

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

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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 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.

- 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 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.

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 transparency of the peer-review.

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

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