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Comment on "Blue light emission from barium doped zinc sulfide nanoparticles"

1. Introduction

After checking many scientific papers, we encountered the same error either in the application of the Tauc model or on the lecture of the UV–vis absorbance spectra. This confusion makes us pessimistic concerning the given (obtained) optical energy band by using this useful model. Actually, in their recent paper titled "Blue light emission from barium doped zinc sulfide nanoparticles", Pathak et al. [1] have reported on the elaboration of ZnS nanoparticles with Ba^{2+} doping through chemical route, namely the chemical precipitation method at room temperature. However, we perceive that some confusion exists about the graphical exploitation in determining the optical energy gap. We express concern about the obtained values by the authors. The purpose of this comment is to correct this error, which has unfortunately been promulgated through scores of papers as mentioned above.

Let us start by looking at Fig. 1 [1]; one can see that a clear absorption edge is apparent in the curves at about 340 nm. This corresponds logically to the transition band of ZnS material.

To determine the band gap, the authors used Tauc's model, in which the optical data is solicited. While this approach appears scientifically correct, graphical exploitation presents challenges. Indeed, one of the main principal errors comes

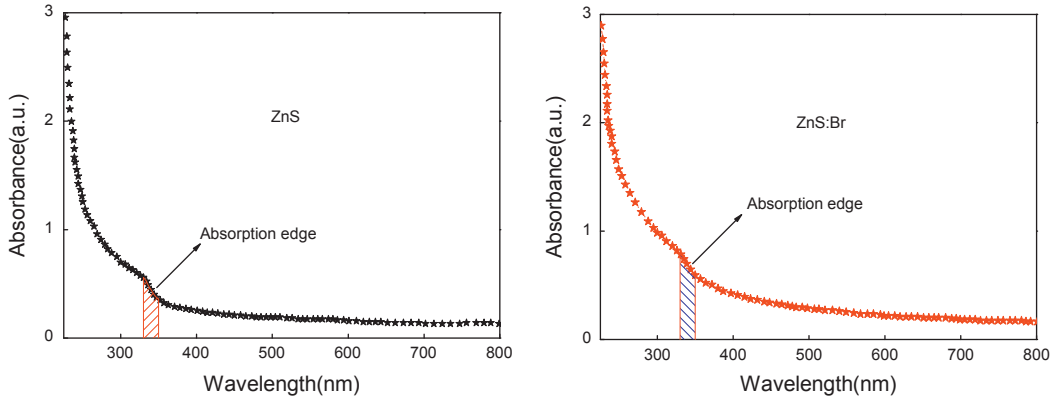

Fig. 1. The retraced UV–visible absorbance spectra [1].

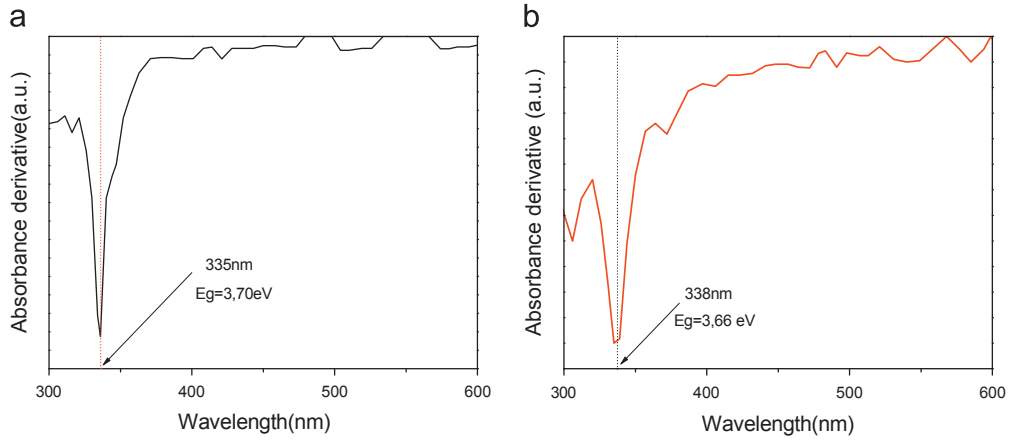

Fig. 2. Absorbance derivative curves: (a) ZnS and (b) ZnS:Br.

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within the plot scale choice [2], so it is necessary to carefully select the appropriate scale.

To respond firmly to this paper, we started by digitalizing (extracting the data) the absorbance curves, for more details see Ref. [3]. As we can see from Fig. 1, the retraced absorbance spectra fit well with the original ones (reported by the authors). With a closer look at Fig. 1, one can predict that the optical band can move into the hatched zone. To locate the cut-off wavelength (or energy), mathematical models (or tools) should be used. The band gap of the synthesized ZnS nanoparticles can be ascertained by differentiating i.e. d (Abs)/d($h\nu$) [4]. The peak position corresponding to the minima of the first derivative of the UV–vis absorbance spectra (shown in Fig. 2) yields the optical band gap. The real and exact values are 3.70 and 3.66 eV for pure and Br-doped zinc sulfide material respectively. On the other hand, it is not possible to confirm by simply looking at the UV–visible absorbance spectra the formation of ZnS nanoparticles!

Finally, we hope that this comment enlightens the readership to stop this confusion, to know how to interpret the UV–vis absorbance data and on how to apply the Tauc model. Also, the editors, reviewers, readers and authors should take care on assuming their full responsibility regarding the scientific knowledge.

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