Dear Editor,

We are grateful to the reviewers for the positive assessment of our work and for constructive suggestions regarding improvement of this paper.

A general criticism from both referees is that there is not enough statistical description of distributions of defect parameters obtained in this work. We have amended the manuscript to include more statistical descriptors of our data. We have also included a paragraph in our methods section explaining that our statistical analysis is not representative of the entire set that could exist in silicon dioxide:

We studied the distributions of defect properties by performing calculations for different a-SiO2 models as well as at different sites in the same model. For some of these properties, we have created large data sets, and where appropriate we use statistical descriptors to characterize the distributions obtained. However, some data sets are more limited due to computational costs, such as the reaction barriers. In these cases we do not use statistical descriptors, but rather give the range of the obtained parameters. We note that some of the defects, such as hydroxyl E' centers, are created at particular precursor sites in the amorphous structure as a result of a thermally activated process and their properties depend on the local and medium range environment of a small part of the amorphous structure. The distributions described in the paper are therefore representative of only those configurations of such defects that we have been able to calculate rather than the entire defects' population in a-SiO2.

All changes to the manuscript are highlighted in the 'changes.pdf' file. We have addressed the referees' comments in the manuscript as described below:

Referee A

Referee A's comments are very supportive of the work. Their main criticism centered around the use of the average as the sole descriptor for a number of the hydrogen induced defects' properties. We have included more statistical descriptors for properties where we have a large enough data set. These are highlighted in the 'changes.pdf' which shows where changes have been made to the manuscript. However, we refrained from giving statistical descriptors to the data sets that are rather small, such as all the calculated barriers and the binding energy of the Si-H bond in the hydrogen bridge.

Referee B

Referee B's comments are also rather supportive of this work, with criticisms also centered around the use of statistical descriptors. Their comments consist of:

1. "The range and the average value measure different things. The former is a measure of the spread, whereas the latter is a measure of the central tendency. I would suggest using the average value together with standard deviation (or median together with the interquartile distance)."

   We have included the standard deviation for our large data sets, as mentioned for the previous referee's comments.
2. "There seems to be an inconsistency in the values of formation energies. The total energy of

[SiO4 /H]0 center ranges from being 0.2 eV more to 0.1 eV less than the energy of the interstitial H atom (as stated on page 4). The E' center is more stable than the [SiO4 /H]0 center by 1.1 eV on average (as stated on page 5). Hence the E' center should be about 1 eV more stable than the hydrogen interstitial. In Fig. 4, however, the difference in the formation energy between the neutrally charged interstitial H atom and the E' center is 0.45 eV. The authors should explain this discrepancy."

Fig. 4 shows the formation energy vs. Fermi level for a single configuration of the hydroxyl E' center. It is not the average formation energy from all configurations. It is meant to show that configurations of the hydroxyl E' center can be stable across the Si band gap in an Si/SiO2 system. This has been made clearer in the manuscript with the description:

The formation energy as a function of the Fermi level position for one particular defect configuration, which is stable across the Si band gap, is shown in Fig. 4b).

3. "3. The authors characterize the statistical distribution of one-electron levels, thermodynamic transition levels and bond lengths but not of formation energies. Since the difference in the formation energy of various hydrogen configurations is the main result of this work, the authors should provide basic statistics or plot histograms of formation energies for at least neutrally charged defects."

   We have included the average and standard deviation of the formation energy of a neutral vacancy with the Fermi level set to the top of the silicon dioxide valence band.

4. "In Tab. I, distribution of reaction barriers are characterized by the minimum, maximum and average. Minimum and maximum values are sensitive to sample size. Because only 10 configurations are used, I would suggest using more robust measures such as the interquartile distance or, if the distribution is nearly normal, the standard deviation."

   We did not offer a statistical analysis of these data sets as they are rather small. We believe that the range of values provide in Table I qualitatively correctly reflects the important fact that these are wide distributions.

5. "Label D - seems to be missing in Fig. 8."

   This has been fixed.

We believe that we fully addressed the questions and concerns expressed by the reviewers and look forward to publication of this novel and original contribution in PRB.