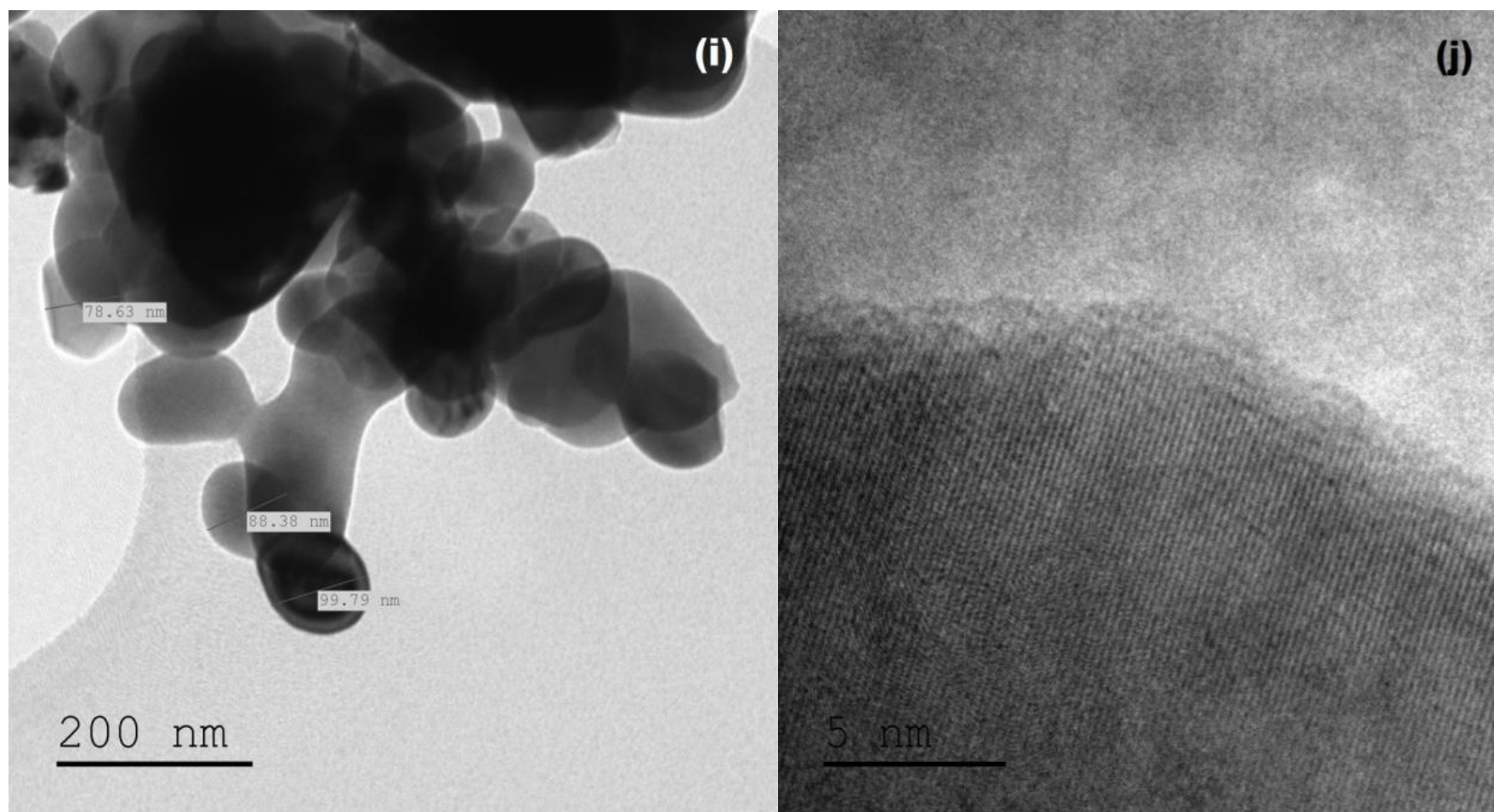


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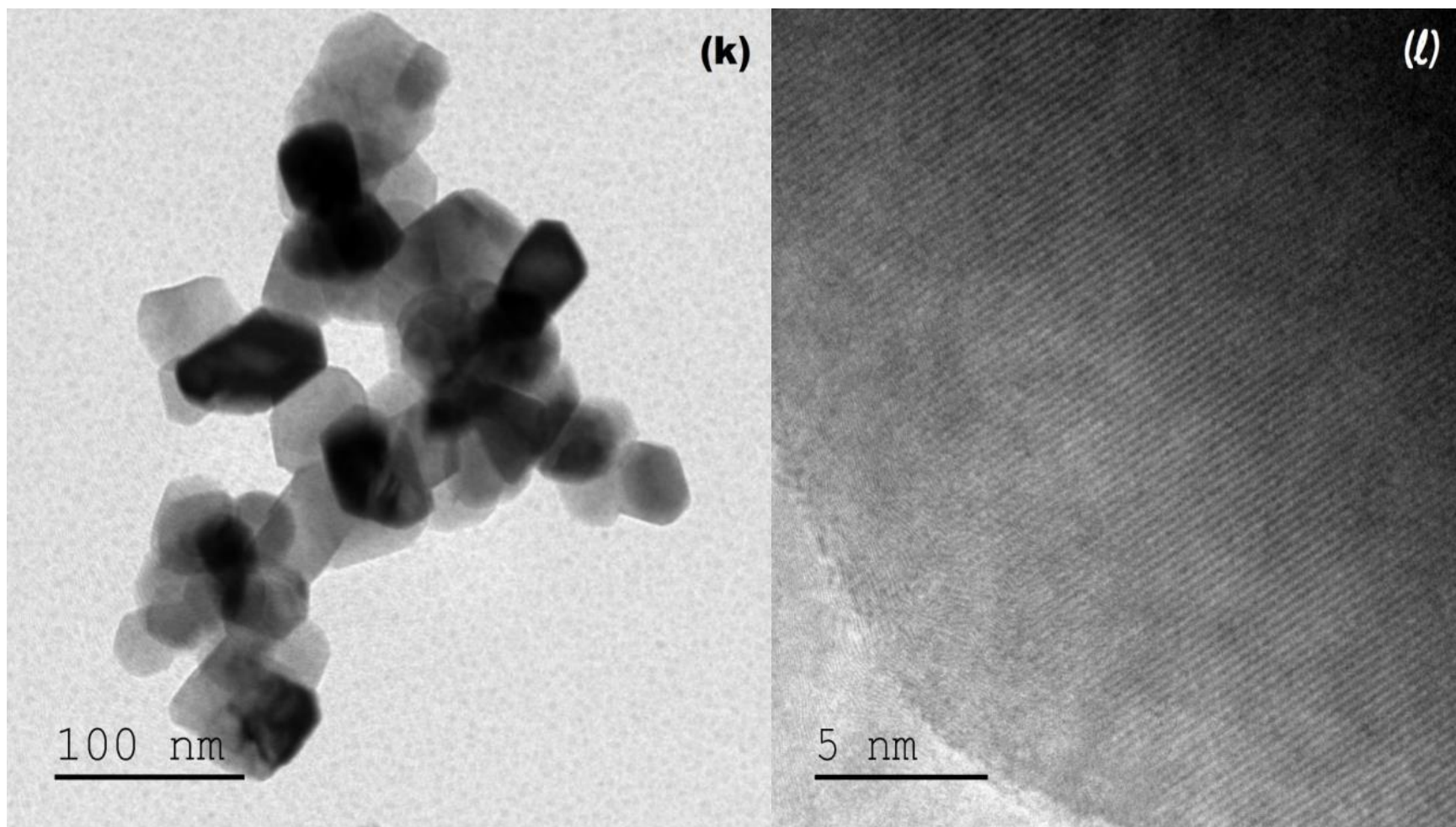


Figure S5. TEM micrographs and high-resolution images, respectively for (a), (b) pure BT sample, (c)-(d) $\text{Ba}_{1-x}\text{Co}_x\text{TiO}_3$ sample with $x = 0.2$; (e)-(f) $\text{Ba}_{1-x}\text{Co}_x\text{TiO}_3$ sample with $x = 0.4$; (i)-(j) $\text{Ba}_{1-x}\text{Co}_x\text{TiO}_3$ sample with $x = 0.8$, and (k)-(l) $\text{Ba}_{1-x}\text{Co}_x\text{TiO}_3$ sample with $x = 1$ (CoTiO_3 complex).

5. UV-Visible

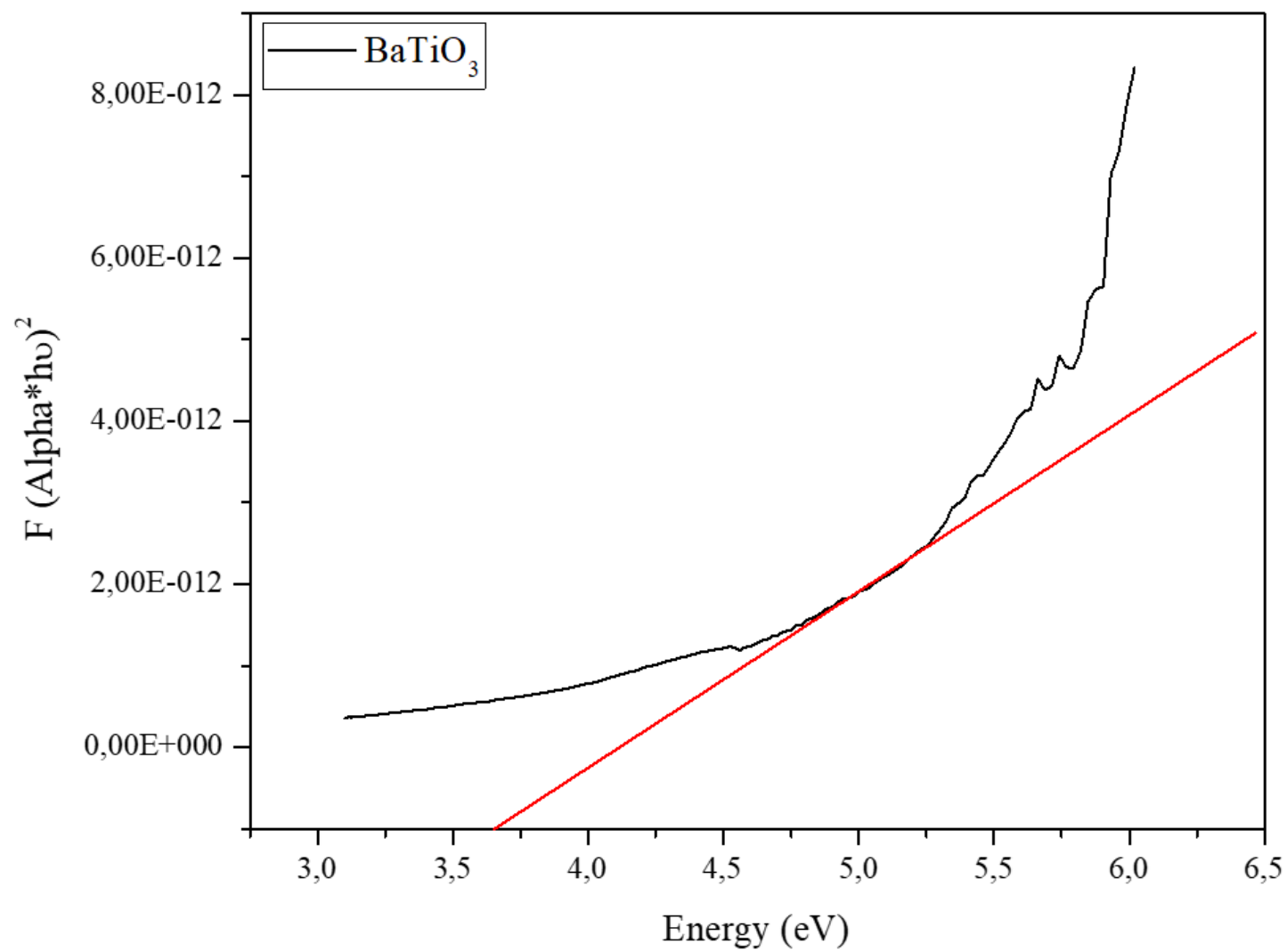
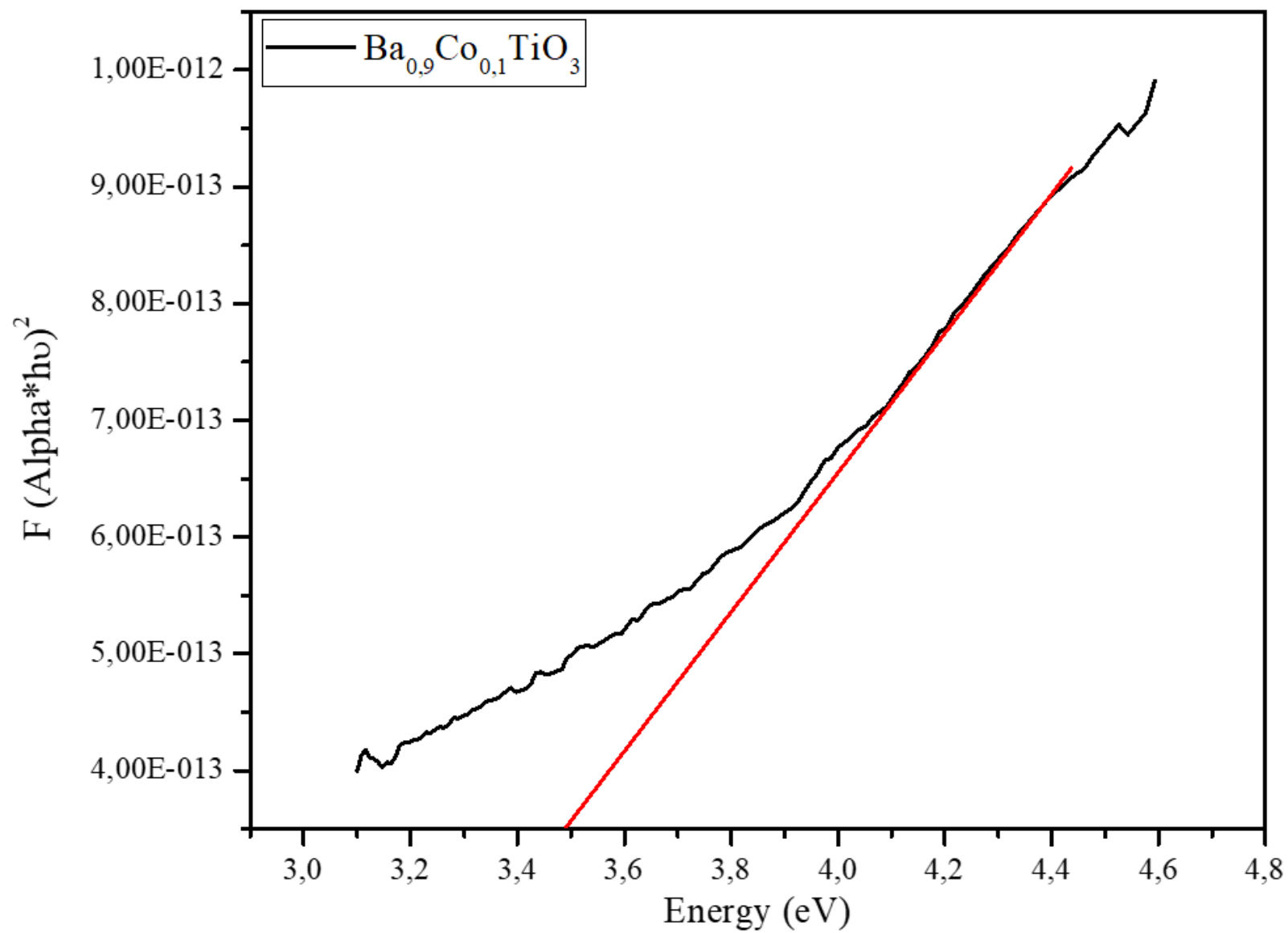
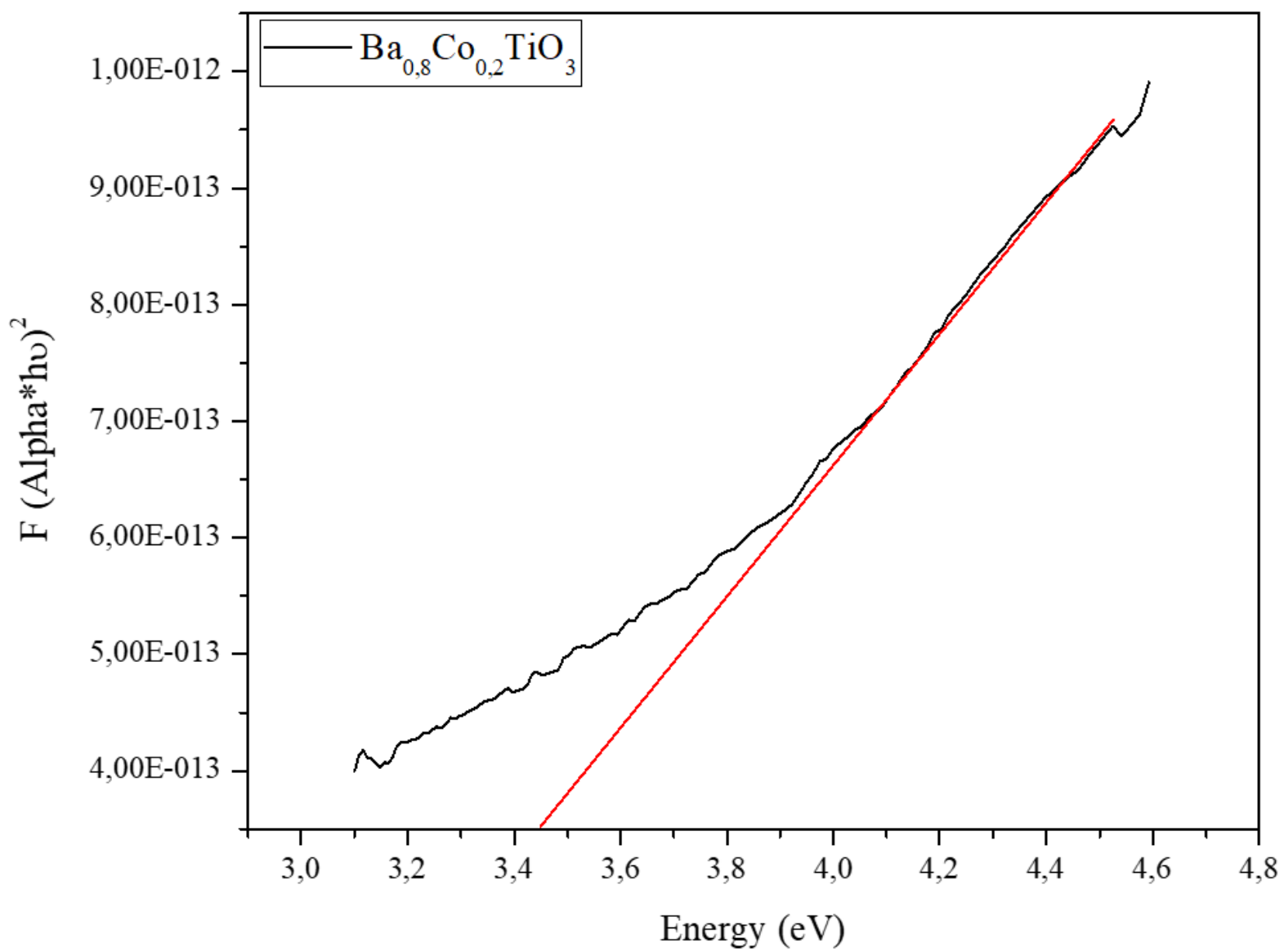


Figure S6. Continued.



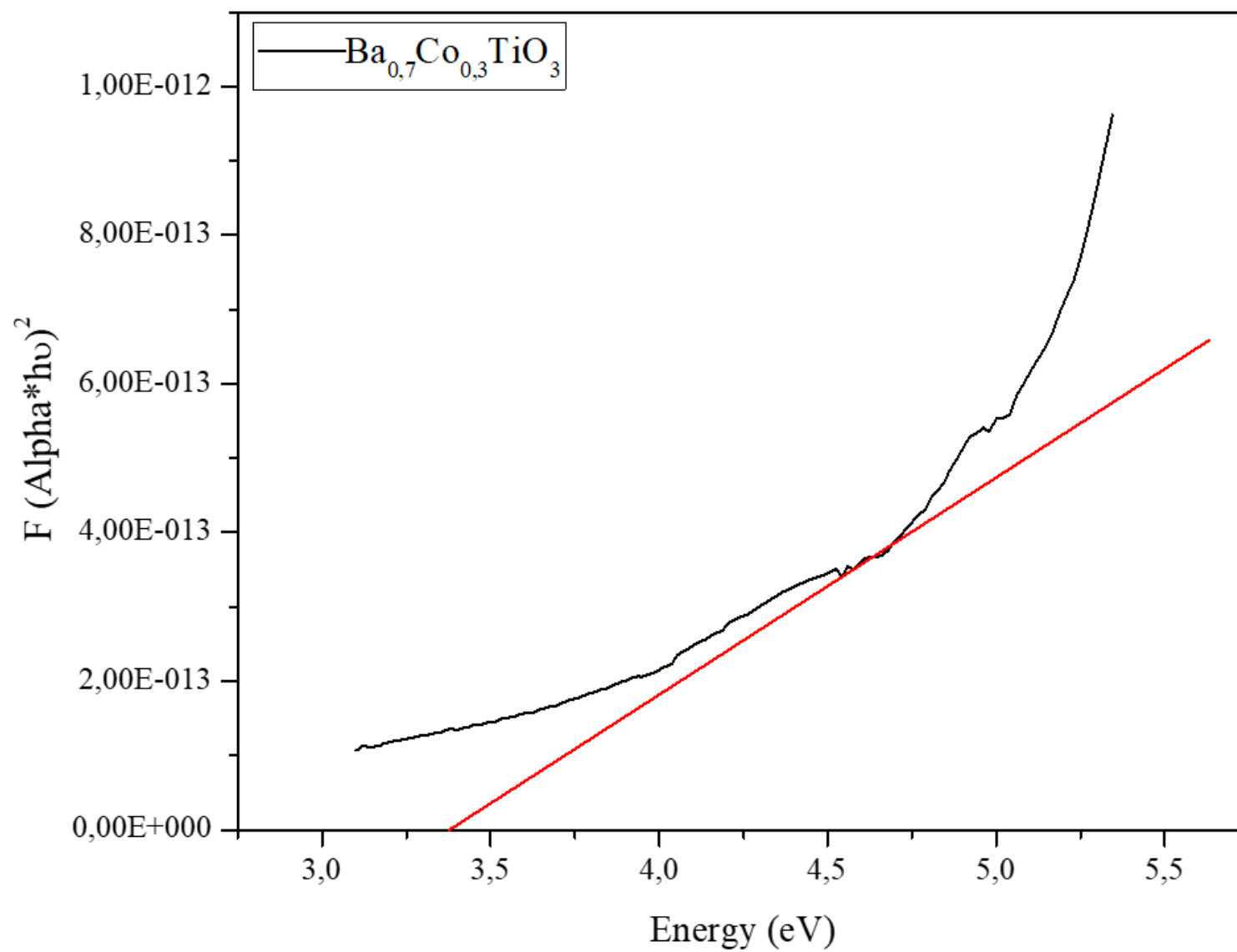
(b)

Figure S6. Continued.



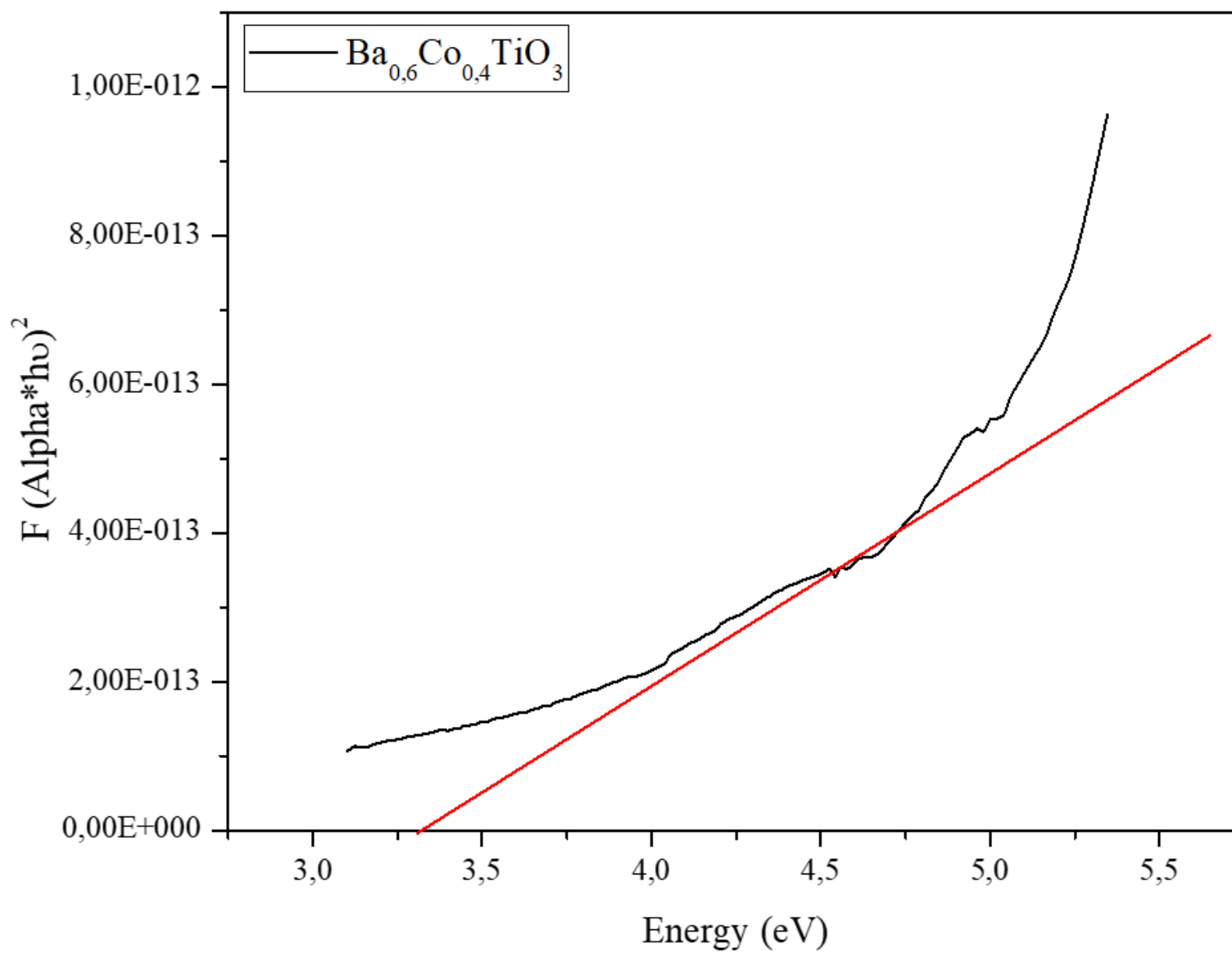
(c)

Figure S6. Continued.



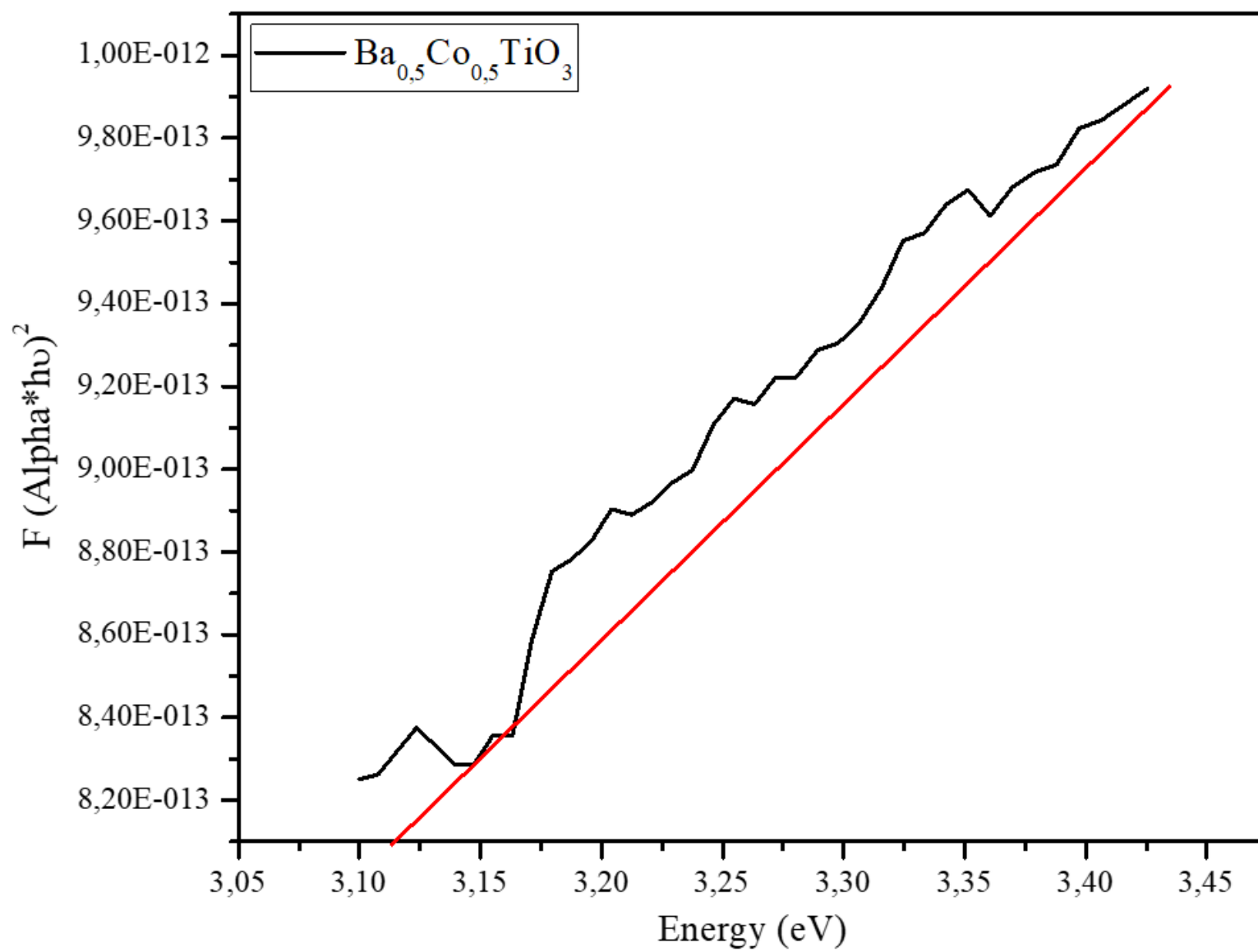
(d)

Figure S6. Continued.



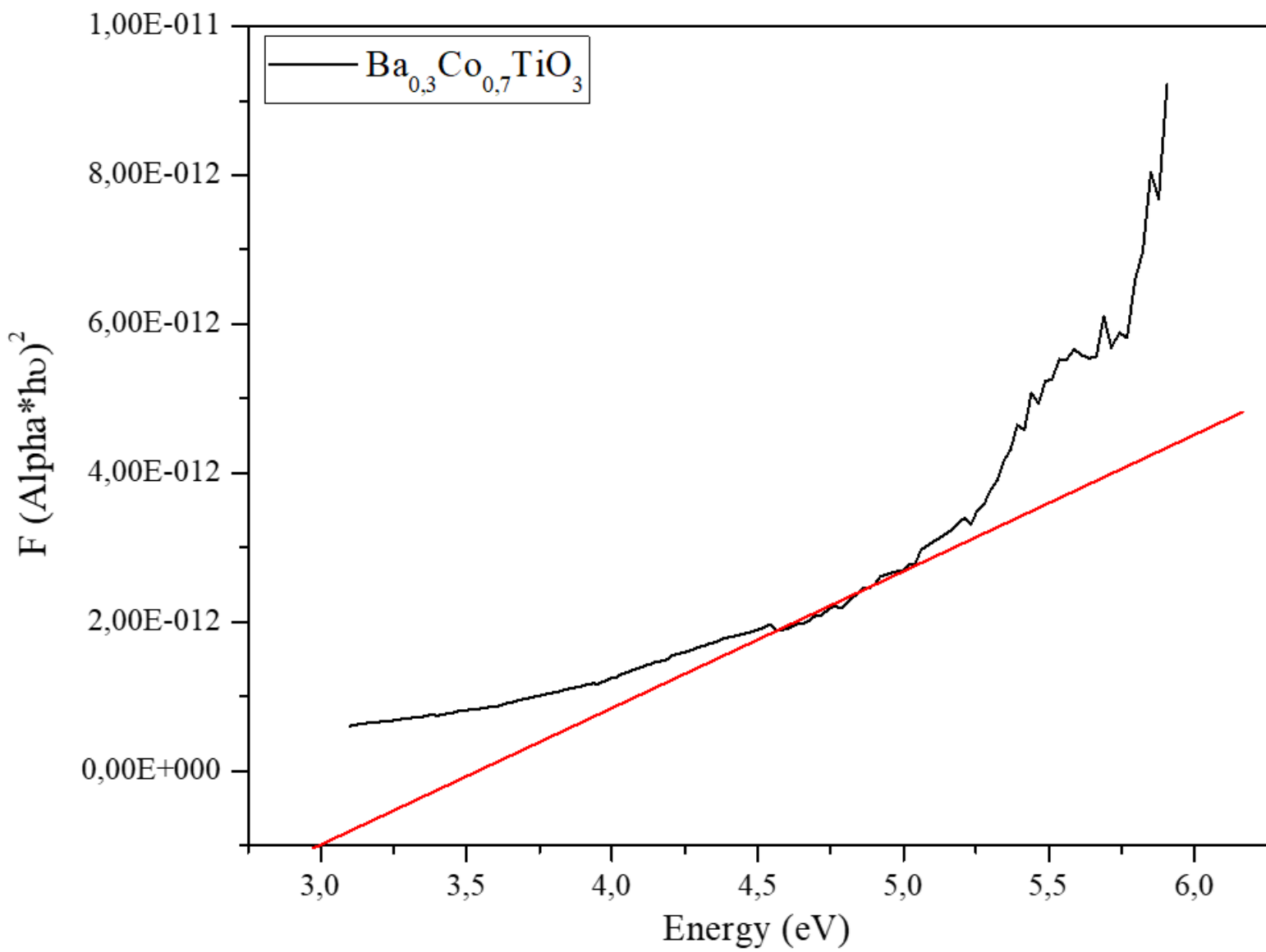
(e)

Figure S6. Continued.



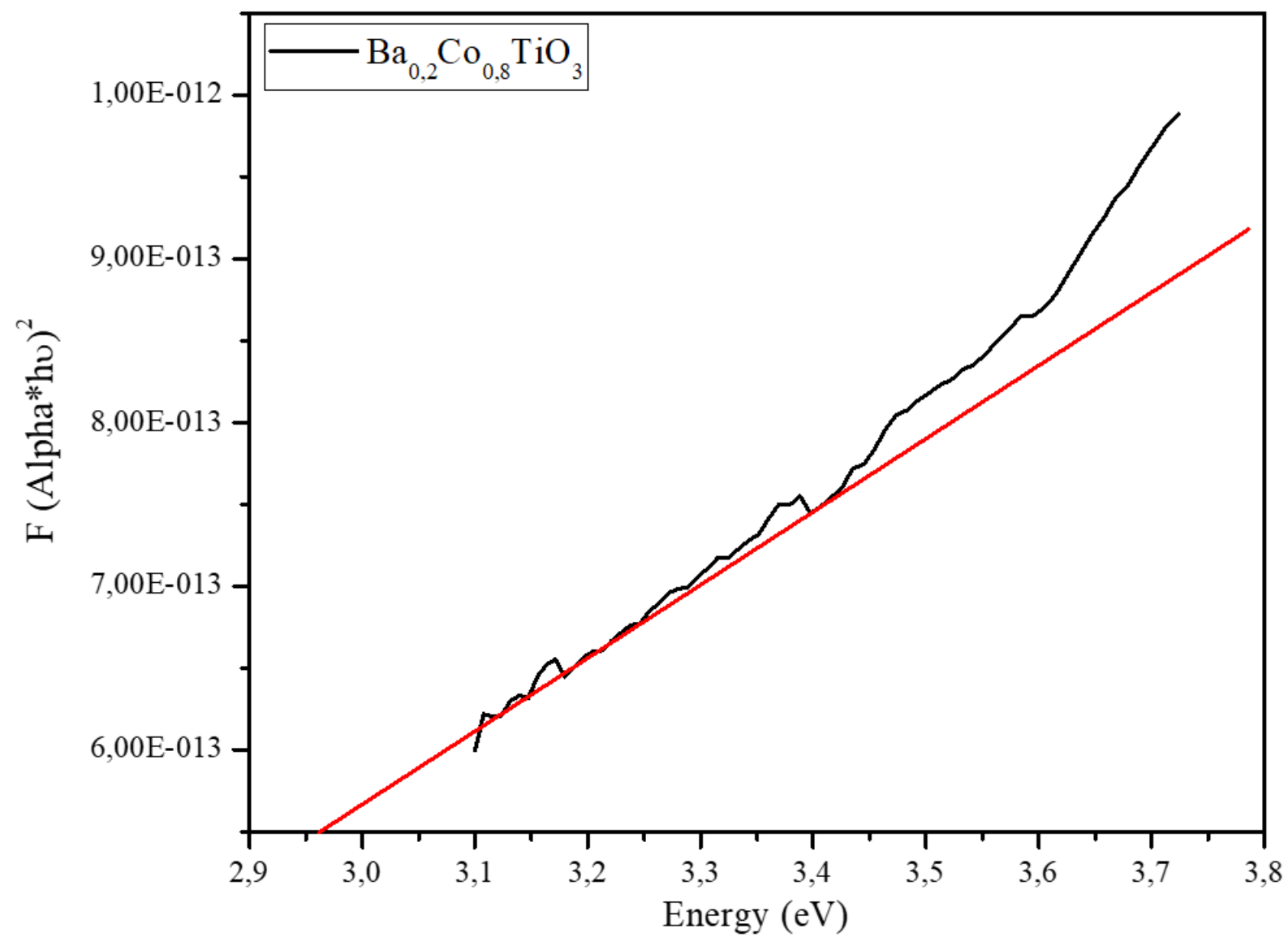
(f)

Figure S6. Continued.



(g)

Figure S6. Continued.



(h)

Figure S6. Continued.

(i)

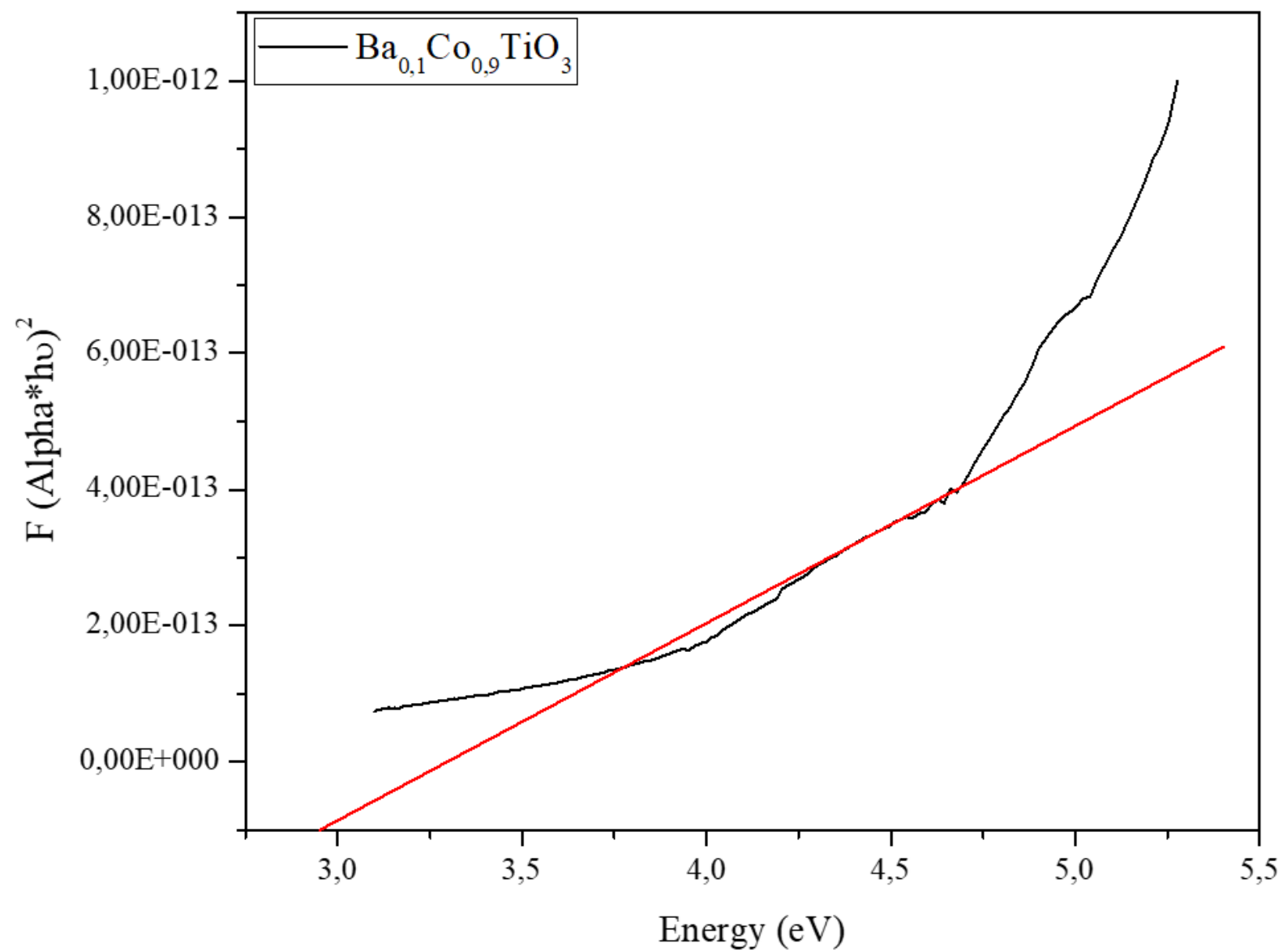
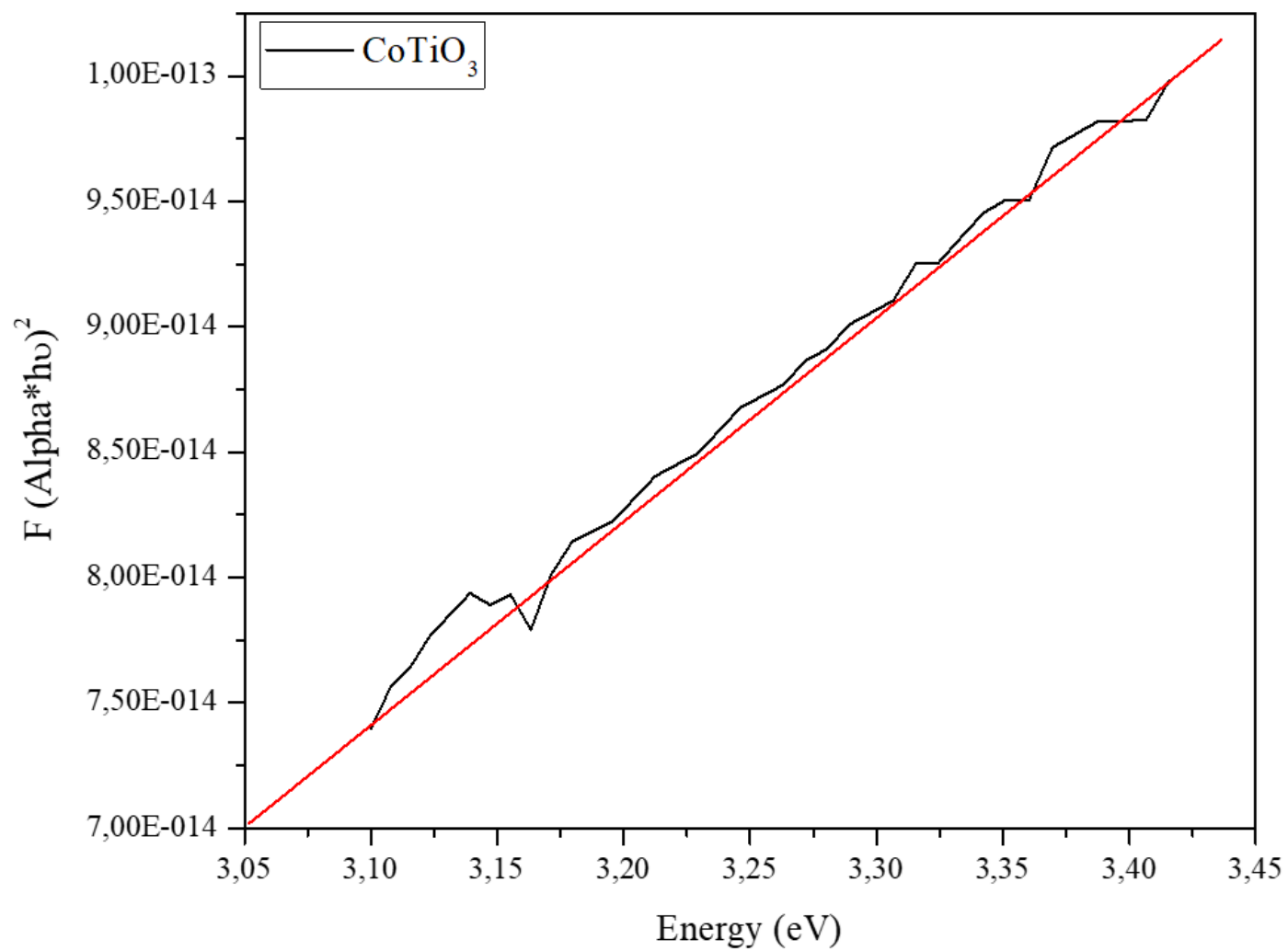


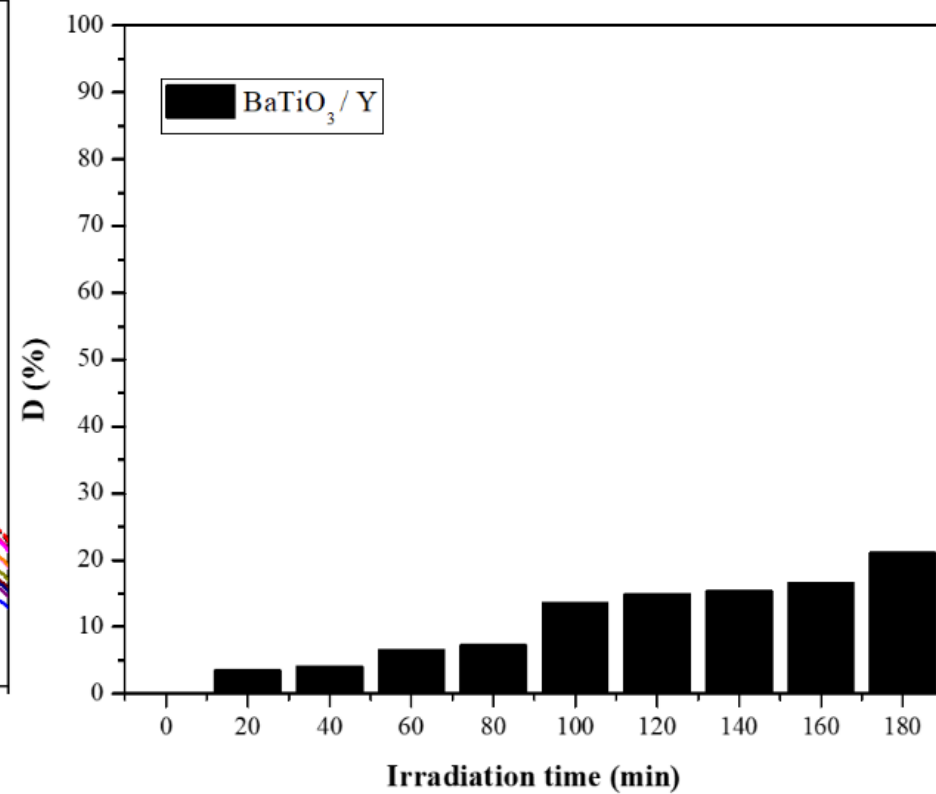
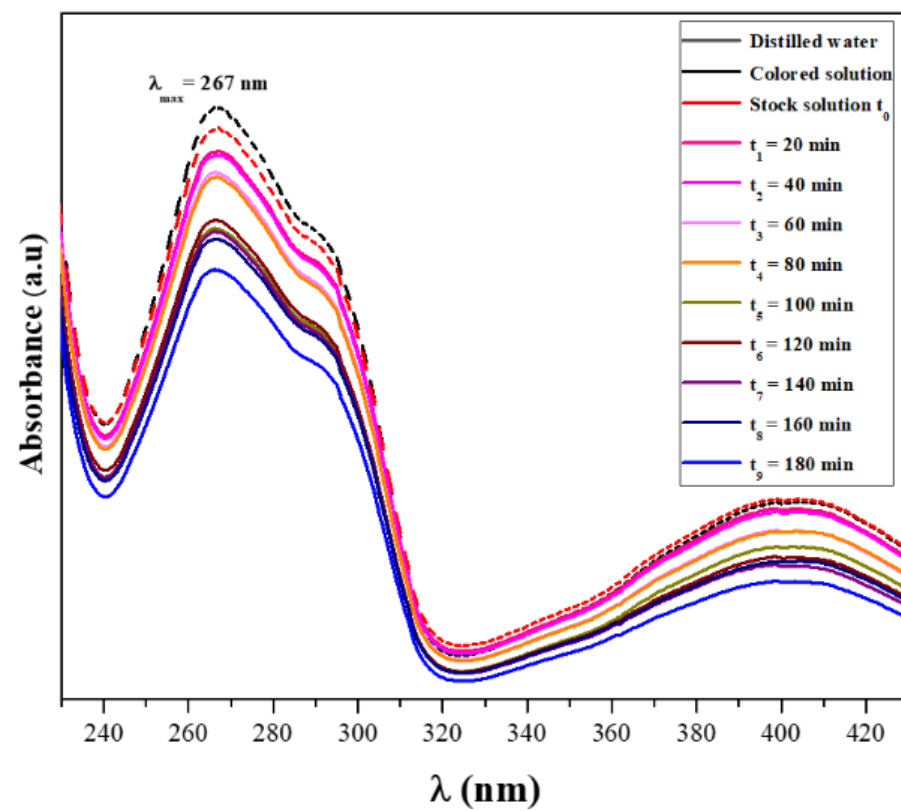
Figure S6. Continued.



(j)

Figure S6. Estimation of band gap energy using Tauc Plot method for $\text{Ba}_{1-x}\text{Co}_x\text{TiO}_3$ $\{x = 0, \dots, 1\}$ samples; (a) BaTiO_3 ; (b) $\text{Ba}_{0.9}\text{Co}_{0.1}\text{TiO}_3$; (c) $\text{Ba}_{0.8}\text{Co}_{0.2}\text{TiO}_3$; (d) $\text{Ba}_{0.7}\text{Co}_{0.3}\text{TiO}_3$; (e) $\text{Ba}_{0.6}\text{Co}_{0.4}\text{TiO}_3$; (f) $\text{Ba}_{0.5}\text{Co}_{0.5}\text{TiO}_3$; (g) $\text{Ba}_{0.3}\text{Co}_{0.7}\text{TiO}_3$; (h) $\text{Ba}_{0.2}\text{Co}_{0.8}\text{TiO}_3$; (i) $\text{Ba}_{0.1}\text{Co}_{0.9}\text{TiO}_3$ and (j) CoTiO_3 .

6. Photocatalytic Application



(a)

Figure S7. Continued.

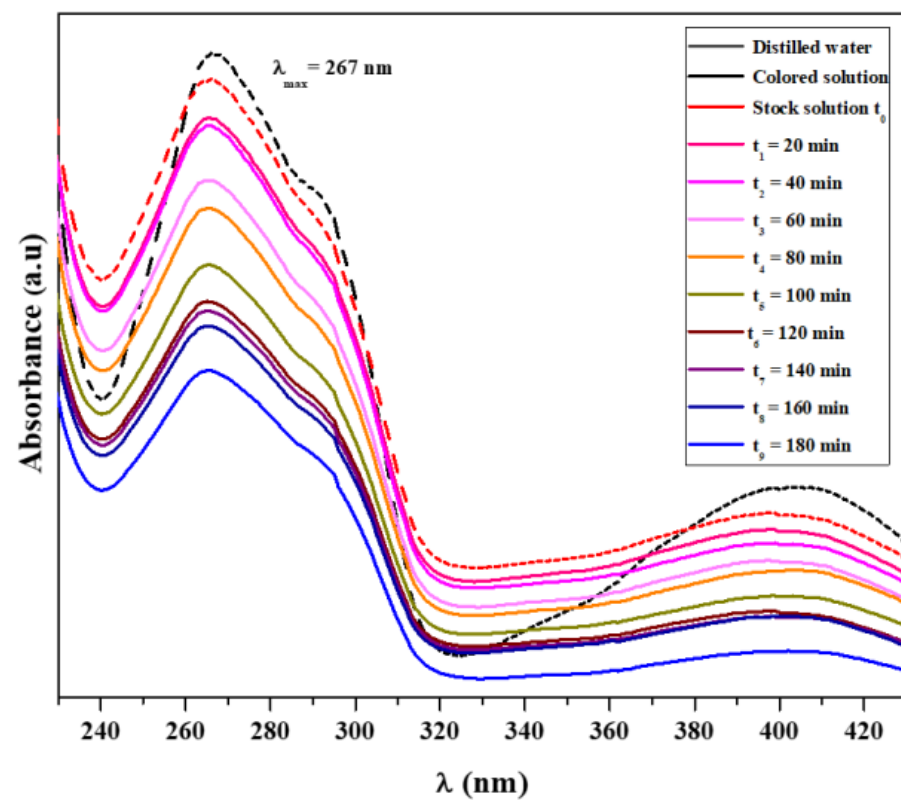
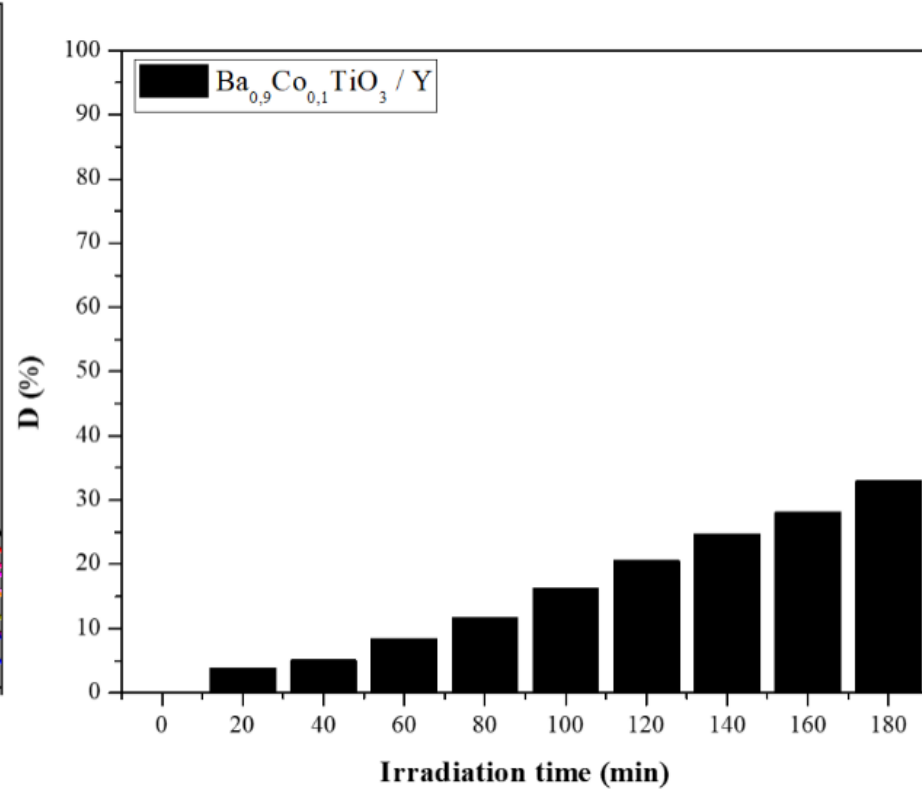


Figure S7. Continued.



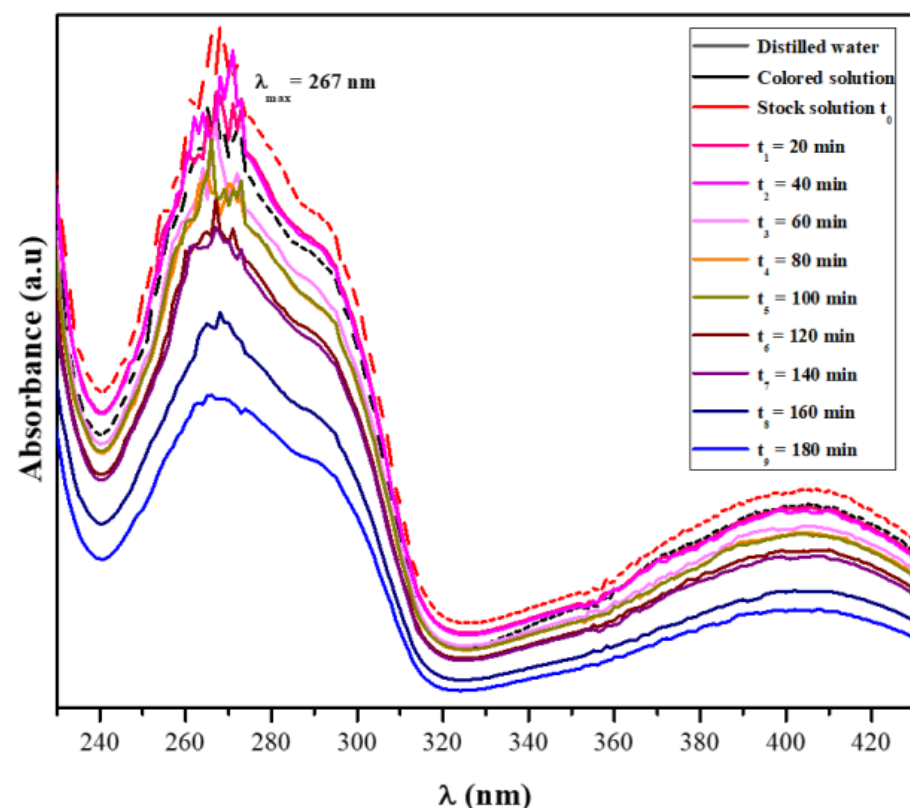
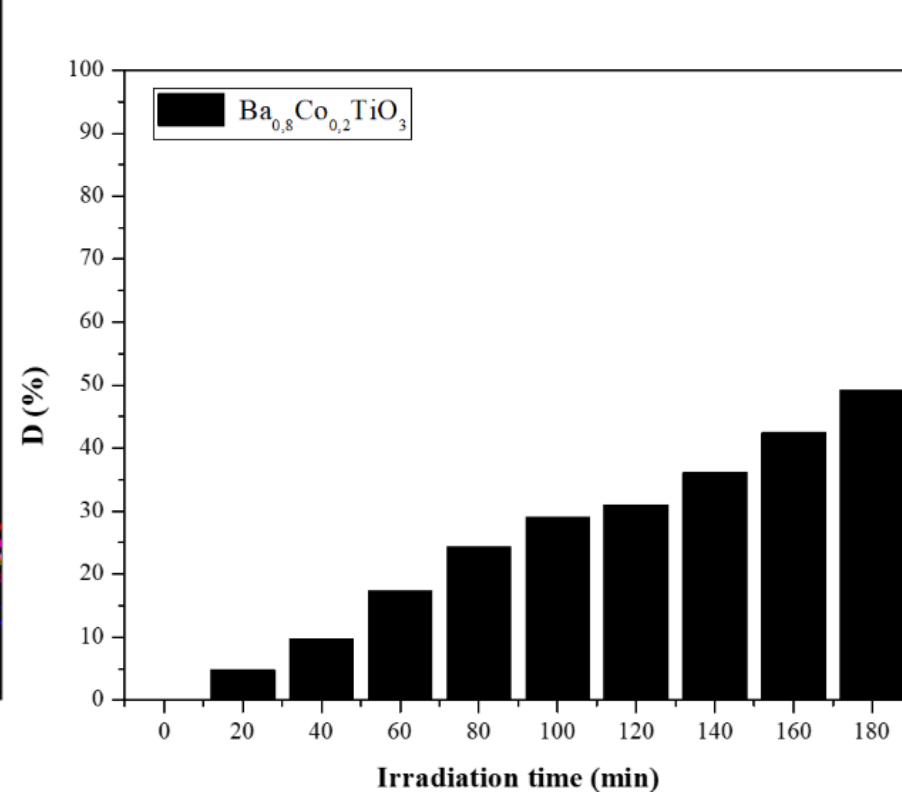
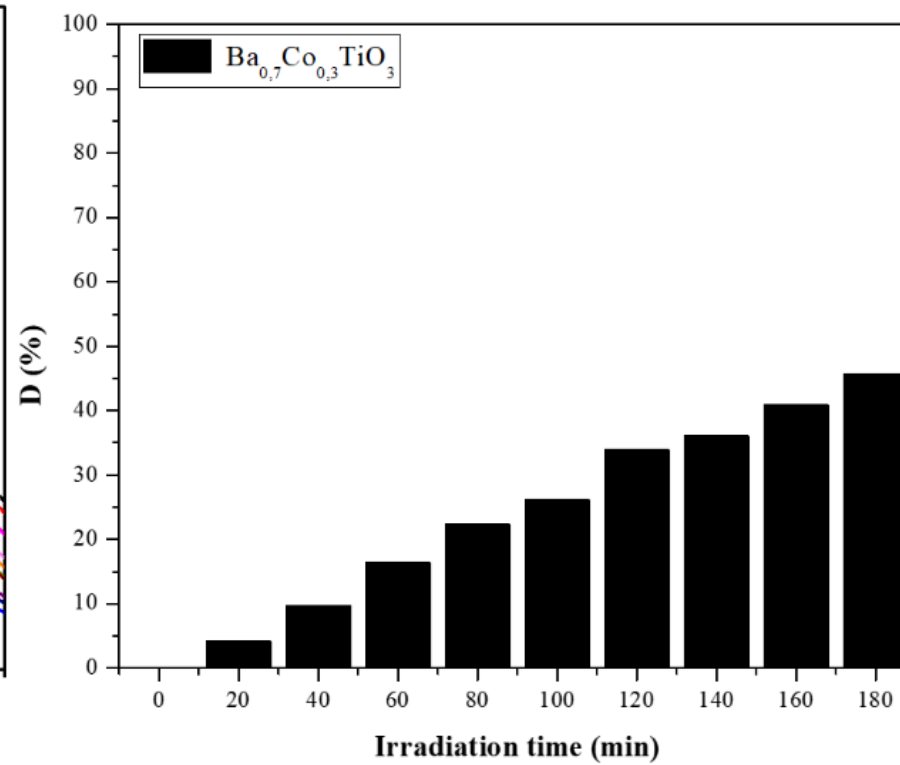
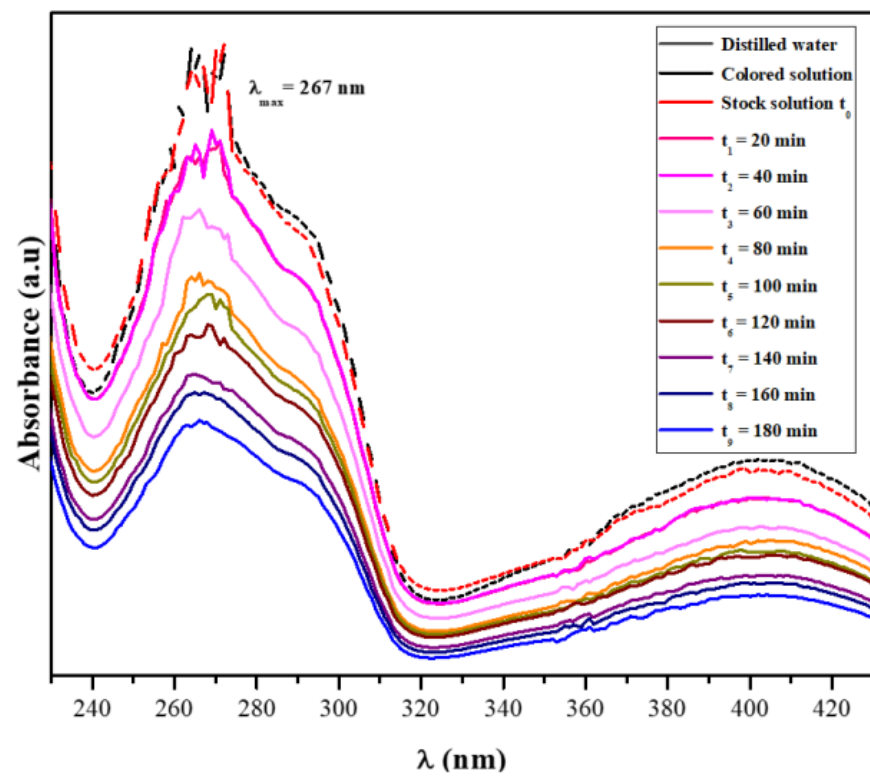


Figure S7. Continued.





(d)

Figure S7. Continued.

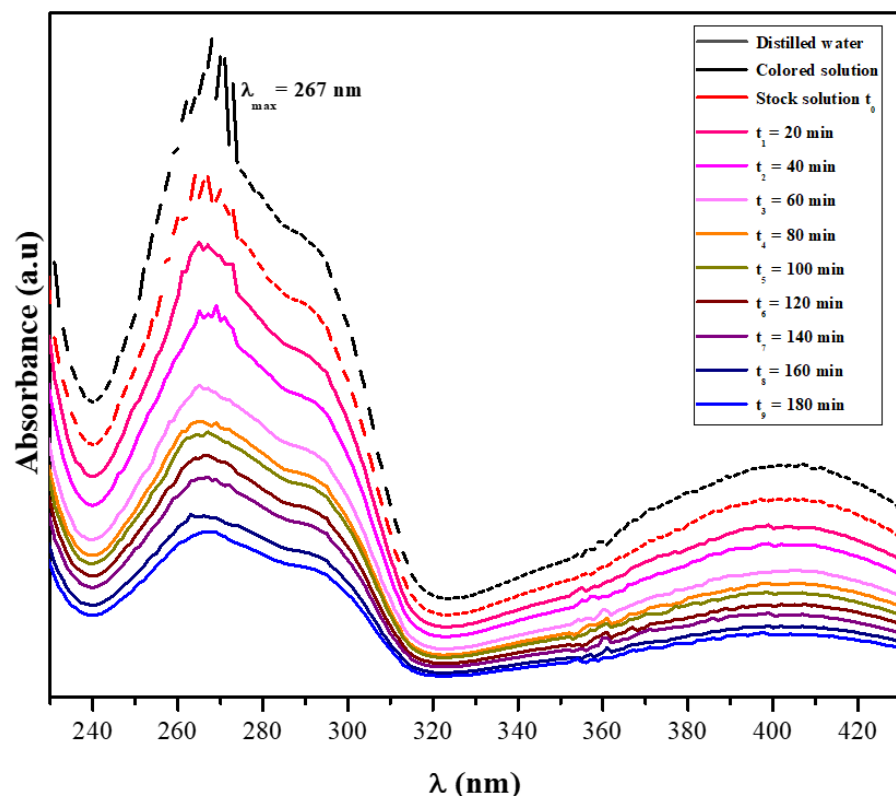
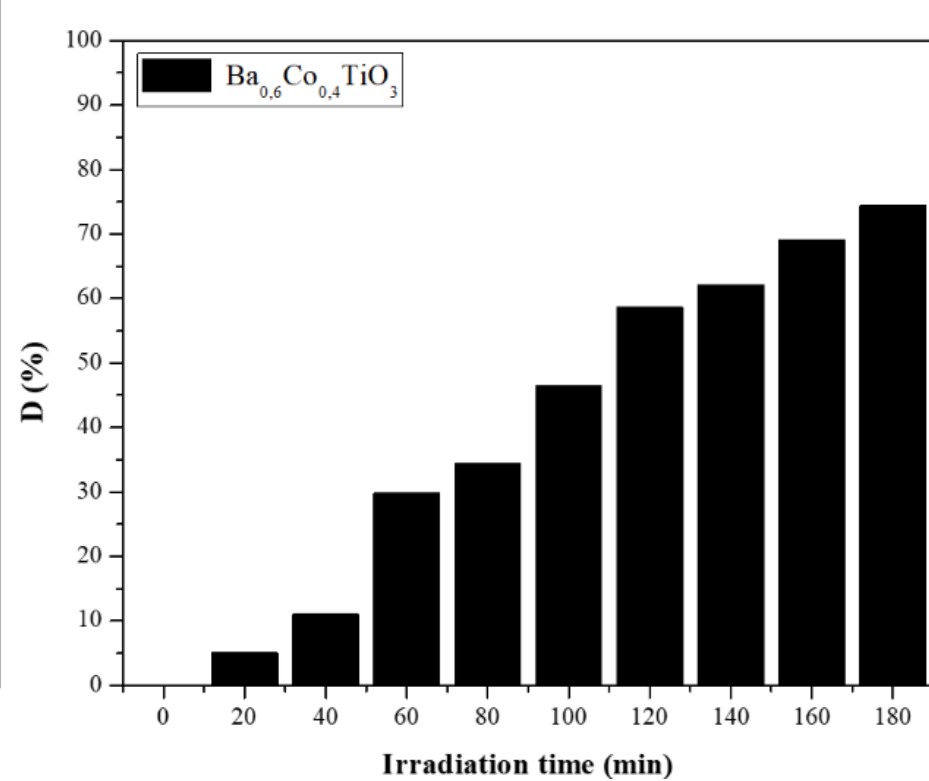


Figure S7. Continued.



(e)

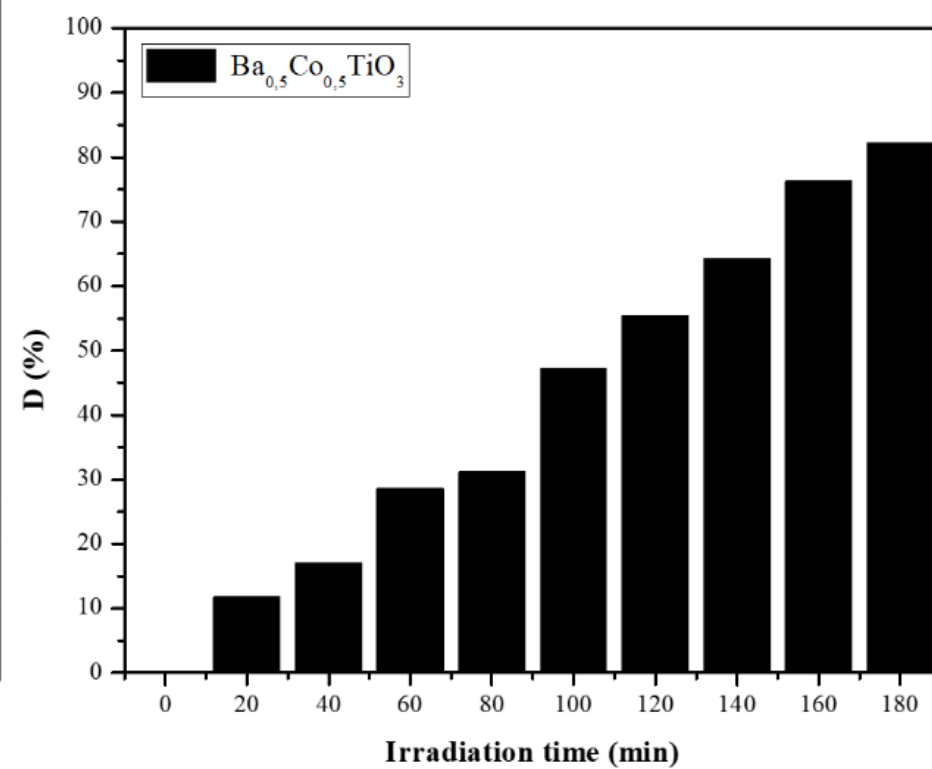
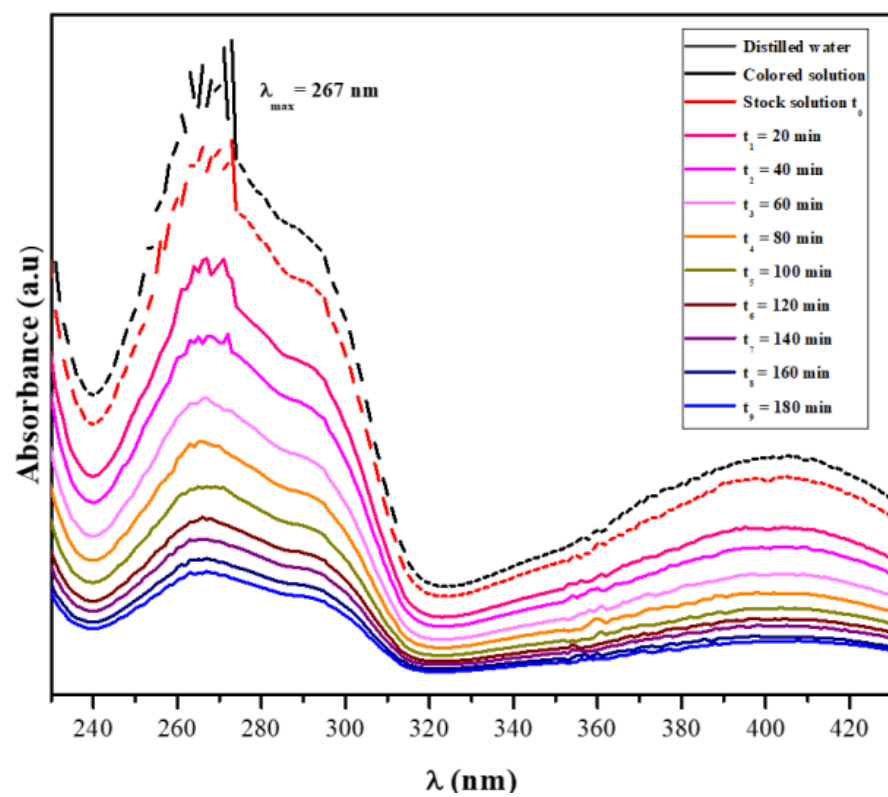


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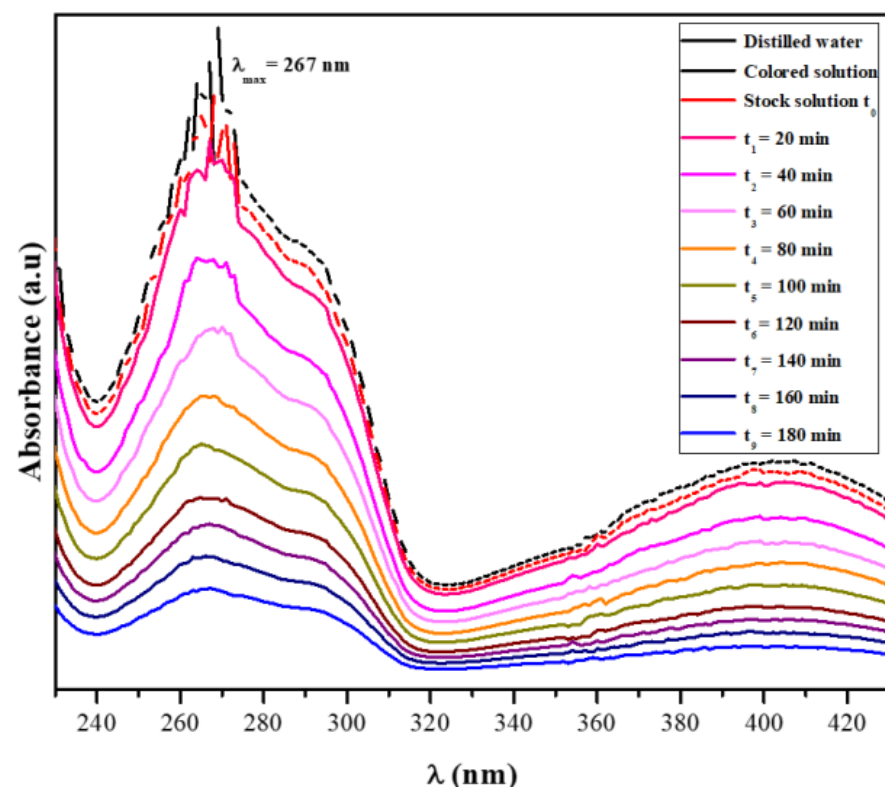
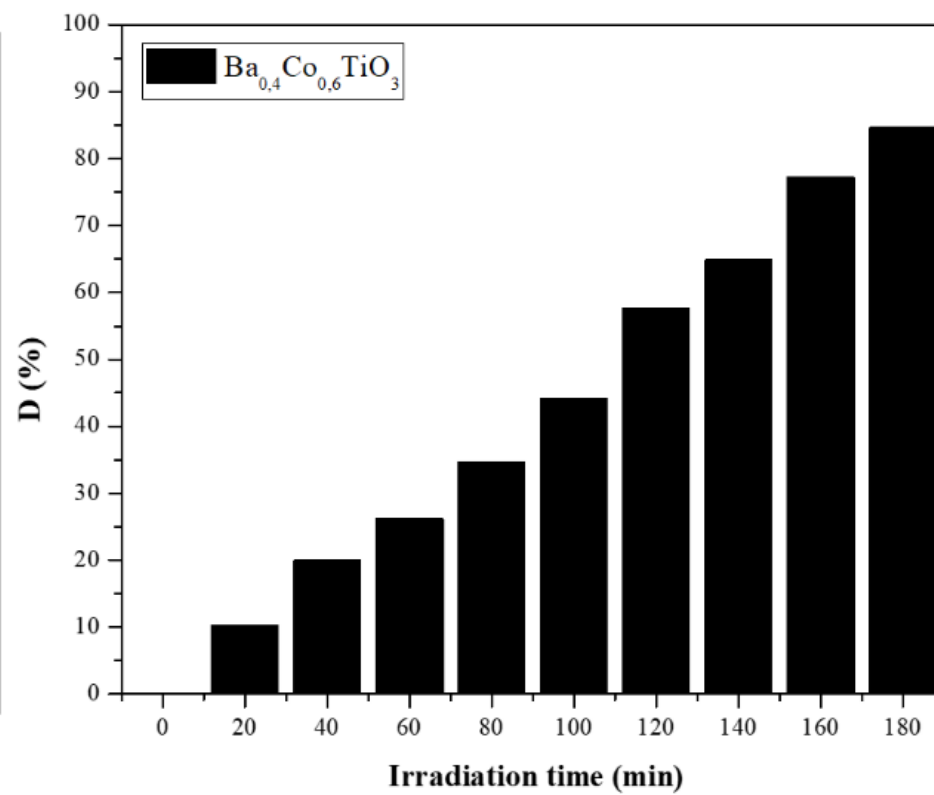
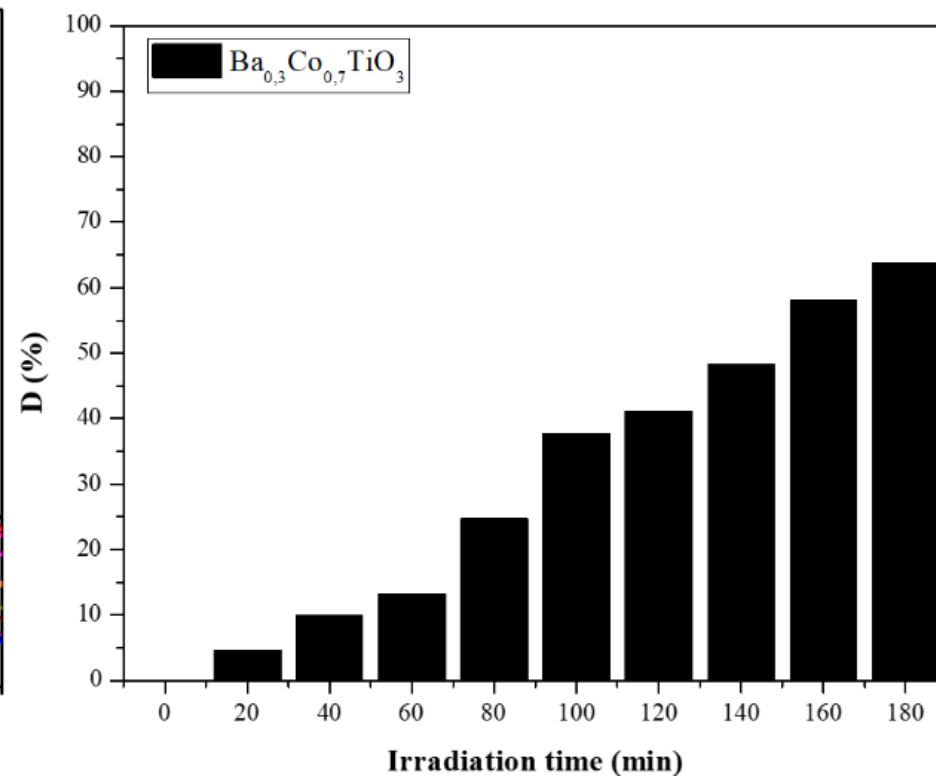
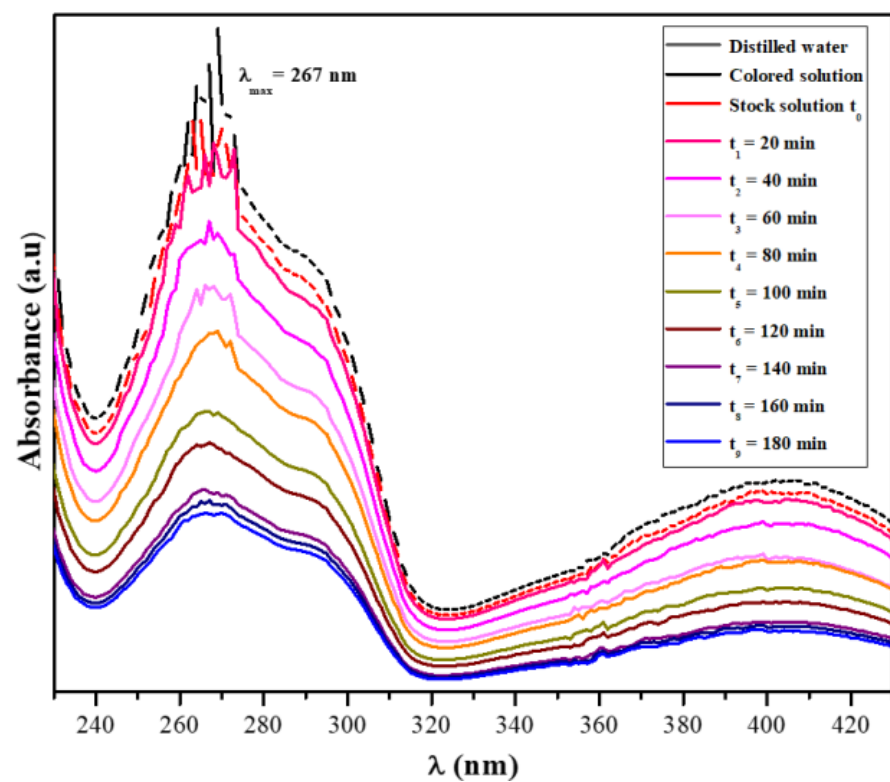


Figure S7. Continued.



(g)



(h)

Figure S7. Continued.

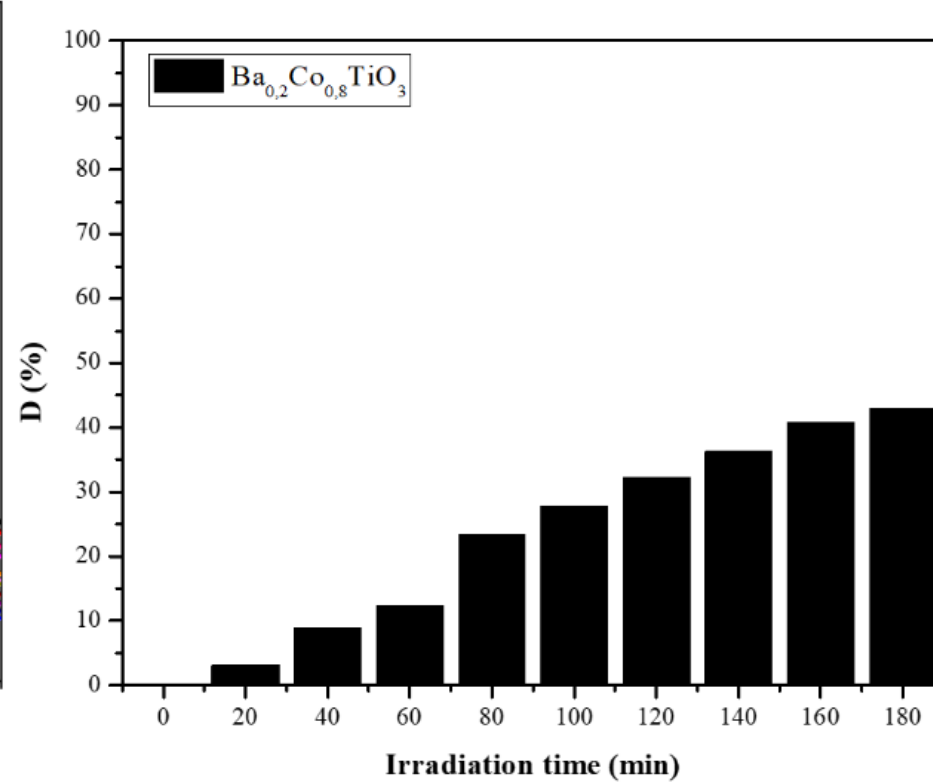
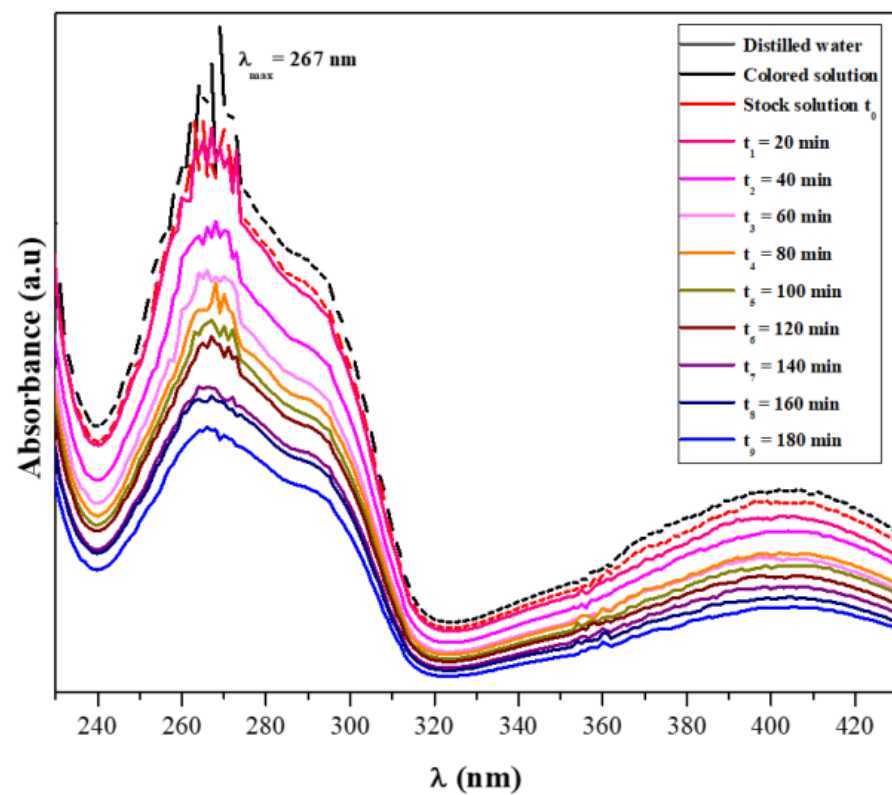
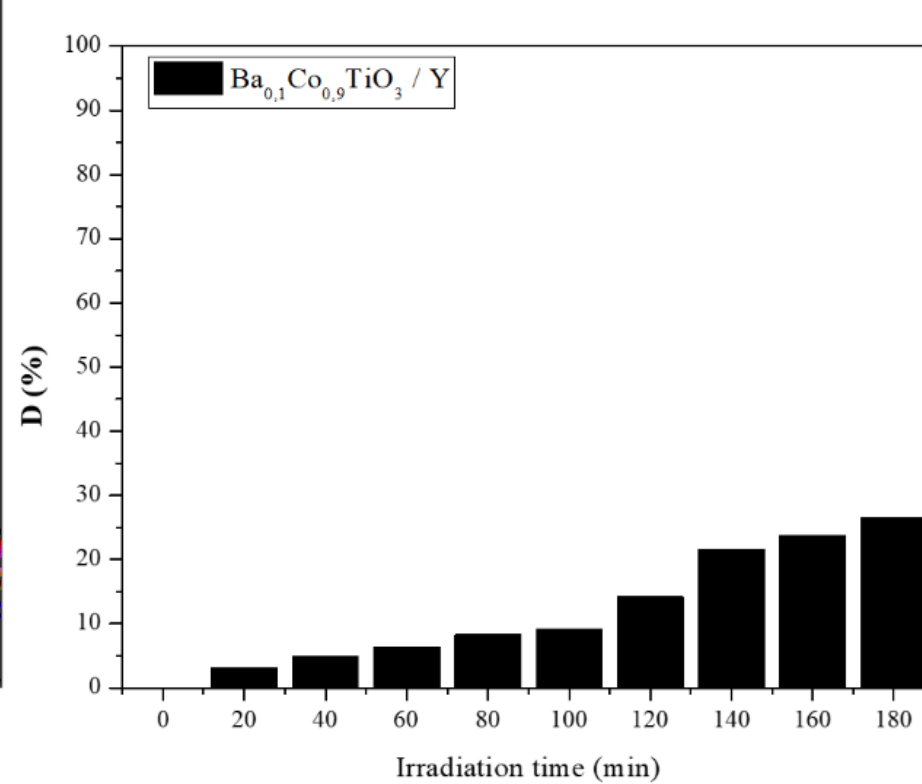
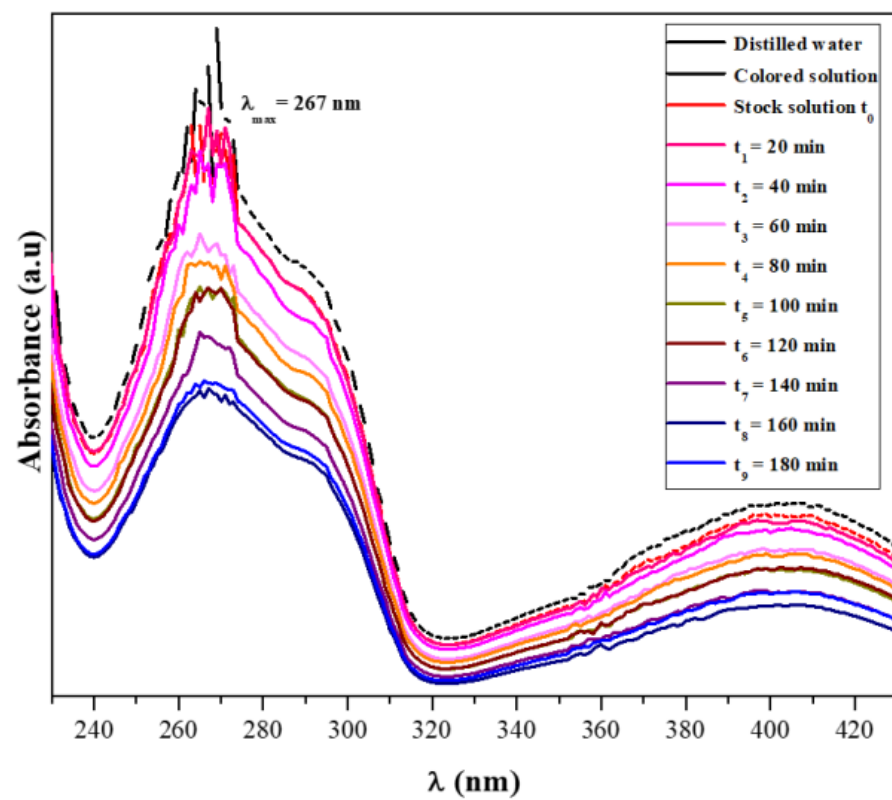
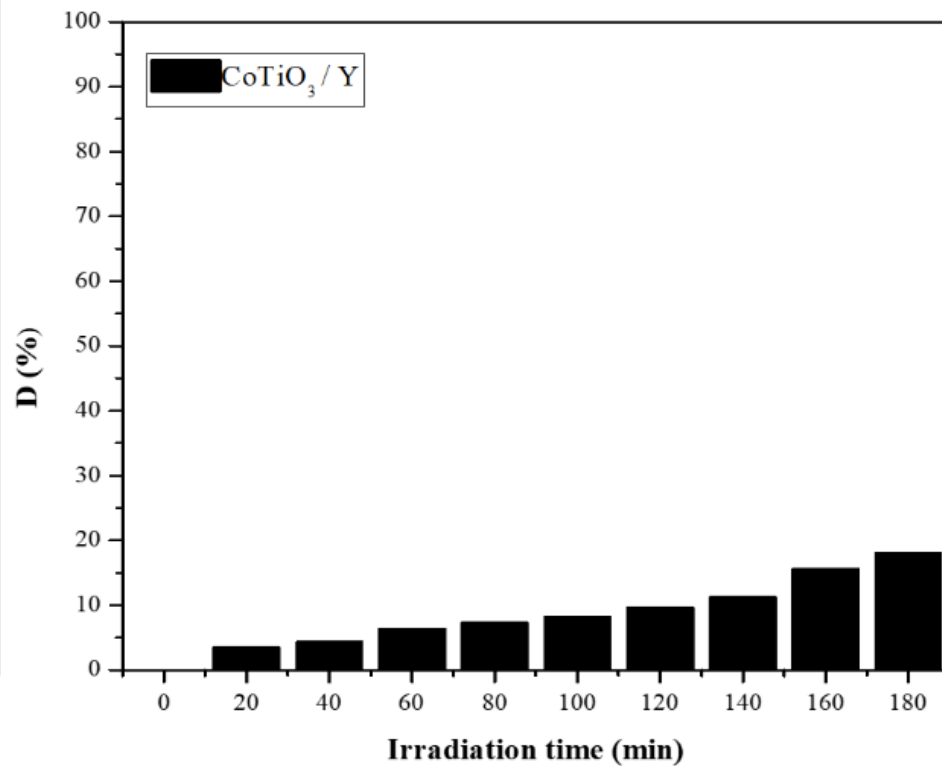
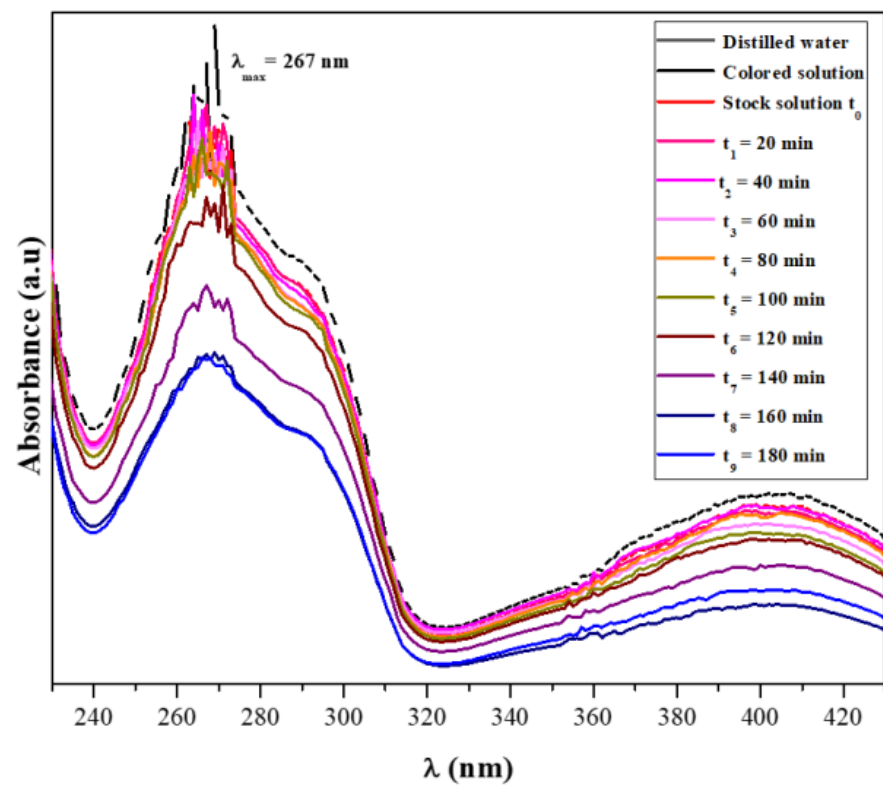


Figure S7. Continued.



(j)

Figure S7. Continued.



(k)

Figure S7. Photocatalytic degradation of CBY 3G-P by $\text{Ba}_{1-x}\text{Co}_x\text{TiO}_3$, $\{x = 0, \dots, 1\}$: (a) BaTiO_3 ; (b) $\text{Ba}_{0.9}\text{Co}_{0.1}\text{TiO}_3$; (c) $\text{Ba}_{0.8}\text{Co}_{0.2}\text{TiO}_3$; (d) $\text{Ba}_{0.7}\text{Co}_{0.3}\text{TiO}_3$; (e) $\text{Ba}_{0.6}\text{Co}_{0.4}\text{TiO}_3$; (f) $\text{Ba}_{0.5}\text{Co}_{0.5}\text{TiO}_3$; (g) $\text{Ba}_{0.4}\text{Co}_{0.6}\text{TiO}_3$; (h) $\text{Ba}_{0.3}\text{Co}_{0.7}\text{TiO}_3$; (i) $\text{Ba}_{0.2}\text{Co}_{0.8}\text{TiO}_3$; (j) $\text{Ba}_{0.1}\text{Co}_{0.9}\text{TiO}_3$ and (k) CoTiO_3 as photocatalyst under 180 min of irradiation.

7. Photocatalytic mechanism

(a)

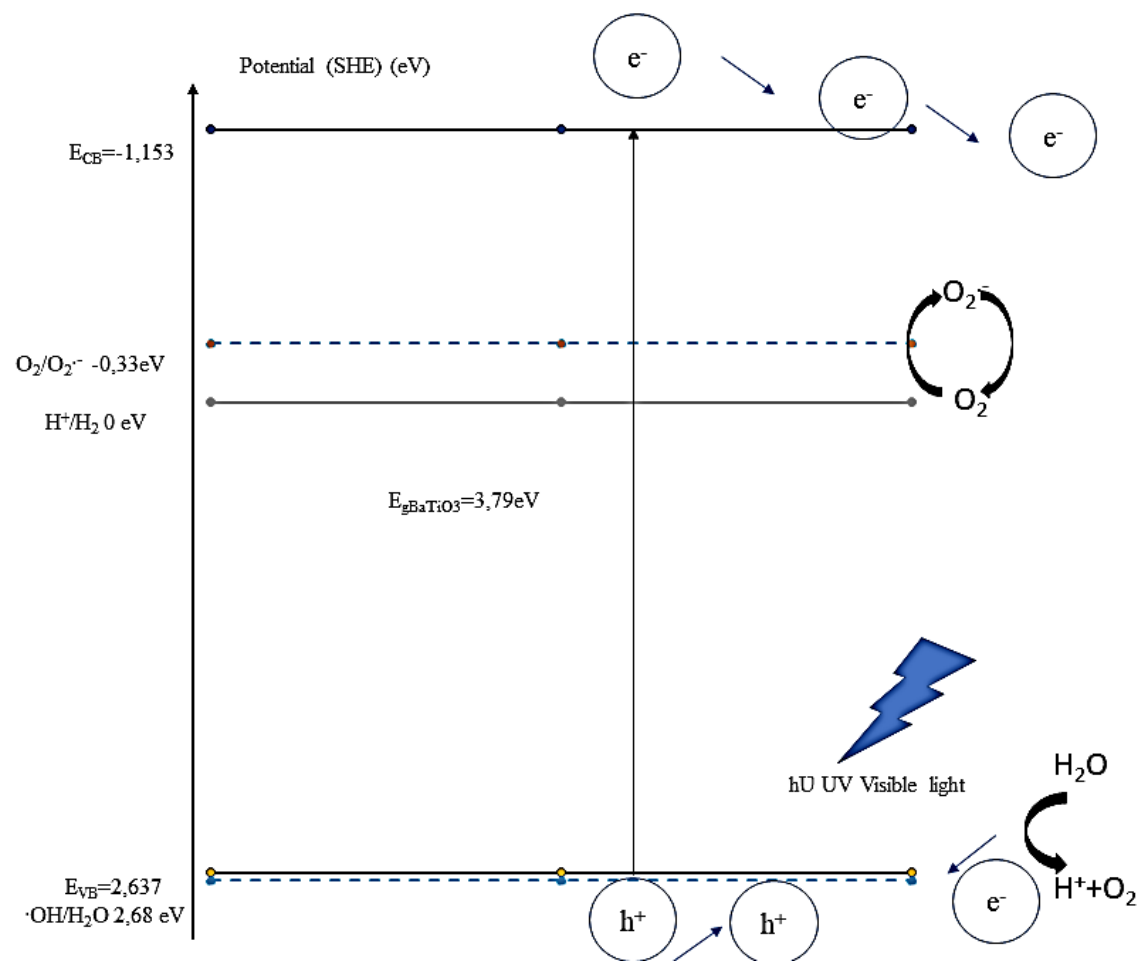


Figure S8. Continued.

(b)

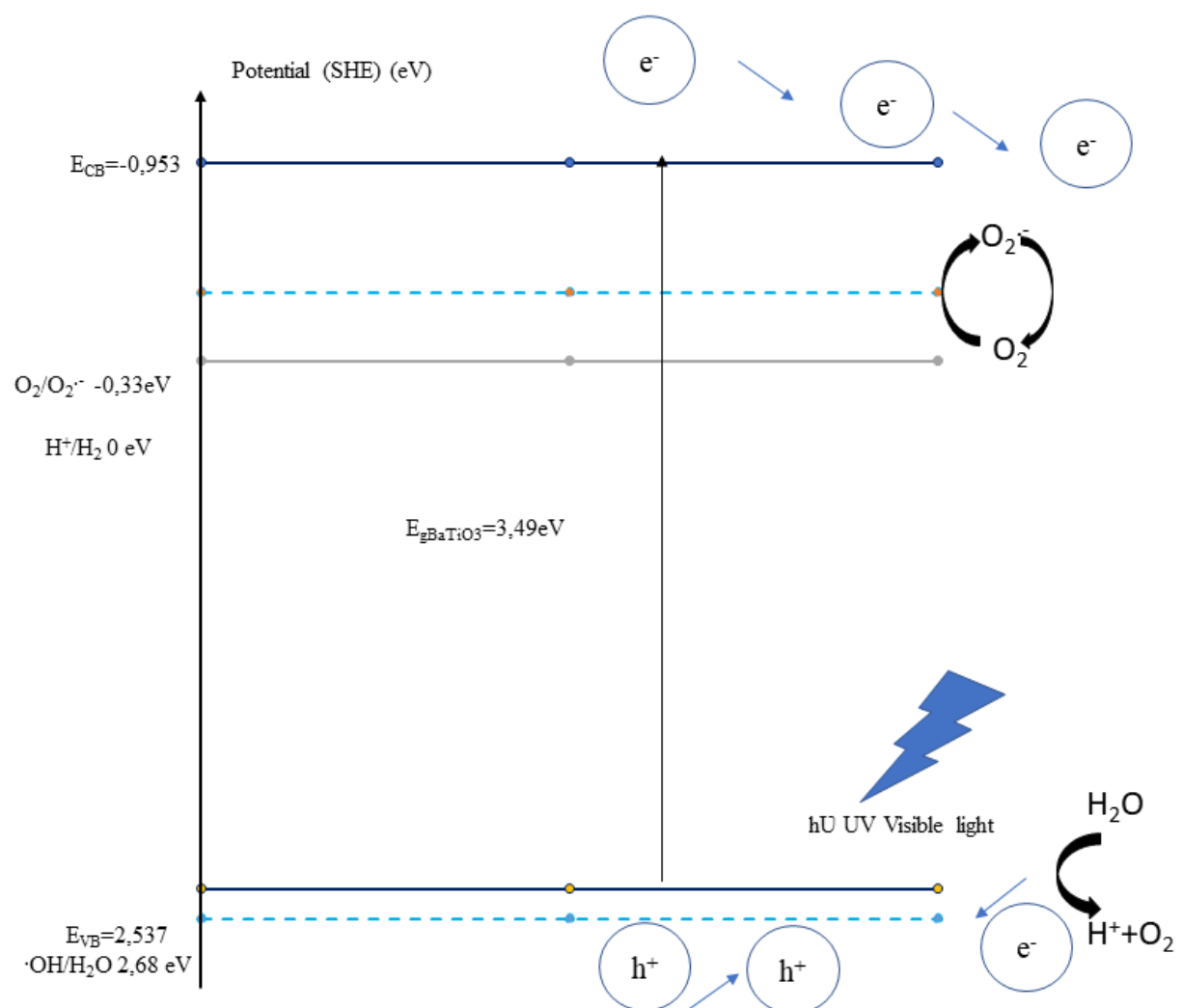


Figure S8. Continued.

(c)

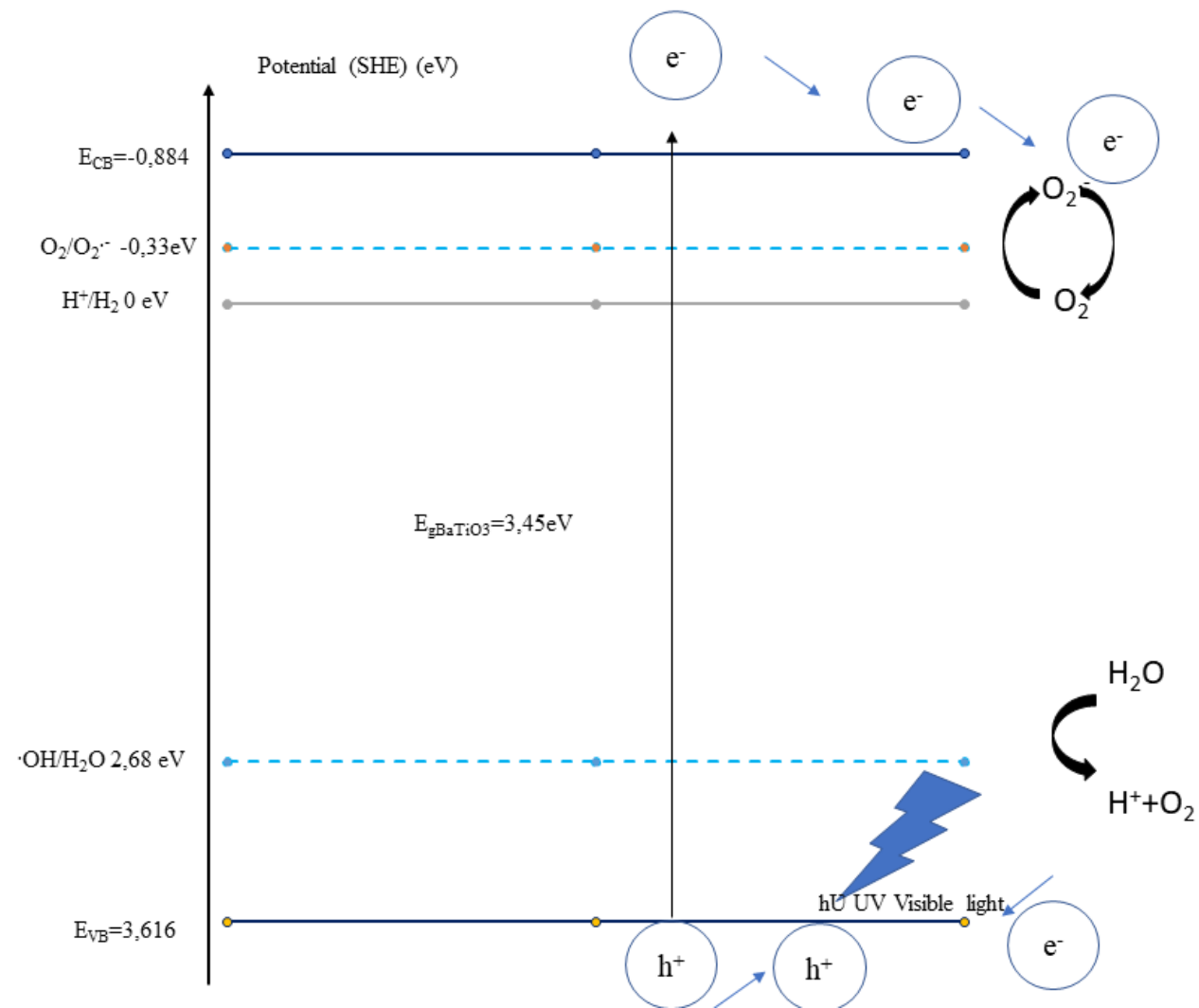


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(d)

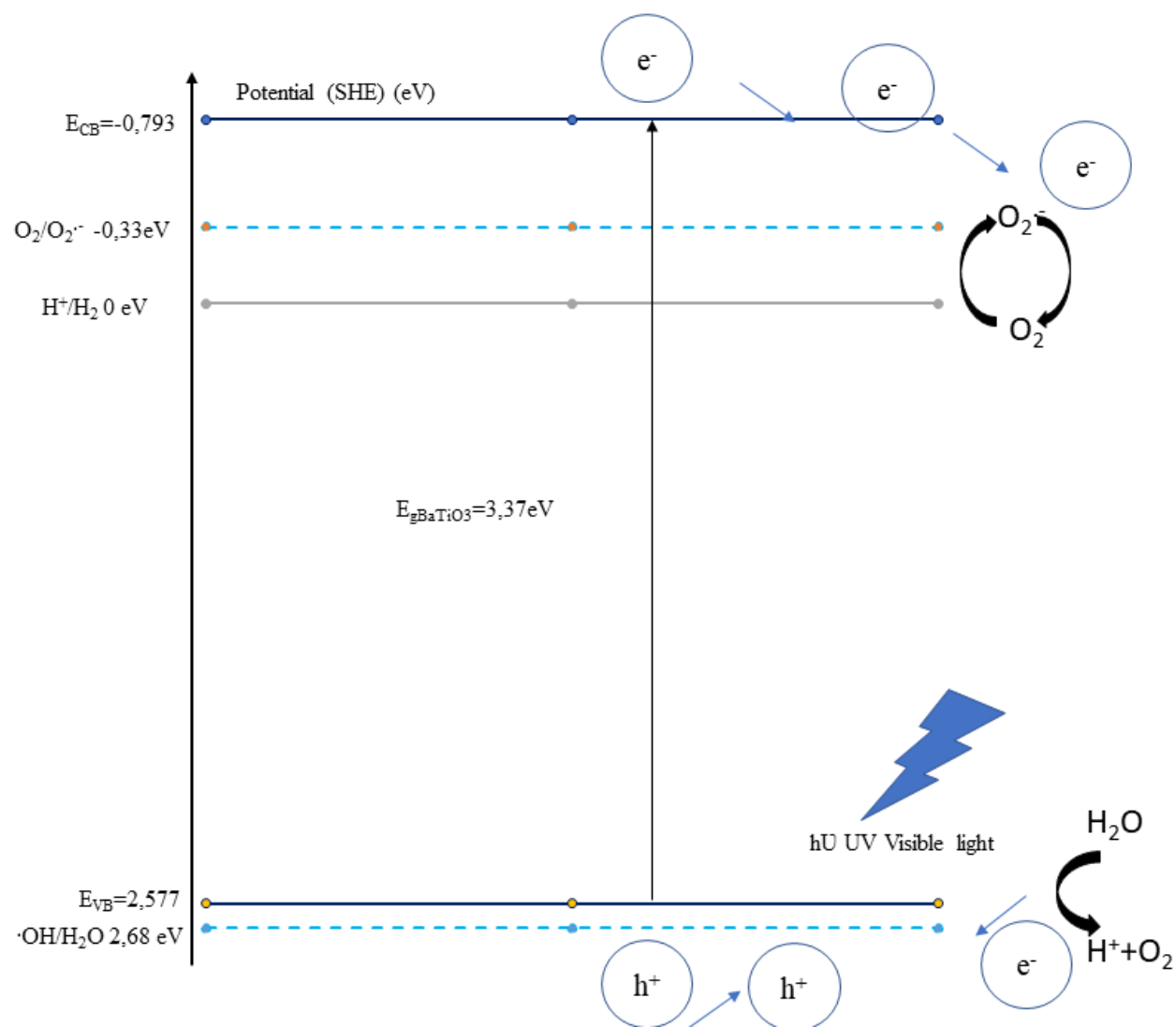


Figure S8. Continued.

(e)

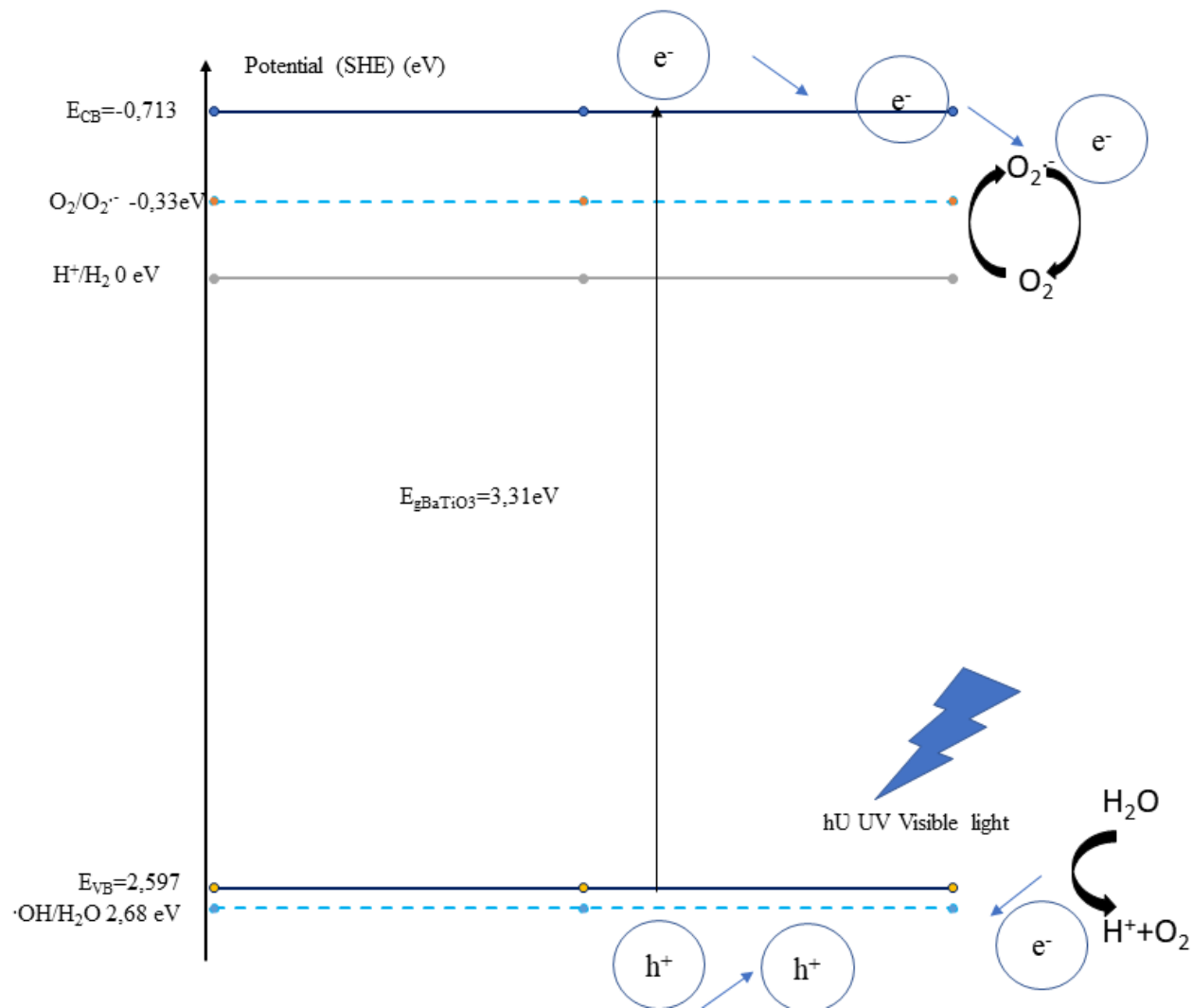


Figure S8. Continued.

(f)

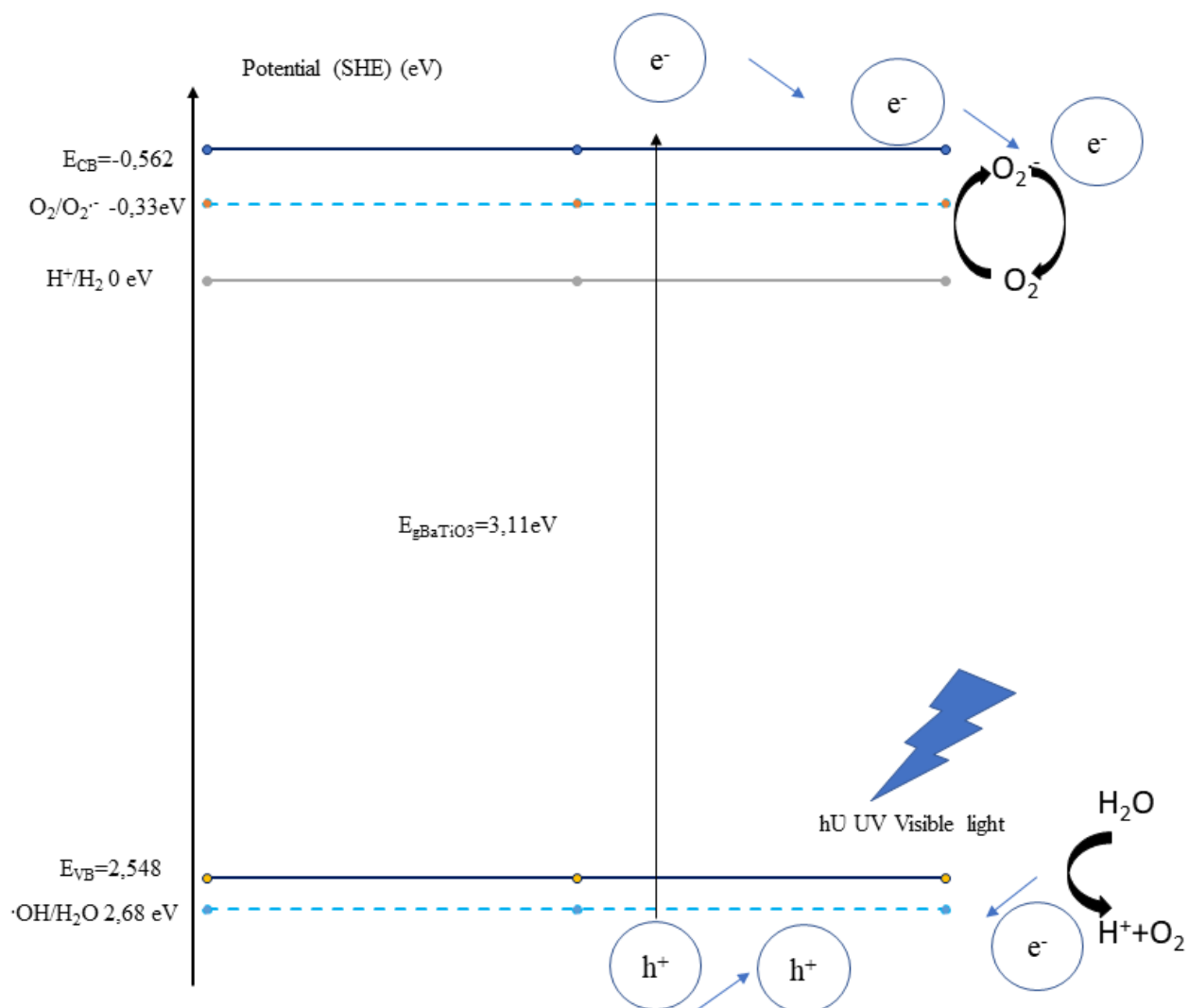


Figure S8. Continued.

(g)

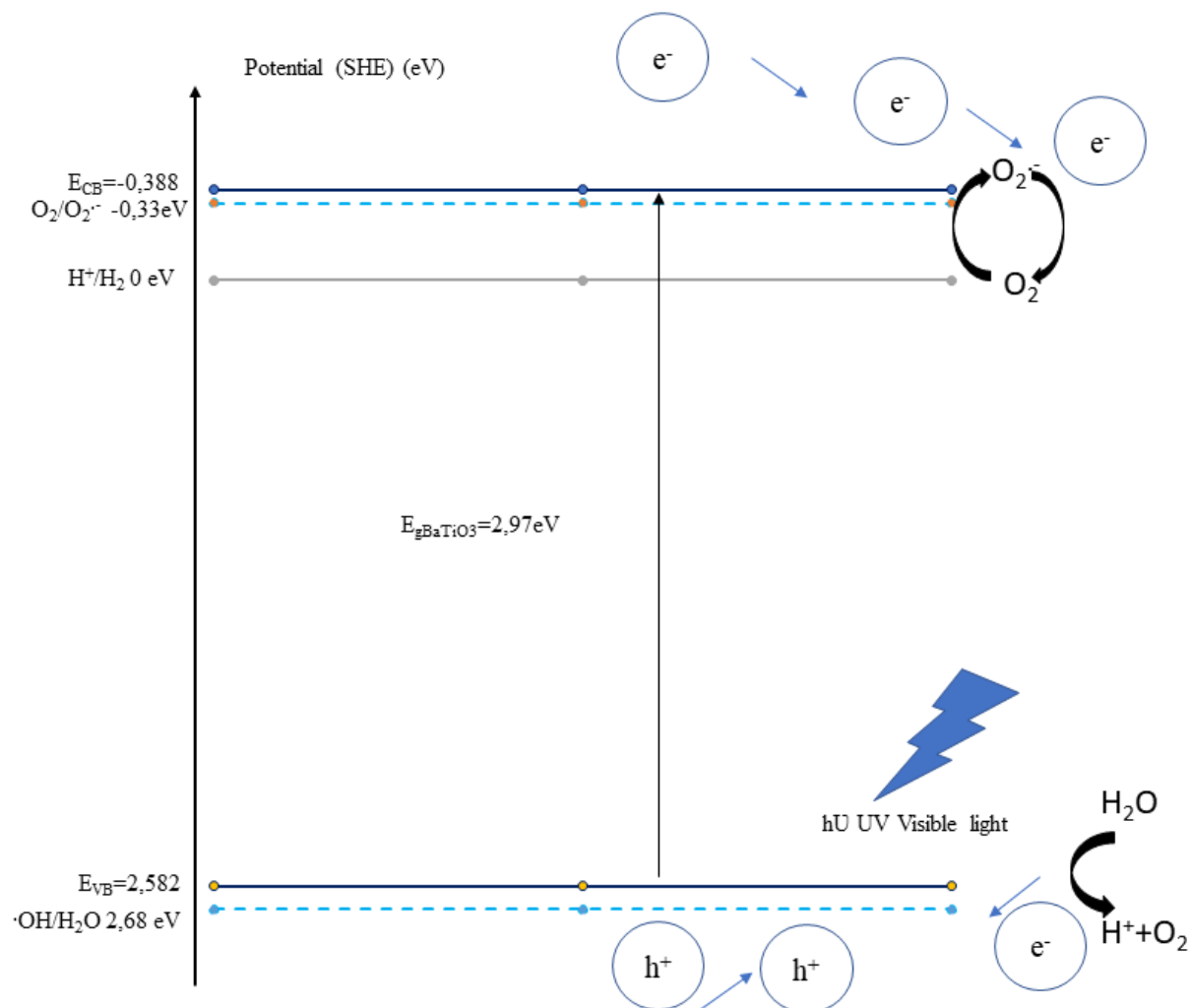


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(h)

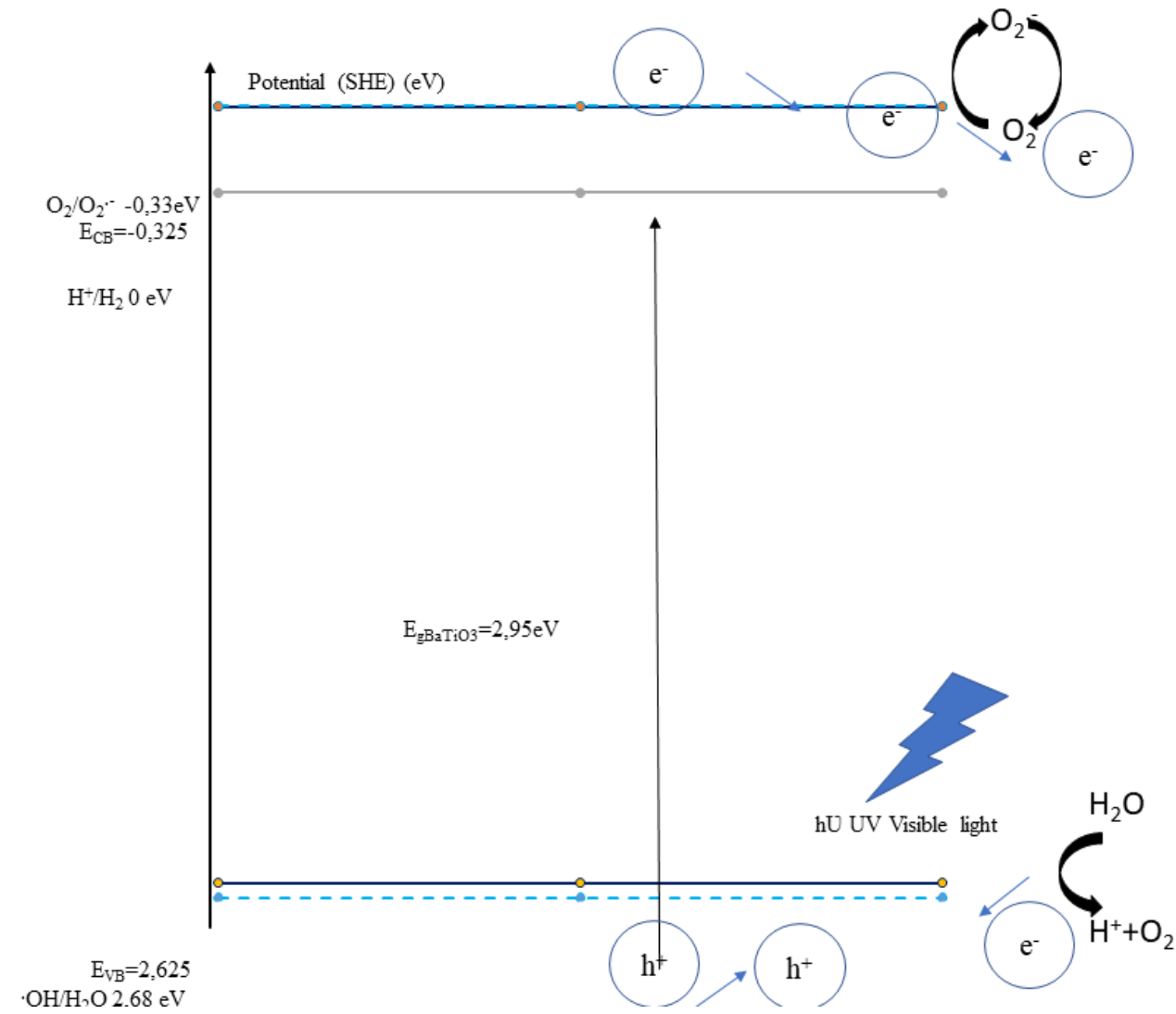


Figure S8. Continued.

(i)

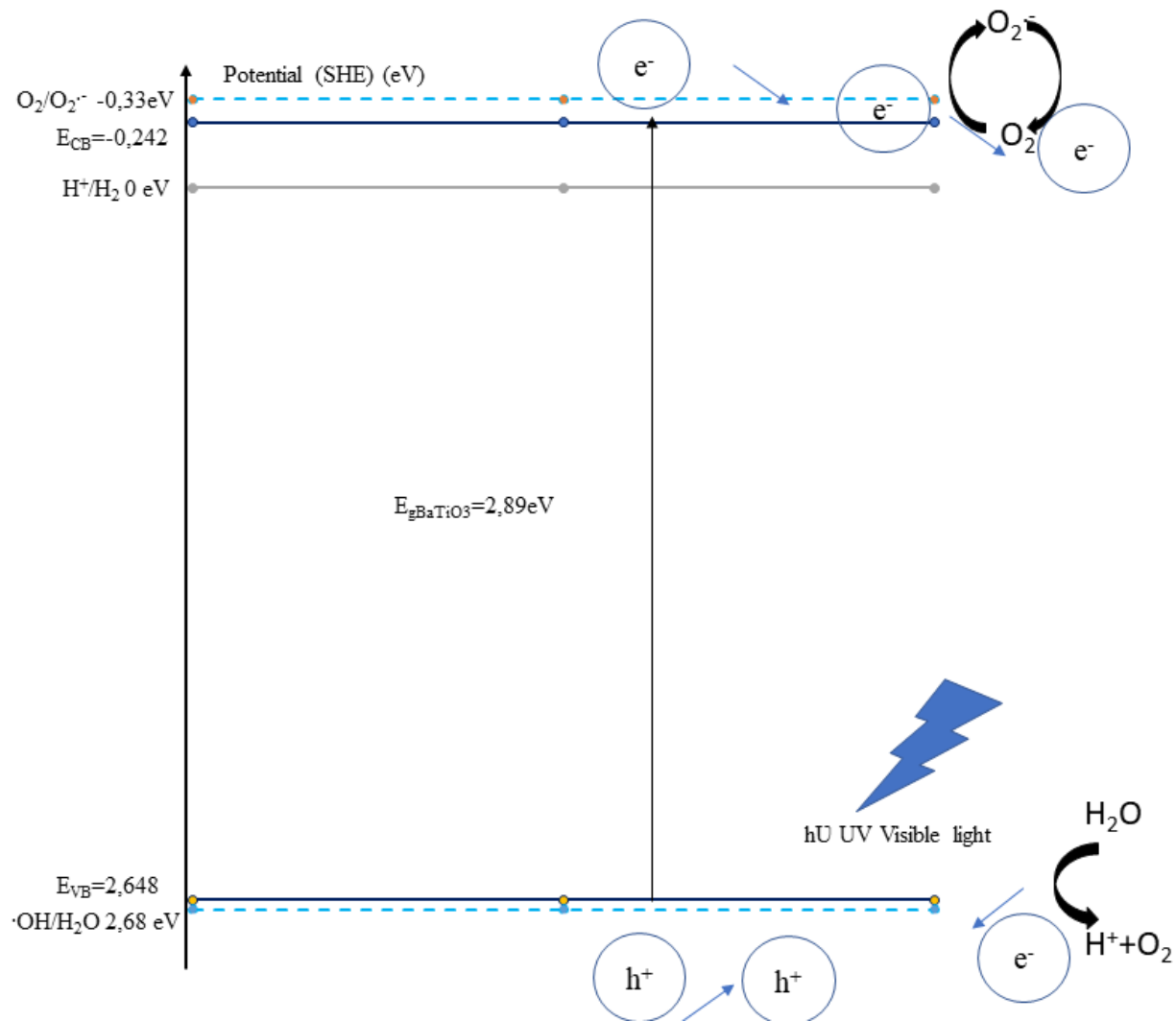
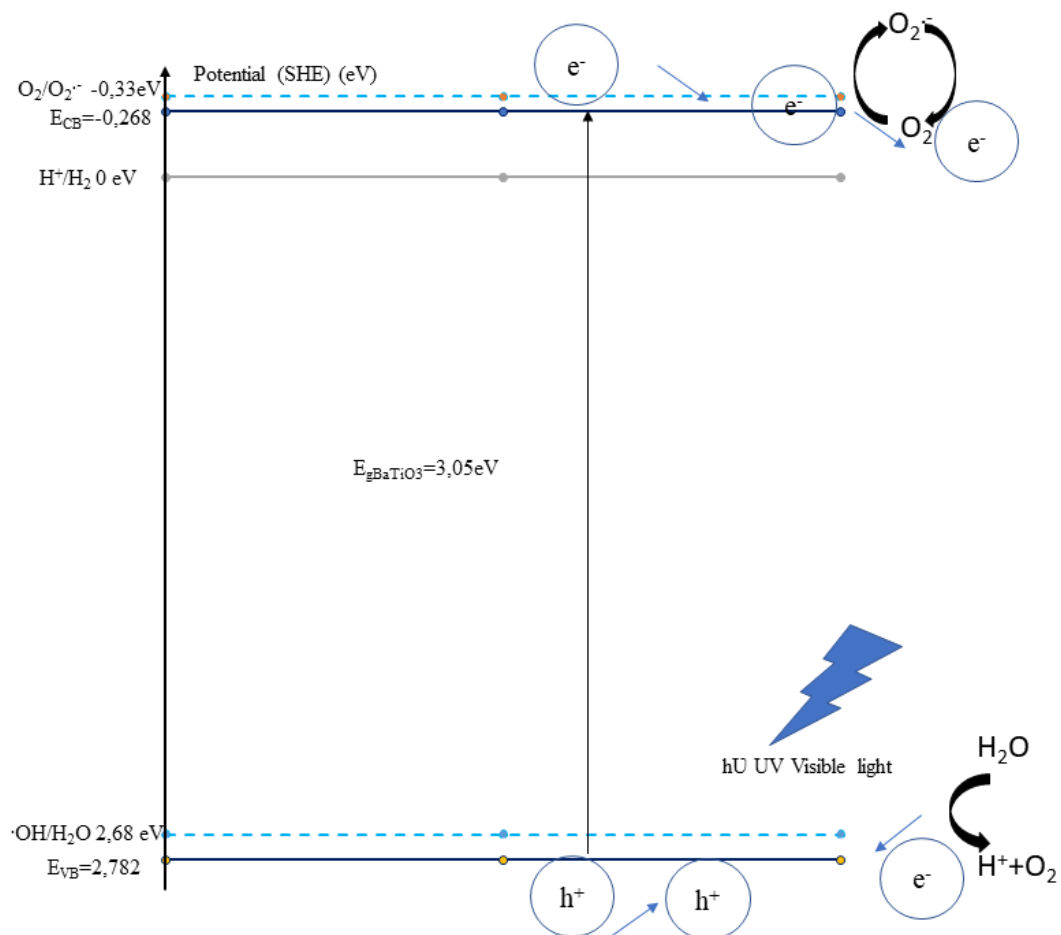


Figure S8. Continued.



(j)

Figure S8. Schematic ELD of $Ba_{1-x}Co_xTiO_3$ with respect to potential for the generation of $(O_2^{\bullet-})$ ($E^\circ_{(OH/H_2O)}$) and $O_2^{\bullet-}$ ($E_{O_2/O_2^{\bullet-}}$) radicals: (a) $BaTiO_3$, (b) $Ba_{0.9}Co_{0.1}TiO_3$; (c) $Ba_{0.8}Co_{0.2}TiO_3$; (d) $Ba_{0.7}Co_{0.3}TiO_3$; (e) $Ba_{0.6}Co_{0.4}TiO_3$; (f) $Ba_{0.5}Co_{0.5}TiO_3$; (g) $Ba_{0.3}Co_{0.7}TiO_3$; (h) $Ba_{0.2}Co_{0.8}TiO_3$; (i) $Ba_{0.1}Co_{0.9}TiO_3$ and (j) $CoTiO_3$.