ABOUT THIS DOCUMENT

Submitting this document is necessary for publication. Even if the article is licensed under a permissive license such as CC-BY, we require this additional license to clarify the rights of the University of Colorado Boulder, as publisher of LiveCoMS, to publish the article. Its role is also to confirm that all authors grant the publisher the right to distribute their article and that the authors are legally entitled to do so for all the material in the article.

This agreement is a license, not a copyright transfer; authors retain the copyright for their works, and therefore authors are not restricted in their own use or distribution of their work in any way by this document.

Only one author needs to sign this form, as under copyright law, each co-author of a joint work can grant non-exclusive publication rights. However, we suggest the signing author get informal agreement from the other authors before signing.

COPYRIGHT LICENSE

In reference to the following article:

F' 4 4 4 4 1 T	Best Practices	£ - :	C	
incert title i	Rest Practices	tor aichemical	tree energy	calcillations
imsert uner	DCSt 1 lactices	ioi aiciiciiiicai	II CC CIICI Gy	Carcarations

For good and valuable consideration, including being acknowledged for my contribution when the University of Colorado Boulder ("UCB") publishes any text or images ("Material") contributed by me, I (the undersigned individual or entity) agree as follows:

- 1. I am the author/creator/developer or co-author ("Contributor") of the Material that I have provided and may in the future provide to UCB for publication in the Living Journal of Computational Molecular Science.
- 2. I grant to UCB, its successors and assigns, a perpetual, non-exclusive, worldwide right, for no fee: to use, copy (an unlimited number of times), display, publish, distribute, transfer, sell (on a cost-recovery basis only) and disseminate the Material (and derivative works) in all media, including the World Wide Web; to create derivative works from the Material; and to sub-license to others all such rights in and to the Material.
- 3. I understand that UCB: i. will publish this material on its own website managed by Scholasticahq.com, or on similar platforms; ii. will offer it to the public under a Creative Commons-By license or a similar license as agreed during the editorial process, or a license with substantially similar terms ("open source license"); and iii. may in the future offer the material under future versions of such open source license.
- 4. I represent and warrant that Material is original (unless otherwise indicated in the Material's text), that I have full authority to grant the rights described in this license, and that UCB's exercise of its rights in the Material (as described in this agreement) will not infringe upon any copyright or any other proprietary right held by another party. I further

agree that to the extent that my Material incorporates material owned by or exclusively licensed to a third party, I am solely responsible for obtaining any necessary authorization from such third party to grant the license contained herein, and I will provide UCB with evidence of such third-party authorization upon request. If any of the representations and warranties in this Section 4 prove to be false, I agree to defend, indemnify, and hold UCB harmless from any resulting claims, demands, damages, costs (including reasonable attorney fees) and liabilities.

- 5. I acknowledge and agree that no monetary or in-kind type of consideration will be paid, nor will any be due and owing to me for the authorization granted hereunder. I will not take any action, whatsoever, which may hinder or restrict, in any manner, UCB in its activities to exercise its rights with respect to the Material and derivative works thereof.
- 6. I understand that UCB may in the future assign UCB's ownership of the Living Journal of Computational Molecular Science to a third-party, which may be a publisher, association, university, or other entity ("successor publisher"). In the case of such assignment, the successor publisher shall be deemed UCB's successor in interest to this license, and shall assume all of UCB's rights hereunder.

Thank you for granting us these rights in your Material. To grant us all of the rights requested in this letter, please sign below and return to:

Living Journal of Computational Molecular Science University of Colorado Boulder 596 UCB Boulder, CO 80309

Email: managing@livecomsjournal.org

Fax: 303-492-8425

11/28/2020 Date of Signature

You can either fax, mail, or scan and email your signed form.

CCEPTED and AGREED TO this 28th day of November	, <u>2020</u>
A May	
Signature of Contributor	
Antonia Mey	
Printed or Typed Name of Contributor	
1 miles of Types I want of Commontor	