

July 08, 2022

Response to Reviewer #2
Manuscript nanomaterials-1804730

Prof. Dr. Fedor Jelezko
Guest Editor
Nanomaterials (Special Issue: Tailored Materials for Quantum Technologies)

Dear Prof. Dr. Jelezko,

on behalf of our coauthors, we would like to thank you for considering our manuscript entitled 'Tailoring the emission wavelength of color centers in hexagonal boron nitride for quantum applications' for Nanomaterials. As requested, we have addressed the comments and questions of the reviewers in a point-by-point response.

We also thank the reviewers for their comprehensive reports, their time and helpful comments. Based on these comments we have improved the quality of our manuscript and hope, that it is now suitable for publication in Nanomaterials. For the aid of the editor and reviewers, we first provide the reviewer's comments (in blue) followed by a detailed response (in black).

Yours sincerely,

Tobias Vogl
Friedrich-Schiller-University Jena

This is a very interesting and well presented paper making a convincing scientific case for specific colour centres in quantum technologies. In this context the paper is extremely topical and has the potential to make a big impact on the field, triggering more extensive experimental investigations and subsequent applications.

We would like to thank the reviewer for providing an accurate summary of our work and his/her comprehensive report.

One extremely minor comment:
Should the figures in Fig 4 not have error bars and thus be smooth curves?

We thank the reviewer for this comment. While we have used the for electronic structures well-suited and accurate hybrid HSE06 functional, the DFT method still has only a finite accuracy. Quantifying this (required for the determining the error bars), however, is not straightforward and potentially would have to be done for each calculation individually. It is possible, that the curve of the S_BV_B defect in 4a or Al_BV_B defect in 4d would then turn into a smooth linear curve. On the other side, this would not happen for the In_BV_N defect in 4a or Er_BV_B defect in 4c. As mentioned in the main text, the relationship between strain and transition energy can have nonlinear effects, consistent with previous reports by P. Dev (Phys. Rev. Res. 2020, 2, 22050, or Ref. [58]) and G. Grosso et al. (Nat. Commun. 2017, 8, 705 or Ref. [61]), but we believe these nonlinearities have a larger effect than the error of our DFT calculations. We have clarified this by expanding the section discussing these effects with:

'[...] Therefore, the eigenvalues of H also nonlinearly depend on s . We note that even using the hybrid HSE06 functional, the DFT method still has a finite accuracy. It is therefore possible that e.g.

the trend of the $S_B V_B$ defect in Figure 4(a) is purely linear. The afore mentioned nonlinear effects e.g. on the $ln_B V_N$ defect in Figure 4(a), however, are larger than this accuracy, implying that the error of our DFT calculations is not aliasing as a nonlinear strain-wavelength relationship'.