



AMERICAN CHEMICAL SOCIETY  
JOURNAL PUBLISHING AGREEMENT  
Form A: Authors Who Hold Copyright and Works-for-Hire  
Control #2015-10-1

Manuscript ID, if Available

Received Date (Office Use Only)

### SECTION I: Copyright

**1. Submitted Work:** The Corresponding Author or designee below, with the consent of all co-authors, hereby transfers to the ACS the copyright ownership in the referenced Submitted Work, including all versions in any format now known or hereafter developed. If the manuscript is not accepted by ACS or withdrawn prior to acceptance by ACS, this transfer will be null and void.

**2. Supporting Information:** The copyright ownership transferred to ACS in any copyrightable\* Supporting Information accompanying the Submitted Work is nonexclusive. The Author and the ACS agree that each has unlimited use of Supporting Information. Authors may use or authorize the use of material created by the Author in the Supporting Information associated with the Submitted or Published Work for any purpose and in any format.

\*Title 17 of the United States Code defines copyrightable material as "original works of authorship fixed in any tangible medium of expression" (Chapter 1, Section 102). To learn more about copyrightable material see "Frequently Asked Questions about Copyright" on the Publications Division website, at [http://pubs.acs.org/page/copyright/learning\\_module/module.html](http://pubs.acs.org/page/copyright/learning_module/module.html).

### SECTION II: Permitted Uses by Author(s)

**1. Reuse/Republishing of the Entire Work in Theses or Collections:** Authors may reuse all or part of the Submitted, Accepted or Published Work in a thesis or dissertation that the Author writes and is required to submit to satisfy the criteria of degree-granting institutions. Such reuse is permitted subject to the ACS' "Ethical Guidelines to Publication of Chemical Research"

*Continued on Page 2*

### SIGNATURES

Signing this agreement constitutes acceptance by the Author(s) and, in the case of a Work-Made-for-Hire, the company/employer of all contents contained herein, including the attached Appendix A: Author Warranties, Obligations, Definitions, and General Provisions.

Yannick CARISSAN

Name of Corresponding Author or designee

Signature

Date

2017 October, 6th

Employer/Organization (Work-for-Hire only)

Authorized Signature(s) of Employer/Organization (Work-for-Hire only)

Date

U.S. Government Contract #, if available

### INSTRUCTIONS FOR FORM A

Form A should be signed **ONLY** by Author(s) who hold Copyright or who have created Works-for-Hire.

This manuscript will be considered with the understanding you have submitted it on an exclusive basis. You will be notified of a decision as soon as possible.

1. Complete all information in the **Manuscript Details** section.
2. Sign and date the form.
3. Submit **ALL PAGES OF THIS FORM** to the Editor's Office or upload it in ACS Paragon Plus.

### MANUSCRIPT DETAILS

Name of ACS Publication:

Journal of Computational and Theoretical Chemistry

Manuscript Title:

Atomic pseudo-potentials for sp<sup>2</sup> carbon atoms

Corresponding Author's Name and Address:

Yannick CARISSAN  
Aix Marseille Université  
Campus St Jérôme - service 561 - iSm2  
13013 Marseille

List Names of ALL Author(s):

Alexander Punter  
Paola Nava  
Yannick Carissan