In this manuscript A. V. Ivanov and co-workers applied time-dependent variational density functional theory to describe the electronic excitations of a prototypical defect, the negatively charged nitrogen-vacancy center in diamond. They used 4 local and semi-local density functionals and compared their results with previous density functional based calculations, high-level many-body calculations and available experimental data.

They report that their method is more robust and predictive than DFT based calculations, since a correct ordering of the low-lying triplet and singlet states is obtained, in qualitative and quantitative agreement with the aforementioned high-level methods.

The resolution of the correct order controversy raised by previous studies is the major advance of the paper.

The paper is well written, interesting and it deserves to be published, but in my opinion it should go to Scipost core, as it's not a breakthrough. Here are my comments and remarks.

1) The authors used a 512 atoms supercell, how did the authors check if the supercell is "big enough" ?

2) It seems to me that people in the literature claim that the correct order of the low lying triplet and singlet states is not recovered because of the fact that the methods used are not able to describe multi-configurational states. However, as far as I understand, the Delta SCF method is also based on a single determinant state. So then what is the strength of this method? Is it the fact that the orbitals are variationally optimised and then the forces can, in principle, be calculated analytically?

3) Did the authors rely on this point to optimize the triplet excited states and calculate the ZPL?

4) From Fig. 2 and the discussion, it seems that the A_1 state is most affected by the type of calculation, do the authors have an opinion on this?

5) The most complex functional r^2SCAN gives vertical excitations in very good agreement with quantum embedding calculations beyond the random phase approximation (called Emb. bRPA). What makes this method so similar to the Emb. bRPA?

6) What geometry did the authors impose for the evaluation of the vertical excitation of the singlet states? They say that the energy decrease due to changes in atomic coordinates was not evaluated.

7) Would it be possible to provide a pictorial view of the electronic energy surfaces, with saddle points, position of triplet and singlet state geometries and the ZPL? I think that even a simple sketch would also help to follow the discussion.