ID_247 paper corrections

Note: expanding and including more material increases the number of pages to beyond 6 pages. The maximum number of pages required is 6 according to the guidelines. We have tried to accommodate the reviewer's suggestions but we were forced to remove some material to maintain a maximum of 6 pages.

Title

1. Title has been changed to " Study of lattice defects in BaF2 at elevated temperatures using positron annihilation and X-ray diffraction methods".

Abstract

2. First sentence in the abstract has been modified to read," Different experimental techniques used in this study have clearly…..
3. S-parameter has been given the context in the abstract
4. In line 11 of the abstract, the word "provided" was changed to "gave"

Introduction

5. Elaborated on the " wide band gap" and added "….. meaning that their electronic properties fall between the insulators and the conventional semiconductors……".
6. On page 2, temperature range was specified as (300-900) K.

Method of calculation

7. LDA was given a context in terms of Two-component density functional theory
8. Added "positron-electron correlation energy" instead of just " correlation energy.
9. Reference (8) was changed to "[8]".
10. All equations have been changed to conform to the requirements.

Experimental

11. First sentence was added as suggested by the reviewer, " The experimental setup for the positron annihilation investigation is shown figure 1 and comprises ….."
12. In line 3, " sized" was added
13. Diagram 1 was changed to give a more general setup diagram showing detector positions.
14. On page 3, we elaborated on coincidence arrangement
15. [111] is the crystal orientation.
16. Added "The data represents 45 diffraction pattern measurements……" as per reviewer's suggestions in line 11 on page 4.
17. "EVE program" was changed to "EVA program (for phase analysis)".

Results and discussion

18. Grammatical errors were corrected as per the reviewer
19. In figure 5, consistency means keep the low momentum window constant because it represents the area of the annihilation centroid. This statement is added in the caption.

20. Figure 6 shows the requested graph of s-parameter vs temperature with error bars. Figure 6 caption was edited according to the reviewer's suggestion
21. Journal abbreviation applied across all references for consistency.

22. Reference [2,3] changed to [2, 3]
23. Reference [5,6] changed to [5, 6]
24. Graph that shows lattice parameters as a function of temperature is included
25. Error margin of S-parameter is included
26. In the abstract," the theoretical approaches……." has been changed to give more context as per reviewer and read thus," Generalized gradient approximation in the framework of local density functional theory is used to calculate the Doppler broadening spectra".
27. In Methods of calculation, we have added the very first sentence which reads thus," Two component density functional theory (TCDFT) is used to obtain both positron and electron densities necessary to estimate positron lifetimes and the calculations of positron-electron momentum densities.