## Editor's comment for "Turning chemistry into information for heterogeneous catalysis"

Matteo Cavalleri<sup>1</sup>

<sup>1</sup>Wiley

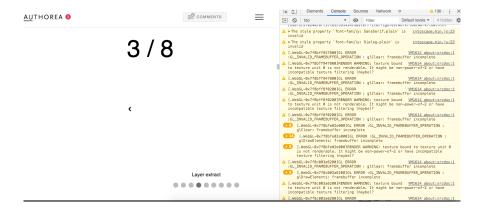
June 10, 2020

Dear Nuria,

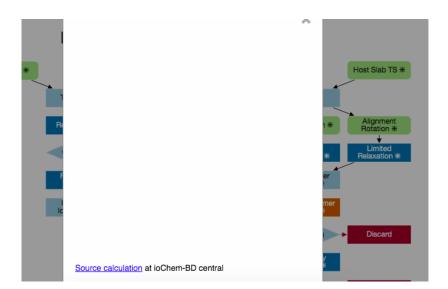
Thank you for your patience. We are ready to accept the paper (the first-ever using Authorea!) for publication.

Before I can do that, there are few aspects that need to be clarified or corrected.

- Minor Issues:
- 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)
- 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.
- 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 idenfied 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.
- If you need to add a Funders Information to the article, please do so in a section above the References
- Major Issues:
- 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 slub 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 brower 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.



- 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:



- 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 interactive 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).

Please let me know if you have any questions or concerns. As soon as the issues above are resolved (with a revision in Authorea, and providing the static figures) we will accept the paper. Referee reports (one

reviewer has elected to remain anonymous, one has signed the report) and your response to the referees will be also published alongside the article for trasparency of the peer-review.

Thank you all for your patience. I think the final published article will be worth the pain.

Matteo

Dr. Matteo Cavalleri|he/him|Editor-in-Chief International Journal of Quantum Chemistry John Wiley & Sons, Inc., Hoboken, NJ 07030