

## Messerly, Richard A. (Fed)

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**From:** notifications=scholasticahq.com@scholasticahq.com on behalf of Living Journal of Computational Molecular Science <notifications@scholasticahq.com>  
**Sent:** Tuesday, October 02, 2018 12:06 AM  
**To:** Messerly, Richard A. (Fed)  
**Subject:** Living Journal of Computational Molecular Science has made a decision concerning your manuscript: Best Practices for Computing Transport Properties 1. Self-Diffusivity and Viscosity from Equilibrium Molecular Dynamics v1

Congratulations!

The editorial staff at LiveCoMS has accepted your article, "Best Practices for Computing Transport Properties 1. Self-Diffusivity and Viscosity from Equilibrium Molecular Dynamics v1", pending minor changes noted below, for publication in the Living Journal of Computational Molecular Science.

After addressing the comments below, the authors should perform a careful readthrough of the manuscript for errors, as no additional typesetting or proofing will be done after that point. We suggest rereading the writing style and editing section of the authors instructions.

After being published as an ASAP article, the authors will have one final chance to fix minor typos and inaccuracies before the article is published in the next regularly scheduled issue. Beyond that, any typos will remain in the LiveCOMS version until the next peer-reviewed version. Changes can of course be made at any time in the authors' maintained version on GitHub, which is linked from the article itself.

Before publication you must also send a signed copy of the contributor license release form to [managing@livecomsjournal.org](mailto:managing@livecomsjournal.org). As a reminder, this license does not transfer any copyright, but makes it easier for LiveCoMS to publish the article by clarifying that author does indeed have the right to distribute the article open source. See copyright licence section for more information. In the case of this article, since one author is at NIST, it will be important to also check the public domain statement suggested in the licensing section and verify that something equivalent is included.

Editorial issues to address are listed below. I will be happy to assist with other questions (perhaps best through GitHub issues) on any other changes as your author team performs final proofing.

Again, congratulations!

Michael Shirts

Editor, Living Journal of Computational Molecular Science

Editorial issues to address:

- The title should be in the form: (title) [Article v1.0]
- In the other resources section, in the introduction, put titles in italics in references, or otherwise set them apart, additionally, it probably makes sense to list just the name of person for class notes (I'm open to other suggestions).
- Figures should have their first sentence rephrased as the conclusion that the figure shows, so that the point the figures make is self-contained. For example, in figure 5,
- Figure 5: rephrase the first sentence as a conclusion, such as "viscosity obtained with the Green-Kubo relationship is only weakly dependent on system size in the range studied".
- Generally, the figures should be examined to ensure they are self-contained. In many cases, the figures refer to the paper the figure came from itself, which is acceptable for the data on how the figures are generated, but the meaning of the figures should be self-contained in the caption. Also, thanks for seeking out permission to use those figures.
- Figure 1: MD and YH not defined in caption.
- Figure 2: This is a bit confusing, as the linear fits are to points that appear to be outside the graph. Red dotted line does not have a label. The notation  $E_{\text{tors}}$  is not explained.
- Figure 8: the inset is not described as such.
- Table 1: Variables (such as  $\gamma$  and  $\xi$ ) should be explicitly defined in the table, not just in the context.
- Section 5.4 and 6.4: Suggest something more specific than "special topics"
- ACS style guide says do not leave a space between a number and a percent; this happens a number of times in the article.

- Acknowledgements should be updated to include anyone who has contributed (other than the author and the editors) to improve the paper.
- Reference 23 has an improperly formatted DOI.
- Preference is that citations are abbreviations, but the regardless style must be consistent; there are citations that are both abbreviations and full journal entries.
- For references 14-17, see if there is a way to split the html without losing the link (check href package options?)

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## Publication Decision Details

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### Manuscript Title

Best Practices for Computing Transport Properties 1. Self-Diffusivity and Viscosity from Equilibrium Molecular Dynamics v1

### Journal

Living Journal of Computational Molecular Science

### Publication Decision

Accept

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