ACS Publications
Most Trusted. Most Cited. Most Read.

THE JOURNAL OF PHYSICAL CHEMISTRY B
A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Last updated: January 10, 2024 View the latest guidelines online

Manuscript Submission Requirements Checklist

This checklist is provided to assist authors in the initial submission of their manuscript to *The Journal of Physical Chemistry A/B/C*. It serves as a quick reference guide to aid authors in the submission process and to avoid potential delays with the review process. While these requirements are recommended before the submission, the points mentioned in **bold** are mandatory, in the absence of which the manuscript will be unsubmitted.

- Mark the corresponding author(s) with an asterisk in the manuscript's author list, and include this person's e-mail address and phone number. Maintain consistency with the author names in the manuscript with the entries in the ACS Paragon Plus submission.
- Label the sections. For a regular article, this includes (in this order) Abstract, Introduction, Methods, Results, Discussion, Conclusions, Supporting Information, Acknowledgments, References, and TOC Image. Other acceptable names for the Methods section include Experiment/Experimental Section, Theory, and Computational Details. The Results and Discussion sections could be presented as a single combined section.
- 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 a 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.
- References can be provided in any style. **Importantly, manuscript titles should be included in the references and there should only be one reference per citation**.
- If the manuscript includes any references to unpublished work (e.g., manuscripts in preparation or submitted for publication), upload such documents as Supporting Information for Review Only.
- Provide sufficient experimental and/or computational data for the reproducibility of results. Refer to the "Data Requirements" section for more information related primarily to theoretical and computational studies

Cover Letter should include

- Journal Part and Section, e.g., Part A, A4: New Tools and Methods in Experiment and Theory (Please note that the final decision on Journal Part and Section is up to the Editor handling the manuscript.)
- **A brief explanation of the manuscript's significance, including its originality, new physical insights, appropriateness for *JPC*, and contribution to new knowledge in the field.** Submission history should be provided if relevant.
- List of 5 recommended reviewers (institution, telephone number, and e-mail), with a short description of their relevant expertise. Provide the professional e-mail address for recommended reviewers rather than "gmail" or other non-professional electronic addresses. For more information refer to the "Cover Letter" section.

When submitting the manuscript in ACS Paragon Plus…

- Ensure that the Journal Part and Section match correctly in the submission site.
- List all authors with their correct professional e-mail addresses. It is essential to provide

accurate e-mail addresses as the co-authors will be notified about the submission. Entering inaccurate e-mail addresses will delay the review process.
- Ensure that all co-authors are aware of the submission. Refer to the Appendix for appropriate Ethical Guidelines.
- The submitting author should enter his/her ORCID identifier.
- Do you have a cover art proposal? Refer to the “Cover Art” section for more details.
- Authors using LaTeX must provide a PDF version of the manuscript and upload as the “Manuscript PDF File”, in addition to the LaTeX source files (which may be archived as a zip file). Refer to the LaTeX manuscript preparation webpage for more details.

Sections and Scopes of the Journals

The Journal of Physical Chemistry A: Molecules, Clusters, and Aerosols

Sections:
- A1 Structure, Spectroscopy, and Reactivity of Molecules and Clusters
- A2 Aerosols; Environmental and Atmospheric Chemistry; Astrochemistry
- A3 Combustion and Plasma Chemistry
- A4 New Tools and Methods in Experiment and Theory

Scope:
The Journal of Physical Chemistry A (JPC A) publishes experimental, theoretical, and computational research on the physical chemistry of molecules, ions, radicals, clusters, and aerosols. *JPC A* emphasizes applications in the areas of atmospheric and environmental chemistry, aerosol processes, molecular geochemistry, combustion, astrochemistry, plasmas, cold molecules, catalysis, and energetic materials, among others. *JPC A* also publishes manuscripts that describe new tools or methods that are of broad interest to the physical chemistry community. If you are unsure about whether your manuscript fits within the scope of *JPC A*, please contact Deputy Editor T. Daniel Crawford (crawford-office@jpc.acs.org) or Executive Editor Andrew Orr-Ewing (orr-ewing-office@jpc.acs.org). Further information about preparing manuscripts can be found here, and some tips for creating high impact manuscripts are given here. Editorials with guidelines on computational and theory research can be found here and here.

An essential criterion for acceptance of research articles in the *Journal* is that they provide new physical insight. Please refer to this Virtual Issue on what constitutes new physical insight. Manuscripts that are essentially reporting data or applications of data are, in general, not suitable for publication in *JPC A*. However, section A4 includes articles on New Tools and Methods in Experiment and Theory where the requirement for new physical insights is relaxed.

The Journal of Physical Chemistry B: Biophysics, Biomaterials, Liquids, and Soft Matter

Sections:
- B1 Biophysical and Biochemical Systems and Processes
- B2 Biomaterials and Membranes
- B3 Liquids; Chemical and Dynamical Processes in Solution
- B4 Soft Matter, Fluid Interfaces, Colloids, Polymers, and Glassy Materials

Scope:

The Journal of Physical Chemistry B (JPC B) publishes experimental, theoretical and computational research in the area of biophysics, biochemistry, biomaterials, and soft matter. Examples of topics of special interest include: biomolecules (proteins, nucleic acids, membranes, enzyme catalysis); biomaterials (including nano-biomaterials); polymers and colloids; liquids (properties of liquids, ionic liquids, deep eutectic solvents, and fluid interfaces, and solid-liquid interfaces, bulk studies of electrolytes); surfactants; glasses; and spectroscopy, charge, and energy transfer of molecules in solution. If you are unsure about whether your manuscript fits within the scope of *JPC B*, please contact Deputy Editor Martin Zanni (zanni-office@jpc.acs.org) or Executive Editor Pavel Jungwirth (jungwirth-office@jpc.acs.org). Further information about preparing manuscripts can be found here, and some tips for creating high impact manuscripts are given here. An editorial with guidelines for computational and theory research can be found here.

The Journal of Physical Chemistry C: Energy, Materials, and Catalysis

Sections:

- C1 Energy Conversion and Storage
- C2 Chemical and Catalytic Reactivity at Interfaces
- C3 Spectroscopy and Dynamics of Nano, Hybrid, and Low-Dimensional Materials
- C4 Physical Properties of Materials and Interfaces

Scope:

The Journal of Physical Chemistry C (JPC C) publishes experimental, theoretical and computational research on the physical chemistry of nano, low-dimensional and bulk materials; chemical transformations at interfaces; and energy conversion and storage. Examples of topics of special interest include: heterogeneous catalysis and electrocatalysis, solar energy cells, fuel cells, novel materials for batteries and capacitors, steady-state and time-resolved spectroscopy of nano- and 2D materials, plasmonic and photonic materials, studies of chemical transformations at solid surfaces, and observations and predictions of novel material and surface properties. If you are unsure whether your manuscript fits within the scope of *JPC C*, please contact Deputy Editor Gregory Hartland (hartland-office@jpc.acs.org) or Executive Editor William Schneider (schneider-office@jpc.acs.org). Further information about preparing manuscripts can be found here, and some tips for creating high impact experimental and theory/computational manuscripts are given here. An editorial with guidelines for computational and theory research can be found here.

Manuscript Types

Note that all Letters or Communications should be submitted to *The Journal of Physical Chemistry Letters*.

Articles should report original research having significant new physical insight that is expected to have a definable impact on the advancement of science, technology, and the field of physical chemistry. Manuscripts should cover the research with thoroughness and clarity but should be as concise as possible. Articles are scheduled for publication in the order of acceptance within limitations of available space. A table of contents (TOC) graphic is required for use in the Web edition of the journal.

Featured Articles are usually published by invitation. However, authors in important and active research fields of interest to physical chemists are encouraged to propose such articles.

Two-page proposals should be sent to the Deputy Editor of the corresponding journal section for

consideration. Contact information for the Deputy Editors can be found on the journal's homepages or the masthead of each journal section.

For Featured Article submissions, the author should provide a clear, concise, and critical status report of the field as an introduction to the article. The author's own contribution and its relationship to other work in the field should constitute the main body of the article. Controversies, if they exist, should also be outlined. Possible future directions and the significance of the research area to the field of physical chemistry should be pointed out. Featured Articles are limited to ~8 printed pages (equivalent to ~40 pages of double-space-typed text with figures, tables, references). A brief biography for each author of the Featured Article must be included. Photograph(s) may also be included with the biography. A TOC graphic is required for use in the Web edition of the journal. Authors of Featured Articles will be invited to provide an image to appear on the cover of the issue in which the Featured Article appears at no cost to the author.

Reviews are published by invitation. They are strictly reviews of active and rapidly changing fields with little or no new data reported. They are ~8 pages long (~40 typed pages). Authors are encouraged to submit two-page proposals to the Deputy Editor of the corresponding journal section for consideration. A brief biography for each author of the Review must be included. Photograph(s) may also be included with the biography. A TOC graphic is required for use in the Web edition of the journal. Authors of Reviews will be invited to provide an image to appear on the cover of the issue in which the Review appears at no cost to the author.

Mini-Reviews are invited short reviews that focus on a specific area. They are ~4 pages long (~20 typed pages), and include a brief biography. Authors must submit a proposal to the Deputy Editor of the corresponding journal section for consideration. A TOC graphic is required for use in the Web edition of the journal.

Perspectives present an experienced researcher's take/opinion on emerging trends in a particular field. The manuscript should discuss the importance of certain topics, methodologies, and/or techniques with highlights on new ideas. Perspectives can have an experimental, computational, or theoretical focus, and should emphasize new physical insights, tools, or methods.

Perspectives should be written with *JPC*'s broad audience of physical chemists in mind, presenting the topic in a way that is accessible even to those who are not experts in the particular field. The Perspective should be approximately 4-6 journal pages long (~20-30 typed, double-spaced pages) and should include a brief abstract (150 words maximum), approximately 50 references, and a TOC graphic. References should draw from research that has been performed over the last two years. A brief biography for each author of the Perspective Article must be included. Photograph(s) may also be included with the biography.

Perspectives are primarily by invitation only. Interested authors should contact the Deputy Editor of the appropriate journal part (A, B, or C) if they are interested in submitting a Perspective.

Viewpoints are typically 1–2 journal page editorial content written by experts in the field who can provide insight and commentary on topics of broad interest for the community. Topics range from opinions about experimental or theoretical methods, assessment of policy issues or educational topics, and information about past meetings. Interested authors should contact the Editor-in-Chief or one of the Deputy Editors.

Comments are significant remarks on work previously published in *JPC A/B/C* and are restricted

to approximately one page (1000 words or equivalent) including tables, figures, and text. There is no abstract. Comments are subject to critical review. If Comments are concerned with the work of other authors, the Editors will generally permit those authors to reply if approved by the Reviewers. It is essential that the discussion focus on scientific issues in both the Comment and the Reply. Comments on papers more than five years old, or to papers in other journals, are not allowed.

Special Issues are published throughout the year. These issues may be a Memorial, Festschrift, or collection of papers from a Meeting or Symposium. *JPC A/B/C* also publishes Special Sections, which are placed at the front of an issue (followed by regular journal content). Suggestions for Special Issue or Special Section topics may be directed to the Deputy Editors of the corresponding journal section. As a general guideline, full Special Issues contain at least 40 Articles, and Special Sections have approximately 20 Articles. **Virtual Special Issues** are special issues in which the manuscripts are published soon after they are accepted, and the collection exists as a webpage rather than a single issue of the journal. For Virtual Special Issues, the front matter and editorial material will be published as part of a regular issue and will serve as an announcement of the availability of the Virtual Special Issue. We are currently transitioning Special Issues to be Virtual Special Issues, with all *JPC A* Special Issues now being virtual.

Virtual Issues are online collections selected by Editors to highlight previously published research on areas of current scientific interest. The collections not only span the different parts of *JPC* but also include content from other ACS journals. They are designed as an informative tool for experienced investigators and students about diverse areas of the chemical sciences. A full Virtual Issue typically contains 25 articles, with related cover art and an editorial by the Editors.

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.
- 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.

Please use official letterhead of the author’s affiliation that lists the telephone number, fax number, and e-mail address. The cover letter must include all of the following points:

- Manuscript title.
- For all authors, provide name (full name preferred), address, telephone number, and current institution e-mail address. All authors must have accounts in ACS Paragon Plus. The corresponding author is preferably a senior author (Professor, Research Associate, or similar), rather than a student.
- Manuscript type (Article, Featured Article, Review, Comment, Special Issue, or Addition/Correction).
- Journal Part and Section that is most appropriate for your manuscript based on scope. [Please note that the final decision on Journal Part and Section remains with the Editors.]
- **Explanation of the manuscript’s significance, including its originality, new physical**

insights or method development, appropriateness for *JPC*, and contribution to new knowledge in the field.

- **List five recommended reviewers for the manuscript, and provide a short description of their relevant expertise.** Include the institution, telephone number, and professional e-mail addresses (if possible avoid using gmail addresses) for each suggested Reviewer. Do not suggest *JPC* Editors as reviewers. The Editors may also use reviewers of their own choosing.
- Note if there are back-to-back or other multipart manuscripts being submitted. However, the submission of more than two coupled manuscripts is greatly discouraged.
- Notification if the manuscript contains a dedication statement.
- Notification if the manuscript has been uploaded to an electronic archive, with details.

When submitting manuscripts in ACS Paragon Plus, authors should do the following, some of which duplicates the information in the Cover Letter:

- Ensure that the Journal Part and Section match. [Please note that the final decision on Journal Part and Section is up to the Editor handling the manuscript.]
- List all authors and correct title (e.g., undergraduate student, graduate student, Post Doc, Research Associate, Professor) in ACS Paragon Plus with correct e-mail address.
- List all authors on the manuscript correctly with current and accurate e-mail addresses for each. It is essential to provide correct e-mail addresses for coauthors because ACS Paragon Plus will notify these authors via e-mail that the manuscript has been submitted. Entering inaccurate e- mail addresses will delay the review process if coauthors cannot be contacted. Use of fictitious e-mail addresses will be considered an ethical violation.
- Ensure that all coauthors are aware of the submission. [See Ethical Guidelines for details.]
- If the manuscript is written in Microsoft Word, turn off the “Line Numbers and Track Changes” feature (after accepting or rejecting all changes) before uploading into ACS Paragon Plus.
- Accurately answer custom questions about prior submission history.

Include a Table of Contents Graphics image. TOCs should not contain offensive material, and copyright permission may be required if material has been published elsewhere.

Manuscript Text Components

The various sections of the manuscript should be assembled in the following sequence:

- Manuscript Title (in Title Case), Authorship, and Affiliations (single page)
- Abstract (single page, labeled)
- Introduction
- Experimental and/or Theoretical Methods
- Results and Discussion
- Conclusions
- Supporting Information Description
- Acknowledgment
- References (Manuscript titles should be provided and they should be in Title Case or sentence case. Mixed cases are not acceptable.)
- Table of Contents Image (at the end of the manuscript) and labeled accordingly.
- Author Biographies (for Featured Articles & Reviews only)
- Supporting Information: submitted as separate files and not repeated in the manuscript (proposed cover art images should be submitted as Supporting Information for Review Only)

Please note that graphics of each type (figures, tables, schemes, charts) should be presented in numerical order. In addition, graphics of each type (figures, tables, schemes, charts) should be mentioned in the manuscript text in numerical order.

Title

The title should be specific and informative and be in Title Case. Using keywords in the title assists in effective literature retrieval. The title, authorship, and institutional affiliations should be included on a single page. Avoid using common phrases such as “investigation”, “study”, “demonstration”, or “performance evaluation”, uncommon acronyms, and words such as “First”, “Novel”, “Facile”, and “One Pot” in the title and abstract.

Authorship

Be consistent in authorship designation on the manuscript and on all correspondence. First name, middle initial, and last name are preferred for correct identification, but omit titles. Give the complete mailing address of the institution where the work was conducted and identify the affiliation of each author. If the current address of an author is different, include it in a footnote on the title page. The corresponding author to whom inquiries about the paper should be addressed must be marked with an asterisk; provide the telephone number and e-mail address of this correspondent. All authors are notified by e-mail when the manuscript is assigned to an Editor.

Abstract

The abstract should be a clear, concise, one paragraph summary (100200 words). It should be informative rather than descriptive, giving scope, purpose, experimental approach, significant results, and major conclusions. Do not cite references or refer to tables, figures, or other sections of the paper in the abstract. Do not use graphics, equations, or tables in the Abstract because this material will not display in secondary sources (e.g., *Chemical Abstracts*). Abbreviations and acronyms should be defined upon first usage. Authors’ abstracts are used directly for *Chemical Abstracts.*

Introduction

Discuss relationships of the study to previously published work but do not reiterate or attempt to provide a complete literature survey. The purpose or reason for the research being reported and its significance, originality, or contribution to new knowledge in the field should be clearly and concisely stated. Do not include or summarize current findings in this section.

Experimental and/or Theoretical Methods

General Information. Complicated chemical equations, schemes, and structures should be supplied as artwork, ready for publication. Schemes and charts should be numbered consecutively with Arabic numbers. Capital, lowercase, and Greek letters should be easily discernible or identified if ambiguity might result. Complicated superscripts and subscripts should be avoided. Tables, Figures, and Figure Captions should be embedded within the Experimental/Theoretical Methods section.

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.

Results/Discussion

Results and Discussion may be presented in separate sections or combined into a single section, whichever format conveys the results in the most lucid fashion. The author should discuss the significance of observations, measurements, or computations and should also point out how these contribute to the scientific objectives indicated in the Introduction. Tables, Figures, and Figure Captions should be embedded within the text.

Conclusions

A brief summary should be given for the principal conclusions of the work.

Appendices

The inclusion of appendices is generally discouraged and should only be used when a specific equation or result needs to be derived and when there is a compelling reason for not including that information in the Supporting Information.

Acknowledgment/Dedication

Acknowledgments of financial assistance for the conduct of research, citations of theses, or indications of presentation at a research meeting should be brief and placed in this section. Acknowledgments to specific individuals who contributed to the science are allowed. Dedications are not recommended and must reference scientific contributions. Statements deemed inappropriately personal will be removed by the Journal office staff.

Author Biographies

Featured Articles and Reviews (and Mini-Reviews) include a brief biography for each author of the paper. Biographies should contain approximately four to five sentences describing the author's education, previous and current positions, and scientific interests. Photograph(s) are optional but welcome. Photos of authors posed individually are acceptable; however, if more than five authors wish to include photographs, a group picture is required. Biographies (and photographs) are to be submitted as part of the manuscript.

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: ^{1}H 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

Reproducibility of Results

It is essential that papers provide enough information so that calculations and experiments can be reproduced by others. We encourage authors to use Supporting Information for this purpose, which is publicly available free of charge on the internet upon publication, regardless of whether or not the accompanying article is made open access.

Guidelines for Computational Results

Below are the general guidelines from *Pure Appl. Chem.* 1998, *70*, No. 10, 2047–2049 (http://dx.doi.org/10.1351/pac199870102047) for manuscripts reporting the results of electronic structure calculations, force field parameters, and other potential energy surface information. Further details are listed in the guidelines authored by J. E. Boggs (*Pure Appl. Chem.* 1998, *70*, No. 4, 1015–1018 (http://dx.doi.org/10.1351/pac199870041015). Both sets of guidelines can be viewed online at http://iupac.org/publications/pac/reports/year/1998/. While these papers refer to electronic structure and molecular dynamics calculations, the concepts stated below apply to all calculations.

- If a paper mentions any calculations that are integral to the study (i.e., the precise quantitative results are central to the conclusions drawn) computational details must be described.
- Reproducibility of computations should be a defining goal in reporting computational results. Sufficient technical details should be provided to allow a reader to reproduce the results of any calculations. Of course, strict reproducibility of computations may be precluded by differences among computers (e.g., differences in operating systems, host-based algorithms, machine precision, etc.), software (e.g., installation procedures and programming modifications), and applications (e.g., for probabilistic methods such as Monte Carlo calculations).

- A description of the results of any published calculation must be available for scientific scrutiny by other investigators. Ordinarily this will best be achieved if the authors place full details of the calculation (e.g., structures, energies, frequencies, dynamical quantities, etc.) in a repository (such as Supporting Information to the paper) that is accessible via the Internet. Otherwise, it is the responsibility of the investigator to make such information available upon request. Depending on the specific circumstances, the appropriate data to be deposited might be final output structure(s) or the input structure(s) that would allow another investigator to replicate the computational experiment.
- Electronically deposited structures should be written in a format that is machine readable by readily available modelling or translating programs.
- An adequate specification of the computer program used to carry out the calculations is essential. If the calculations were carried out with commercially available software, the investigator must list the source, version number, and force field employed. Any program modifications and any differences from the published version (including changes in parameters) must be fully described or available to other investigators upon request. Changes in parameters, program options (e.g., dielectric constant, nonbonded cutoffs, etc.) affecting reproducibility of the calculation, and program constraints must be fully described in the article. If the program is not available, commercially or otherwise, the authors must specify sufficient detail that the calculation could be reproduced.
- The issue of convergence must be adequately addressed. An iterative calculation is considered to have converged when further iterations will not significantly alter the results. Convergence criteria should be reported (e.g., energy change per iteration or energy gradient for geometry optimization of a single structure).

Guidelines for Experiments

Authors are expected to provide sufficient detail to enable a trained professional to reproduce routine measurements and synthetic procedures. Authors are required to provide crystallographic or surface structure data as Supporting Information in crystallographic information file (CIF) format. For quantitative optical measurements, the specifics and usable range of the photodetector should be reported.

Teams of ACS editors have identified best practices in certain fields to guide authors in the reporting of experimental results. Please refer to them, as needed:

- Best Practices for the Reporting of Colloidal Inorganic Nanomaterials (http://pubs.acs.org/doi/abs/10.1021/acs.chemmater.5b02323)
- Best Practices for Reporting on Heterogeneous Photocatalysis (http://pubs.acs.org/doi/abs/10.1021/am504389z)
- Best Practices in Perovskite Solar Cell Efficiency Measurements. Avoiding the Error of *Making Bad Cells Look Good* (http://pubs.acs.org/doi/abs/10.1021/acs.jpclett.5b00289)
- Best Practices for Reporting on Energy Storage (http://pubs.acs.org/doi/abs/10.1021/acsami.5b06029)
- Best Practice in Photocatalysis: Comparing Rates of Apparent Quantum Yields? (http://pubs.acs.org/doi/abs/10.1021/acs.jpclett.5b00521)

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 Artwork Editing and Graphical Abstract services generate publication-ready figures and Table of Contents (TOC) graphics that conform to your chosen journal's specifications. For figures, this includes changes to file type, resolution, color space, font, scale, line weights, and layout (to improve readability and professional appearance). For TOC graphics, our illustrators can work with a rough sketch or concept or help extract the key findings of your manuscript directly for use as a visual summary of your paper.

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 Physical Chemistry 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. 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. The use of a preprint service will not bias reviewing/acceptance of the paper in *JPC*. Upon publication, authors are advised to add a link from the preprint to the published paper via the Digital Object Identifier (DOI). Redundant publication, such as the use of a repository for *published* versions of papers, is subject to the Journal Publication Agreement and generally requires copyright permission.

Editorial Policies

Editorial Peer Review Process

The Editors may exercise their prerogative to reject a manuscript without peer review if that paper is judged to be outside the scope of the Journal, poorly written or formatted, fragmentary and marginally incremental, lacking in significance, or containing no obvious new physical insight.

All submitted manuscripts are reviewed and handled by the Editor-in-Chief, Deputy Editors, and/or Senior Editors. The Senior Editor and his or her Editorial Assistant are then responsible for the assigned manuscripts, including acknowledging receipt, evaluating the content of the paper, selecting reviewers, monitoring the progress of the review process, evaluating the comments of reviewers and forwarding them to the authors for their response, communicating ultimate acceptance or rejection to the corresponding author, carrying out a final check of accepted manuscripts for appropriate format and style, and forwarding accepted manuscripts to the publications office.

The Editors seek the scientific advice of reviewers who are active in the research area covered by the manuscript. The reviewers act only in an advisory capacity, and the final decision concerning a manuscript is the responsibility of the Editors. The reviewers are asked to comment on the following: (1) significance and originality of the work, (2) broad appeal to physical chemists, (3) how well the conclusions are supported by the data, (4) clarity of the paper, and (5) the extent to which the paper provides new physical insights. All reviews are anonymous, and the reviewing process is most effective if reviewers do not reveal their identities to the authors. An exception arises in connection with a manuscript submitted for publication in the form of a Comment on the work of another author. Under such circumstances, the author whose work is being commented on will, in general, be allowed to review the communication and to write a Reply if deemed necessary. The Reply and the original communication will be “refereed” and, if accepted, will be published together in the same issue.

A manuscript sent back to an author for revision should be returned to the Editor without delay. Manuscripts that are not returned by the date given in the Editor's decision letter will expire. When a manuscript expires, it will no longer be available on the author’s Paragon Plus homepage. When this occurs, the revised manuscript must be resubmitted as a new submission. The cover letter should indicate the previous manuscript number and offer a response to the comments of the reviewers. The manuscript will be processed as a revision with a new manuscript number and date of submission.

Revised manuscripts are generally sent back to the original reviewers, who are asked to comment on the revisions. If only minor revisions are involved, the Editor may examine the revised manuscript in light of the recommendations of the reviewers without seeking further opinions. The author should provide a cover letter with the revised manuscript containing responses to all of the reviewers’ comments and detailing, in a point-by-point manner, the revisions to the manuscript. The dates of receipt of the original and the revised manuscripts will both appear in publication. If using highlighting, bolding, italics, or markings of any kind to indicate changes made in response to the reviews of your manuscript, we ask that you upload the marked-up copy as “Supporting Information for Review Only” and provide an unmarked version as the official revised manuscript submission.

Providing Potential Reviewer Names

Please suggest five 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.

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.

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.

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.

To expedite 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.

Criteria for authorship can be found in Part B of the Ethical Guidelines to Publication of Chemical Research. Artificial intelligence (AI) tools do not qualify for authorship. The use of AI tools for text or image generation should be disclosed in the manuscript within the Acknowledgment section with a description of when and how the tools were used. For more substantial use cases or descriptions of AI tool use, authors should provide full details within the Methods or other appropriate section of the manuscript.

If any change in authorship is necessary after a manuscript has been submitted, confirmation is required that all of the authors (including those being added or removed) have been notified and have agreed to the change. To provide this confirmation, authors are asked to complete and sign an authorship change form and provide the completed form to the appropriate editorial office.

Authors with a single name: If you, or any of your coauthors, have only one name, please follow these steps for proper submission to ACS Paragon Plus:

1. First (Given) Name Field: Enter an asterisk (*) into the "First (Given) Name" field.
2. Last (Family) Name Field: Enter your single name into the "Last (Family) Name" field.

If your paper is accepted, the asterisk (*) will be removed from the published version of the paper.

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 completing the Journal Publishing Agreement or 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.

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.

- **Citation Diversity Statement:**The citation diversity statement should appear in the Acknowledgements section of the manuscript. ACS recommends including the following: (1) the importance of citation diversity, (2) the proportion of citations by gender and race/ethnicity for the first and last authors, (3) the method used to determine those proportions and its limitations, and (4) steps taken to by the authors to improve citation diversity in the article. We recognize that one limitation of the current methods is that it cannot account for intersex, non-binary, and transgender people, or Indigenous and mixed-race authors. (Adapted from BMES/Springer Guidelines)
- **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

Consult the Guidelines for Table of Contents/Abstract Graphics for specifications.
Our team of subject-matter experts and graphical designers can also help generate a compelling TOC graphic to convey your key findings. Learn more about our Graphical Abstract service.

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

The Journal of Physical Chemistry A/B/C 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. Images chosen for the front cover will be published at no cost to the author. 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.

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. Photos of people or nonscientific images such as cartoon characters and clip art are not acceptable. Cover art images may be submitted with any type of manuscript, although publication preference for front cover art will be given to Featured Articles, Reviews, and Perspectives.

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 8.19 in. x 9.74 in. (or 20.80 cm x 24.74 cm). Please note that the journal title will cover the top 2.5 in. (6.35 cm) of the image. Authors should submit the cover image, along with a short, clear legend 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.