Electronic and structural properties of engineering CdSe@TiO_2 nanotubes arrays

R. G. Freitas [a] (PQ), R. A. Mendes [a] (PG), F. W. S. Lucas [b] (PG), M. A. Santanna [b] (PG), G. L. C. Souza [a] (PQ), L. H. Mascaro [b] (PQ), E. C. Pereira [b] (PQ)

[a]*Department of Chemistry, Federal University of Mato Grosso, 78060-900, Cuiabá-MT, Brazil*
[b]*Department of Chemistry, Federal University of São Carlos, 13560-970, São Carlos-SP, Brazil*

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INTRODUCTION

TiO_2 nanotubes emerge as a promising class of semiconductors[1], especially when tuned with CdSe quantum dots [1]. TiO_2-anatase crystalline structure can be obtained at 450°C. Therefore, this work describe the structural and electronic parameter for CdSe deposited inside TiO_2NT previously (TiO_2NT-PTT) and later thermally treated (TiO_2NT-LTT).

METHODS

Rietveld refinement[2] was performed using the General Structure Analysis System program[3] suite. Based on the results of Rietveld refinement, TiO_2-anatase CIF inputs for the band structure and density of states (DOS) were obtained. DFT calculation for electronic structures of TiO_2 unit cell were carried out within the generalized gradient approximation (GGA) using the PWscf code included in the Quantum-Espresso package[4]. For this surface, a 4x4x4 Monkhorst-Pack and 49 *k*-points mesh was utilized for energy and electronic calculations.

RESULTS AND DISCUSSION

Rietveld refinement for TiO_2NT-PTT and TiO_2NT-LTT can be observed in Figure 1 with good statistical agreement.

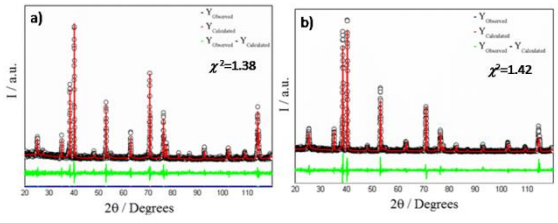

Figure 1. Rietveld refinement for a) TiO_2NT-PTT and b) TiO_2NT-LTT nanostructured materials.

Structural parameter obtained were a=b=3.756(4)Å, c=9.441(7)Å and a=b=3.796(2)Å, c=9.502(6) Å for TiO_2NT-PTT and TiO_2NT-LTT respectively.

The band structure and DOS for the TiO_2NT-PTT and TiO_2NT-LTT can be observed in Figure 2. It is possible to notice that the top of valence band is located at point *Z* for both crystalline structure.

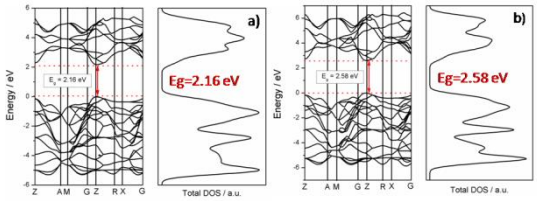

Figure 2. Band structure and DOS obtained for a) TiO_2NT-PTT and b) TiO_2NT-LTT nanostructured materials.

Moreover, direct band gaps can be observed. Experimental band gap values were 2.20eV and 2.65eV for TiO_2NT-PTT and TiO_2NT-PTT respectively. These data are in agreement with theoretical one.

CONCLUSIONS

Electronic structures derived from the models obtained using Rietveld refinement allows calculated electronic energy band gap, as well as energy band structure that were consistent with experimentally determined optical band gap.

ACKNOWLEDGMENTS

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