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Scope of the Journal

The *Journal of Chemical Theory and Computation* publishes papers reporting new theories, methodology in quantum electronic structure, molecular dynamics, and statistical mechanics and/or their important applications. Specific topics include advances in ab initio quantum mechanics, density functional theory, design and properties of new materials, surface science, Monte Carlo simulations, solvation models, QM/MM calculations, biomolecular structure prediction, and molecular dynamics in the broadest sense, including gas-phase dynamics, ab initio dynamics, biomolecular dynamics, and protein folding/phase separation. New theories for quantum computers and their applications are welcome, as well as the combination of data science, theory, and computations relevant to chemistry. We also welcome papers on computational chemistry packages that present innovative methods. The Journal does not consider papers that are straightforward applications on only single-class systems of well-established methods, including DFT, traditional wave function theories, and molecular dynamics. The Journal favors submissions that include advances in theory, methodology, and data science with applications to compelling problems in chemistry and materials science.

Manuscript Types

Articles. Full-length research manuscripts, consistent with the objectives of the *Journal of Chemical Theory and Computation*, are the principal focus of the journal. Authors must follow the instructions for preparation and submission given below.

Letters. Letters are intended for rapid publication of preliminary reports on important findings of novel and timely significance. The major concepts of the paper should not have been published previously. Manuscripts are limited to four journal pages (16 double-spaced manuscript pages including all materials). The abstract is limited to 75 words and should briefly state the purpose of the research, principal results, and major conclusions.

Reviews. Reviews are topical, brief, and of general interest to the *Journal of Chemical Theory and Computation* community. These articles critically evaluate existing work and make the material more easily comprehensible to those who are not experts in the subject matter. Reviews must be ~10,000 words (excluding the References and all graphics).

Perspectives. Perspectives are interpretive accounts on subjects of current interest to the *Journal of Chemical Theory and Computation* community. This series is intended to be a forum for experts to present their perspectives on emerging or active areas of research.

ACS Researcher Resources

While this document will provide basic information on how to prepare and submit the manuscript as well as other critical information about publishing, we also encourage authors to visit [ACS Researcher Resources](#) for additional information on everything that is needed to prepare (and review) manuscripts for ACS journals and partner journals, such as

- [Mastering the Art of Scientific Publication](#), which shares editor tips about a variety of topics

including making your paper scientifically effective, preparing excellent graphics, and writing cover letters.

- Resources on [how to prepare and submit a manuscript](#) to ACS Paragon Plus, ACS Publications' manuscript submission and peer review environment, including details on selecting the applicable [Journal Publishing Agreement](#).
- [Sharing your research](#) with the public through the ACS Publications open access program.
- [ACS Reviewer Lab](#), a free online course covering best practices for peer review and related ethical considerations.
- [ACS Author Lab](#), a free online course that empowers authors to prepare and submit strong manuscripts, avoiding errors that could lead to delays in the publication process.
- [ACS Inclusivity Style Guide](#), a guide that helps researchers communicate in ways that recognize and respect diversity in all its forms.

Manuscript Preparation

Submit with Fast Format

All ACS journals and partner journals have simplified their formatting requirements in favor of a streamlined and standardized format for an initial manuscript submission. Read more about the requirements and the benefits these serves authors and reviewers [here](#).

Manuscripts submitted for initial consideration must adhere to these standards:

- Submissions must be complete with clearly identified standard sections used to report original research, free of annotations or highlights, and include all numbered and labeled components.
- Figures, charts, tables, schemes, and equations should be embedded in the text at the point of relevance. Separate graphics can be supplied later at revision, if necessary.
- When required by a journal's structure or length limitations, manuscript templates should be used.
- References can be provided in any style, but they must be complete, including titles. For information about the required components of different reference types, please refer to the [ACS Style Quick Guide](#).
- Supporting Information must be submitted as a separate file(s).

Document Templates and Format

The templates facilitate the peer review process by allowing authors to place artwork and tables close to the point where they are discussed within the text. Learn more about document templates [here](#).

General information on the preparation of manuscripts may also be found in the [ACS Guide to Scholarly Communication](#).

Acceptable Software, File Designations, and TeX/LaTeX

See the list of [Acceptable Software](#) and appropriate [File Designations](#) to be sure your file types are compatible with ACS Paragon Plus. Information for manuscripts generated from [TeX/LaTeX](#) is also available.

Cover Letter

A cover letter must accompany every manuscript submission. During the submission process, you may type it or paste it into the submission system, or you may attach it as a file.

The cover letter is a word-processor or PDF file that is uploaded at the same time as the manuscript file. The cover letter should include (1) the corresponding author's name, postal and e-mail addresses, and telephone and fax numbers; (2) the title of the manuscript and a brief paragraph pointing out the significance of the reported work; (3) indication of whether the manuscript is being submitted as an Article, Perspective, or Letter; and (4) the names, institutional affiliations, and postal and e-mail addresses of three scientists qualified to act as reviewers. The Editors will also use reviewers of their own choice.

If substantially the same manuscript has been previously submitted to this Journal or to another ACS journal, the author should include copies of the reviews with the submission and explain any revisions in the cover letter. The Editor may accept the manuscript on the basis of those reviews and author remarks or may seek additional reviews.

Manuscript Text Components

Title. The title of the paper should be brief—preferably 12 words or fewer. Readers rarely read and absorb longer titles, so it should be concise. An abstract of 3-4 sentences is required, and as with the title, it should be concise, touching on just the major points about which the author wants to alert the reader.

Text. A list of currently acceptable software packages can be found at <https://pubs.acs.org/page/4authors/submission/software.html>. The article should conform to the usual ACS format, using the article template available online at [ACS Paragon Plus](#). The final version should be prepared in a single word-processor file, with all graphics included.

The word-processor file should be saved in a document format (.wpd or .doc) not in the .txt or ASCII formats, which do not support enhancements such as subscripts. Text should be single-column, fully justified. If a non-Western version of the word-processing software is used, the file should be saved in rich-text format (RTF). Each file should be checked with an up-to-date virus detection program. The presence of a virus may delay publication.

The fonts "Times" and "Symbol" produce the best results. Other fonts, particularly those that do not come bundled with the system software, may not translate properly. All special characters (e.g., Greek characters, math symbols, etc.) must be present in the body of the text as characters and not as graphic representations.

Supporting Information

This information is provided to the reviewers during the peer-review process (for Review Only) and is available to readers of the published work (for Publication). Supporting Information must be submitted at the same time as the manuscript. See the list of [Acceptable Software by File Designation](#) and confirm that your Supporting Information is [viewable](#).

If the manuscript is accompanied by any supporting information files for publication, these files will be made available free of charge to readers. A brief, nonsentence description of the actual contents of each file, including the file type extension, is required. This description should be

labeled Supporting Information and should appear before the Acknowledgement and Reference sections. Examples of sufficient and insufficient descriptions are as follows:

Examples of sufficient descriptions: “Supporting Information: ^1H NMR spectra for all compounds (PDF)” or “Additional experimental details, materials, and methods, including photographs of experimental setup (DOC)”.

Examples of insufficient descriptions: “Supporting Information: Figures S1-S3” or “Additional figures as mentioned in the text”.

When including supporting information for review only, include copies of references that are unpublished or in-press. These files are available only to editors and reviewers.

Research Data Policy

All ACS journals strongly encourage authors to make the research data underlying their articles publicly available at the time of publication.

Research data is defined as materials and information used in the experiments that enable the validation of the conclusions drawn in the article, including primary data produced by the authors for the study being reported, secondary data reused or analyzed by the authors for the study, and any other materials necessary to reproduce or replicate the results.

The [ACS Research Data Policy](#) provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

Data Requirements

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Experimental Safety. Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the experimental details section of the full article or communication.

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The quality of illustrations in ACS journals and partner journals depends on the quality of the original files provided by the authors. Figures are not modified or enhanced by journal production staff. All graphics must be prepared and submitted in digital format.

Graphics should be inserted into the main body whenever possible. Please see Appendix 2 for additional information.

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The *Journal of Chemical Theory and Computation* authors are allowed to deposit an initial draft of their manuscript in a preprint service such as [ChemRxiv](#), arXiv, bioRxiv, or the applicable repository for their discipline prior to submission. Please note any use of a preprint server in the cover letter, and as appropriate, state how the manuscript has been adjusted/updated between deposition and submission. All other prior/redundant publication is forbidden. Upon publication, authors are advised to add a link from the preprint to the published paper via the Digital Object Identifier (DOI).

Editorial Policies

A guide to the proper format for manuscripts is provided on the [Journal's web page](#). Another valuable resource is [The ACS Style Guide](#), 3rd ed. (2006) available from Oxford University Press, Order Department, 201 Evans Rd, Cary, NC 27513. This book deals with all questions relating to manuscript style and provides the standard list of abbreviations for ACS Journals.

Authors must be sure that they are familiar with and abide by the [Ethical Guidelines](#) that are also available on the website and in [The ACS Style Guide](#).

For Supporting Material not submitted to ACS: If the supporting information is not submitted to ACS, it can't be referred to it in the paper as Supporting Information. The author will need to include a paragraph or sentence either at the end of the paper right before the acknowledgment or elsewhere in the paper if it makes more sense to include it there. The author should not include the heading "Supporting Information Available" or refer to the information in the paper as

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Retractions

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- an investigation into alleged misconduct related to the publication either has not been, or would not be, fair and impartial or conclusive;
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Appendix 1: PREPARING FOR SUBMISSION

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Ethical Guidelines

ACS editors have provided [Ethical Guidelines](#) for persons engaged in the publication of chemical research—specifically, for editors, authors, and reviewers. Each journal also has a specific [policy on prior publication](#).

OFAC Compliance

As a U.S.-based non-profit organization, the American Chemical Society (ACS) is required to comply with U.S. sanctions laws and regulations administered by the [U.S. Treasury Department's Office of Foreign Assets Control](#) (OFAC). While these laws and regulations permit U.S.-based publishers like ACS to engage in publishing-related activities with authors located in sanctioned regions in many cases, ACS may be prohibited under U.S. law from engaging in publishing-related activities in some cases, including, but not limited to, instances where an author or the institution with which an author is affiliated is located in a particular sanctioned region or has been designated by OFAC as a [Specially Designated National](#) (SDN) pursuant to certain U.S. sanctions programs. ACS reserves the right to refrain from engaging in any publishing-related activities that ACS determines in its sole discretion may be in violation of U.S. law.

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Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the Experimental Section of a full article and included in the main text of a letter. Statement examples can be found in the [Safety Statement Style Sheet](#) and additional information on communicating safety information from the *ACS Guide to Scholarly Communication* [is freely available here](#).

Conflict of Interest Disclosure

A statement describing any financial conflicts of interest or lack thereof is published in each ACS journal and partner journal article.

During the submission process, the Corresponding Author must provide a statement on behalf of all authors of the manuscript, describing all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest. If the manuscript is accepted, the statement will be published in the final article.

If the manuscript is accepted and no conflict of interest has been declared, the following statement will be published in the final article: "The authors declare no competing financial interest."

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Authorship, Author List, and Coauthor Notification

Authors are required to obtain the consent of all their coauthors prior to submitting a manuscript. The submitting author accepts the responsibility of notifying all coauthors that the manuscript is being submitted.

During manuscript submission, the submitting author must provide contact information (full name, email address, institutional affiliation, and mailing address) for all of the coauthors. Because all of the author names are automatically imported into the electronic [Journal Publishing Agreement](#), the names must be entered into ACS Paragon Plus. (Note that coauthors are not required to register in ACS Paragon Plus.) Author affiliation should reflect where the work was completed, even if the author has since left that institution. Authors may include a note with a current address if their institution has changed since the work was completed.

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Authors are responsible for ensuring that all patent activities and intellectual property issues are satisfactorily resolved prior to first publication (ASAP or in issue). Acceptance and publication will not be delayed for pending or unresolved issues of this nature.

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Diversity and Inclusion Statement

During manuscript submission, ACS journal authors have the option to submit a statement sharing information related to diversity and inclusion that is relevant for their paper. If supplying a diversity and inclusion statement, the corresponding author must provide this on behalf of all authors of the manuscript during the submission process. These statements include but are not limited to analysis of citation diversity and acknowledgment of indigenous land on which research was conducted. Statements expressing political beliefs are not permitted and may be removed by the journal office. All statements are subject to final review by the Editor.

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- **Land acknowledgment:**The land acknowledgment statement should appear in the Acknowledgements section of the manuscript. The statement should link to the institutions' formal land acknowledgments on which the research took place, if possible. Further guidance for creating these statements can be found here: <https://nativegov.org/news/a-guide-to-indigenous-land-acknowledgment/>.

Appendix 2: Preparing Graphics

Resolution

Digital graphics pasted into manuscripts should have the following minimum resolutions:

- Black and white line art, 1200 dpi
- Grayscale art, 600 dpi
- Color art, 300 dpi

Size

Graphics must fit a one- or two-column format. Single-column graphics can be sized up to 240 points wide (3.33 in.) and double-column graphics must be sized between 300 and 504 points (4.167 in. and 7 in.). The maximum depth for all graphics is 660 points (9.167 in.) including the caption (allow 12 pts. For each line of caption text). Lettering should be no smaller than 4.5 points in the final published format. The text should be legible when the graphic is viewed full-size. Helvetica or Arial fonts work well for lettering. Lines should be no thinner than 0.5 point.

Color

Color may be used to enhance the clarity of complex structures, figures, spectra, and schemes, etc., and color reproduction of graphics is provided at no additional cost to the author. Graphics intended to appear in black and white or grayscale should not be submitted in color.

Type of Graphics

Table of Contents (TOC)/Abstract Graphic

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Figures

A caption giving the figure number and a brief description must be included below each figure. The caption should be understandable without reference to the text. It is preferable to place any key to symbols used in the artwork itself, not in the caption. Ensure that any symbols and abbreviations used in the text agree with those in the artwork.

Charts

Charts (groups of structures that do not show reactions) may have a brief caption describing their contents.

Tables

Each table must have a brief (one phrase or sentence) title that describes the contents. The title should be understandable without reference to the text. Details should be put in footnotes, not in the title. Tables should be used when the data cannot be presented clearly in the narrative, when many numbers must be presented, or when more meaningful inter-relationships can be conveyed by the tabular format. Tables should supplement, not duplicate, information presented in the text and figures. Tables should be simple and concise.

Schemes

Each scheme (sequences of reactions) may have a brief caption describing its contents.

Chemical Structures

Chemical structures should be produced with the use of a drawing program such as ChemDraw.

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JCTC authors are encouraged to submit images to be considered for use on the journal's front cover or [Supplementary Covers](#) at the time of the submission of their revised manuscript. If your article is accepted for publication, your suggestion may also be selected for use on one of the journal's covers. If your art is selected for front cover, ACS will send you information about how to request one complimentary 18" by 24" printed poster featuring your work. Images chosen for the front cover will be published at no cost to the author.

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