

Last updated: December 06, 2021 [View the latest guidelines online](#)

Scope of the Journal

The [Journal of Chemical Theory and Computation](#) invites new and original contributions with the understanding that, if accepted, they will not be published elsewhere. Papers reporting new theories, methodology, and/or important applications in quantum electronic structure, molecular dynamics, and statistical mechanics are appropriate for submission to this Journal. Specific topics include advances in or applications of 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. The Journal does not consider papers that are straightforward applications of known methods including DFT and molecular dynamics. The Journal favors submissions that include advances in theory or methodology with applications to compelling problems.

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.

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

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.

ACS Publishing Center

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 the [ACS Publishing Center](#) 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.

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 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” or “Additional experimental details, materials, and methods, including photographs of experimental setup”.

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

ACS Math Style. Authors including math, display or in-text, in their manuscripts are encouraged to consult the [ACS Guidelines for Presenting Mathematical Information](#). This style sheet provides brief discussion of formatting related to the presentation of mathematical formulas, complete with examples of ACS style and layout. This document was developed to help authors anticipate how mathematical expressions will be formatted in the published version of the paper.

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.

Language and Editing Services

A well-written paper helps share your results most clearly. ACS Publications' [English Editing Service](#) is designed to help scientists communicate their research effectively. Our subject-matter expert editors will edit your manuscript for grammar, spelling, and other language errors so your ideas are presented at their best.

Preparing Graphics

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.

Any graphic (figure chart, scheme, or equation) that has appeared in an earlier publication should include a [credit line](#) citing the original source. Authors are responsible for [obtaining written permission](#) to re-use this material.

Figure and Illustration Services

The impact of your research is not limited to what you can express with words. Tables and figures

such as graphs, photographs, illustrations, diagrams, and other visuals can play a significant role in effectively communicating your findings. Our [Figures service](#) generates publication-ready figures that conform to your chosen journal's specifications. This includes changes to file type, resolution, color space, font, scale, line weights, and layout (to improve readability and professional appearance).

Preparing for Submission

Manuscripts, graphics, supporting information, and required forms, as well as manuscript revisions, must all be submitted in digital format through [ACS Paragon Plus](#), which requires an ACS ID to log in. Registering for an ACS ID is fast, free, and does not require an ACS membership. Please refer to Appendix 1 for additional information on preparing your submission

Prior Publication Policy

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 Supporting Information. The information can be referred to as "Additional information" or something similar – just not Supporting Information.

Providing Potential Reviewer Names

Please suggest 6 reviewers. Authors are encouraged to avoid suggesting reviewers from the authors' institutions. Do not suggest reviewers who may have a [real or perceived conflict of interest](#). Whenever possible, suggest academic email addresses rather than personal email addresses.

Manuscript Transfer

If your submission is declined for publication by this journal, the editors might deem your work to be better suited for another ACS Publications journal or partner journal and suggest that the authors consider transferring the submission. [Manuscript Transfer](#) simplifies and shortens the process of submitting to another ACS journal or partner journal, as all the coauthors, suggested reviewers, manuscript files, and responses to submission questions are copied by ACS Paragon Plus to the new draft submission. Authors are free to accept or decline the transfer offer.

Note that each journal is editorially independent. Transferring a manuscript is not a guarantee that the manuscript will be accepted, as the final publication decision will belong to the editor of the next journal.

PRODUCTION AND PUBLICATION

Proofs via ACS Direct Correct

Correction of the galley proofs is the responsibility of the Corresponding Author. The Corresponding Author of an accepted manuscript will receive e-mail notification and complete instructions when page proofs are available for review via [ACS Direct Correct](#). Extensive or important changes on page proofs, including changes to the title or list of authors, are subject to review by the editor.

It is the responsibility of the Corresponding Author to ensure that all authors listed on the manuscript agree with the changes made on the proofs. Galley proofs should be returned within 48 hours in order to ensure timely publication of the manuscript.

Publication Date and Patent Dates

Accepted manuscripts will be published on the ACS Publications Web site as soon as page proofs are corrected and all author concerns are resolved. The first date on which the document is published on the Web is considered the publication date.

Publication of manuscripts on the Web may occur weeks in advance of the cover date of the issue of publication. Authors should take this into account when planning their patent and intellectual property activities related to a document and should ensure that all patent information is available at the time of first publication, whether ASAP or issue publication.

All articles published ahead of print receive a unique Digital Object Identifier (DOI) number, which is used to cite the manuscript before and after the paper appears in an issue. Additionally, any supplemental information submitted along with the manuscript will automatically be assigned a DOI and hosted on Figshare to promote open data discoverability and use of your research outputs.

ASAP Publication

Manuscripts will be published on the “ASAP Articles” page on the web as soon as page proofs are corrected and all author concerns are resolved. ASAP publication usually occurs within a few working days of receipt of page proof corrections, which can be several weeks in advance of the cover date of the issue.

Post-Publication Policies

The American Chemical Society follows guidance from the [Committee on Publication Ethics](#) (COPE) when considering any ethical concerns regarding a published article, Retractions, and Expressions of Concern.

Additions and Corrections

Additions and Corrections may be requested by the author(s) or initiated by the Editor to address important issues or correct errors and omissions of consequence that arise after publication of an article. All Additions and Corrections are subject to approval by the Editor, and should bring new and directly relevant information and corrections that fix scientific facts. Minor corrections and additions will not be published. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work.

Additions and Corrections must be submitted as new manuscripts via ACS Paragon Plus by the Corresponding Author for publication in the “Addition/Correction” section of the Journal. The corresponding author should obtain approval from all coauthors prior to submitting or provide evidence that such approval has been solicited. The manuscript should include the original article title and author list, citation including DOI, and details of the correction.

Retractions

Articles may be retracted for scientific or ethical reasons and may be requested by the article author(s) or by the journal Editor(s), but are ultimately published at the discretion of the Editor. Articles that contain seriously flawed or erroneous data such that their findings and conclusions cannot be relied upon may be retracted in order to correct the scientific record. When an article is retracted, a notice of Retraction will be published containing information about the reason for the Retraction. The originally published article will remain online except in extraordinary circumstances (e.g. where deemed legally necessary, or if the availability of the published content poses public health risks).

Expressions of Concern

Expressions of Concern may be issued at the discretion of the Editor if:

- there is inconclusive evidence of research or publication misconduct by the authors;
- there is evidence that the findings are unreliable but the authors' institution will not investigate the case;
- an investigation into alleged misconduct related to the publication either has not been, or would not be, fair and impartial or conclusive;
- an investigation is underway but a judgment will not be available for a considerable time.

Upon completion of any related investigation, and when a final determination is made about the outcome of the article, the Expression of Concern may be replaced with a Retraction notice or Correction.

Sharing Your Published Article

At ACS Publications, we know it is important for you to be able to share your peer reviewed,

published work with colleagues in the global community of scientists. As sharing on sites known as scholarly collaboration networks (SCNs) is becoming increasingly prevalent in today's scholarly research ecosystem, we would like to remind you of the many ways in which you, a valued ACS author, can [share your published work](#).

Publishing open access makes it easy to share your work with friends, colleagues, and family members. In addition, ACS Publications makes it easy to share your newly published research with ACS Articles on Request (see below). Don't forget to promote your research and related data on social media, at conferences, and through scholarly communication networks. Increase the impact of your research using the following resources: [Altmetrics](#), [Figshare](#), [ACS Certified Deposit](#)

E-Prints

When your article is published in an ACS journal or partner journal, corresponding authors are provided with a link that offers up to 50 free digital prints of the final published work. This link is valid for the first 12 months following online publication, and can be shared via email or an author's website. After one year, the access restrictions to your article will be lifted, and you can share the [Articles on Request](#) URL on social media and other channels. To access all your Articles on Request links, log in to your ACS Publishing Center account and visit the "My Published Manuscripts" page.

Reprints

[Article](#), [journal](#), and [commercial](#) reprints are available to order.

Appendix 1: PREPARING FOR SUBMISSION

We've developed ACS' publishing and editorial policies in consultation with the research communities that we serve, including authors and librarians. Browse our policies below to learn more.

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](#).

Safety Considerations

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."

Plagiarism

In publishing only original research, ACS is committed to deterring plagiarism, including self-plagiarism. ACS Publications uses CrossCheck's iThenticate software to screen submitted manuscripts for similarity to published material. Note that your manuscript may be screened during the submission process.

Further information about plagiarism can be found in Part B of the [Ethical Guidelines to Publication of Chemical Research](#). See also the [press release](#) regarding ACS' participation in the CrossCheck initiative.

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.

If any change in authorship is necessary after a manuscript has been submitted, the Corresponding Author must e-mail a signed letter to the Editor-in-Chief confirming that all of the original coauthors have been notified and have agreed to the change. If the change involves the removal of a coauthor's name, the Corresponding Author must, in addition, arrange for the coauthor involved to e-mail a separate signed letter to the Editor-in-Chief consenting to the change. No changes in the author list will be permitted after a manuscript has been accepted.

To expediate the processing of your manuscript, please format your author and affiliation information according the guidelines in this

link: <https://pubsapp.acs.org/paragonplus/submission/author-address-information.pdf>.

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.)

Patent Activities and Intellectual Property

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.

Open Researcher and Contributor ID (ORCID)

Authors submitting manuscript revisions are required to provide their own personal, validated ORCID iD before completing the submission, if an ORCID iD is not already associated with their ACS Paragon Plus user profiles. This ID may be provided during original manuscript submission or when submitting the manuscript revision. All authors are strongly encouraged to register for an ORCID iD, a unique researcher identifier. The ORCID iD will be displayed in the published article for any author on a manuscript who has a validated ORCID iD associated with ACS when the manuscript is accepted.

ORCID iDs should not be typed into the manuscript. ACS publishes only those ORCID iDs that have been properly verified and linked **before the manuscript is accepted**. After your ORCID iD is linked, it will be displayed automatically in all subsequently accepted manuscripts for any/all ACS journals. We do not publish ORCID iDs provided during proof review or via other communications after a manuscript is accepted for publication.

With an ORCID iD, you can create a profile of your research activities to distinguish yourself from other researchers with similar names, and make it easier for your colleagues to find your publications. If you do not yet have an ORCID iD, or you wish to associate your existing ORCID iD with your ACS Paragon Plus account, you may do so by clicking on “Edit Your Profile” from your ACS Paragon Plus account homepage and following the ORCID-related links. Learn more at www.orcid.org.

Copyright and Permissions

To obtain forms and guidelines for copyright transfer, obtaining permissions from copyright owners, and to explore a Copyright Learning Module for chemists, click [here](#).

Funder Reporting Requirement

Authors are [required to report funding sources](#) and grant/award numbers. Enter **ALL** sources of funding for **ALL** authors in **BOTH** the Funder Registry Tool in ACS Paragon Plus and in your manuscript to meet this requirement.

Open Access Compliance

ACS offers options by which authors can fulfill the requirements for open access and deposition into repositories for funded research. Visit our ACS Open Science site to see [how to fulfill requirements for specific funders](#) and to find out if you are eligible to publish under a [Read + Publish agreement](#) between ACS and your institution. You can also find out more about [Open Access Compliance](#) and [ACS Open Science initiatives](#).

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

Consult the Guidelines for [Table of Contents/Abstract Graphics](#) for specifications.

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.

Cover Art

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.

Cover image submissions should be colorful and visually engaging, with minimal text. The cover image should not resemble a graphical abstract or data figure, but rather should be an artistic and scientifically accurate representation of the manuscript.

Image files should be submitted as TIF, JPG, PNG or EPS files with a resolution of at least 300 dpi for pixel-based images. Images should be 6.79 in × 7.10 in. (or 17.25 cm × 18.03 cm). Authors should submit the cover image, along with a short, clear legend (less than 50 words) explaining the image, as supplementary files to ACS Paragon Plus with their revised manuscript.

If you wish to be considered only for the front cover, and not a paid supplementary cover, please respond NO accordingly to the Journal Covers question in ACS Paragon Plus. For more information on the Supplementary Covers program, please [see this webpage](#). All art submitted for consideration for a supplementary cover will also be considered for a front cover.

Web Enhanced Objects (WEO)

The Web editions of ACS journals allow readers to view multimedia attachments such as animations and movies that complement understanding of the research being reported.

WEOs should be uploaded in ACS Paragon Plus with 'Web Enhanced Object' selected as the file designation. Consult the list of [compatible WEO formats](#).