

Responses to the editor

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February 17, 2020

Dear Matteo,

Thanks a lot for the previous email. We are very happy to see that the issues raised by Reviewers were mostly covered. We have ammended the minor problems, added a few modifications to properly adapt to pdf format and we are also adding a few comments for you and Authorea to ease the process.

We hope that the current version is soon out and we are very proud to be the first ones in this new way of understanding scientific publications.

Best wishes,
Núria

Format convention

To ease the reading, our responses will be written in royal blue, and the actions taken will be in *italics*.

Minor issues

Issue #1

There are still few language issues that need to be resolved. In particular, we note that a couple of the typos signaled by the reviewers has not been corrected (i.e. "Our framework show(s)" in the Abstract, "Niquel" in the caption of Fig.1)

Authors:

Manuscript has been carefully revised searching and correcting typos and grammar errors.

Issue #2

I have no reservations about the use of "avoidhuman". I think the humoristic intent of the term is clear, and in the context of the article it is apparent that it is not meant in an offensive way. My only observation is that avoidhuman only appear in the Abstract and nowhere else in the text. It may be clearer to label the avoidhuman path also in the body of the manuscript.

Authors:

Avoidhumans term was deleted from Section 1. (Introduction) in the previous version. In the current version Introduction has been modified to re-include the term. As the Reviewer indicates there is a humoristic intent.

Issue #3

The caption of Fig. 3 is, in my opinion, still not clear. At the moments it reads "Efficiency of the MER and TS workflows. Additional steps required implies that error checking routines have identified a deficiency in the calculation (i.e. maximum convergence steps reached), instead Manual preparation points out that the calculation failed and requires human intervention (i.e. bond breaking)". I suggest that "Additional steps" and "Manual preparation" are within quote marks. It would be useful to define "Good" also as Regularly terminated calculation. It is still not too clear what "Additional steps" is. Please note that there is typo in "identify". This calls for a final round of language checking.

Authors:

Text in Caption. 3 has been changed to meet the requirements of the Reviewer. Now it "Good" implies "Regularly terminated calculation".

Issue #4

If you need to add a Funders Information to the article, please do so in a section above the References.

Authors:

Thanks to the editor for the advice. *A new Section 5. has been added with the acknowledgments.*

Major issues**Issue #1**

The 3dMol visualization of the slabs in Figure 1 was working in the 1st submission but it is no longer working now. This needs to be fixed. As you can see from the attached screenshot, while the rest of the figure works, the slab does not render and return a white box. Please note that the figure was displaying perfectly until I had to clear my cache. This is how I discovered it. If you clear your browser cache (or use a new browser) you will see it to. This has something to do with the OpenGL libraries and it was a change that happens after the submission of your first version back in October last year. Obviously, this needs to be fixed before we can proceed.

Authors:

We were experiencing two different problems with the figures: (i) 3DMol figures ceased to render due an update from 3Dmol developers and (ii) not all molecules inside the paper were rendered on a mobile device. *3Dmol library has been changed to link a static version instead of the most recent version. The code of the Fig. 1 has been modified to load only a viewer instead of a set of them and change the model depending on the structure.*

Issue #2

I agree that Authorea needs to have an embargoed data management system to allow for the peer-review of not-yet-public data. We are working on this, and thank you and the Reviewer for working on work-arounds to this problem at the moment. However, we need the data to be made public a bit before publication for internal testing before publication. Since this the first article to be published on Wiley Online Library (ever!) with these features we need to manually check things. We will work with you on the timing for this to make sure that users do not get on the data before the paper is out, but please understand that we need this. I assume the embargo is the explanation for molecular structure not displaying in Fig. 2 at the moment? (see screenshot attached)

Authors

We agree with the editor and the embargoed data will be public after acceptance of the article. Fig. 2 was not display due to an error affecting the number of figures that can be loaded at the same time. *Two "datalinks" have been added to Fig. 1 and 2, the first one containing the reduced dataset and the second one containing the full dataset. Code of Fig. 1 has been modified to load only one viewer instead of a set of them, this will allow all the figures to load in any browser (double checked).*

Issue #3

For all 3 Figures we request a static representation (JPG, PDF, etc...) for publication. Can you provide those? These serves two purposes: 1) While readers will read the paper in all its interactive glory online, we will still have a journal typeset PDF of the article. The static version of the figures (with a link to the interactive version in the HTML version) will go in the PDF. 2) The static version will appear online instead of the interactive version IF the default inteactive figure fails to render for whatever reason, or it I displayed in a screen that is too small for the interactive version to work. Please note that the static representation of the figure can mirror the interactive version (this I think will work for Fig 2 & 3), or can be different (for example Fig 1 could be only the diagram without the slabs, or have all the slabs displayed).

Authors

Static versions for all the figures have been added to the manuscript.