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Manuscript Submission Requirements Checklist

- **Submit with Fast Format**: ACS journals have simplified formatting requirements with a streamlined and standardized review-ready format for an *initial* manuscript submission. Include article titles in references.
- Cover Letter: must include a paragraph explaining why your manuscript is appropriate for ACS Physical Chemistry Au, clearly indicating what key advance(s) are described in the work relative to the state-of-the-art, and a statement confirming the manuscript has not been previously published by any of the authors and/or is not under consideration for publication in another journal at the time of submission.
- **Suggested Reviewers**: Submit names and email addresses of at least six scientists from at least three different countries who could evaluate the work. These suggested reviewers must not be former mentors or mentees nor collaborators or co-authors from the past five years.
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- References: Include article titles in references.
- **Safety**: Authors must emphasize any unexpected, new, and/or significant hazards associated with the work.
- Table of Contents graphic:

- required, dimensions of 3.25 inches by 1.75 inches (approx. 8.25 cm by 4.45 cm)
- Cover Art (optional): Authors may submit images to be considered for the cover (TIF, JPG, PNG or EPS files with a resolution of at least 300 dpi for pixel-based images). The image size is 8.19 inches (20.8 cm) wide × 10 inches (25.4 cm) high at 300 ppi.
- Supporting Information (if any): must be included at the time of electronic submission. Include the heading "Supporting Information" followed by the manuscript title, author list, and affiliations. Tables, Schemes, and Figures should be written as Table S1, Figure S1, Scheme S1, etc. All pages of the PDF Supporting Information should be numbered consecutively. Copies of all related works that are "in press", "accepted", or "submitted" for publication or in the late stages of preparation must be uploaded as Supporting Information for Review Only at the time of submission. References that are only available online should be cited by the Digital Object Identifier (DOI).
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<u>ACS Physical Chemistry Au</u> is an open access journal, which publishes original, fundamental and applied research on all aspects of physical chemistry. The journal publishes new and original experimental, computational and theoretical research of interest to physical chemists, biophysical chemists, chemical physicists, physicists, material scientists, and engineers. An essential criterion for acceptance is that the manuscript provides new physical insight or develops new tools and methods of general interest. Some major topical areas include:

Molecules, Clusters and Aerosols; Biophysics, Biomaterials, Liquids and Soft Matter; Energy, Materials and Catalysis

Manuscript Types

Articles should report a significant advance in a subfield of chemistry, being characterized by the editor and referees as an advance representing the top 10% of articles published annually in that field. Articles must be of high scientific quality, originality, significance, and conceptual novelty. Articles that mainly expand findings that were previously published as Letters in *ACS Physical Chemistry Au* or elsewhere and that only incorporate experimental data, without greatly expanded scope and without providing new insights or conceptual breakthroughs, will be declined or recommended for Manuscript Transfer to specialized journals. Similarly, articles that are mainly routine extensions of previously published related work will be declined or recommended for Manuscript Transfer to specialized journals.

Use of the template for Articles is strongly encouraged but is not required. If an author chooses not to use a template to prepare an Article, only Times and Symbol fonts and 1.5 or double line spacing should be used. Other fonts may cause problems when the PDF files used for review are created. Also, if the template is not used, the document mode or its equivalent in the word-processing program should be used; i.e., files should not be saved in "Text Only" (ASCII) mode. If a non-Western version of word- processing software is used to prepare the manuscript, the file should be saved in rich-text format (RTF).

Articles should cover their subjects with thoroughness, clarity, and completeness but should be as

concise as possible. Abstracts to Articles are typically limited to 300 words and should summarize the significant results and conclusions.

Letters are short publications that report results whose immediate availability to the science and engineering community is deemed important. A Letter must convey the scientific findings concisely in a brief abstract, main text, and graphical elements as determined by word count not exceeding 2,200 words, including titles/footnotes/captions of approximately five graphics (typically 2 inches long in a single column). References are not included in word count to allow article titles to be included at submission. To calculate word count within the word processing application, select all text from abstract through end of main text (excluding title, authors, affiliations, and content after main text) and view the word processor's word count data. Letters exceeding the word count limit must be shortened before acceptance. Note: *ACS Physical Chemistry Au* encourages submission of Letters ranging from approximately 1,200-2,200 words (equivalent to 2-4 formatted journal pages), with more concise submissions appropriate for the most urgent new findings of exceptional significance.

All graphics and tables must be placed near the point of first mention in the text of the manuscript (not grouped at the end of the document) and must be sized according to current guidance. Long notes are not permitted in the References section; information not directly germane to the Letter can be included as Supporting Information. Letters can be complete publications, but follow-up publication may be justified when the research is continued and a more complete account of the work is deemed necessary, especially for the most urgent concise Letters noted above. Special efforts will be made to expedite the reviewing and the publication of Letters. The time for proofreading the galley proofs is relatively short. For this reason, authors of Letters should ensure that manuscripts are in final, error-free form when submitted. A template for Letters is available.

Reviews are topical, forward looking, and of general interest to the readership. Length is flexible (6–20 or more pages). A good review critically evaluates existing work of multiple groups in a field or across disciplines, provides a logical organization, and makes the material more easily available to those not expert in the area through clear text and figures. Reviews should lay out the challenges and opportunities that lie ahead. Reviews should contain an abstract and appropriate references. The use of graphics to illustrate key concepts is strongly encouraged. Reviews include a graphical Table of Contents entry. Reviews also include ~8–10 keywords and a vocabulary section in which 5–7 terms extracted from the text are defined in one or two sentences.

Perspectives are personal reviews of a field or area by one or a small team of authors, and they are focused rather than comprehensive. Perspective authors are asked to assess the current status of the field with an emphasis toward identifying key advances being made or those advances that are needed, and with an eye to the future. An *ACS Physical Chemistry Au* Perspective should touch base with the current literature, including key contributors and references, but will primarily serve to inspire and help direct future research efforts. Authors may be invited by the Editor to submit Perspectives. Perspectives may not exceed 10,000 words in abstract, main text, and graphical elements.

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- 1. Proposed Review or Perspective title
- 2. Corresponding author names, affiliations, and websites
- 3. A short (~400 word) description of the focused topic
- 4. A list of 5-10 lead references that will form the foundation of the manuscript
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others, and an explanation of how the proposed review will differ in focus and advance the literature on the subject.

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- 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
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The cover letter must include a paragraph explaining why your manuscript is appropriate for *ACS Physical Chemistry Au*. This paragraph should clearly indicate what key advance(s) is/are described in the work. The letter may suggest the name of an appropriate *ACS Physical Chemistry Au* Associate Editor. However, manuscript assignment to an Associate Editor is ultimately at the discretion of the Editor-in-Chief. Non-preferred Associate Editors and reviewers may be denoted in the cover letter, along with a reason for their designation.

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Abstract. All Articles, Letters, and Perspectives) must be accompanied by an abstract, including an Abstract (TOC) graphic, which should state briefly the purpose of the research, the principal results, and major conclusions. Abstracts of manuscripts may not contain the words "superb", "excellent", "exceptional", "outstanding", or other similar descriptive words unless rigorously supported by a thorough comparison with the state-of-the-art in the manuscript. Like manuscript titles, the words "New", "First", or "Novel" are also generally disallowed in the abstract. The abstract should not generally exceed 200/300 (Letter/Article) words. Pasting the abstract in the text box on the Web submission page does not replace the need for including an abstract in the manuscript document.

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Text (Articles). The first paragraphs of an Article should explain the motivation for and import of the work, where it fits in the development of the field and of chemistry, and perhaps why it should be of interest to chemists in other areas. It should be possible to do this without excessively increasing the length of the Article. Extensive reviews of the literature cannot be accepted. Thoughtful use of schemes and figures (with well-composed captions) is recommended, so that even casual browsers can discern the nature of the work. Well-known procedures should be

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Text (Letters). Section headings (Introduction, Experimental Section, Conclusion, etc.) should not be used in a Letter.

Safety. Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. For each manuscript that reports experimental procedures, authors must include an affirmative statement about safety in the Experimental Section of the full article or the main text of a Letter. Further information may be included or re-introduced in the Supporting Information.

Appendices. Appendix sections must be placed in the Supporting Information.

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Abbreviations. Acronyms and abbreviations that are not broadly familiar to readers in all disciplines of chemistry should be introduced in parentheses following the full term on its first appearance in the text. Do not include a separate Abbreviations list.

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Unnecessarily long lists of references should be avoided, and excessive self-citation is not permitted. However, authors must reference all previous publications in which portions of the present work have appeared. Each literature reference should be assigned one number and placed in the text as a superscript Arabic numeral. Footnotes to the text should be combined with references and numbered in ordinal sequence. Long footnotes should be avoided in Articles and are not permitted in Communications; additional data and peripheral discussion should be placed

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Example of a journal reference:

Yue, Q.; Liu, W.; Zhu, X. n-Type Molecular Photovoltaic Materials: Design Strategies and Device Applications. *J. Am. Chem. Soc.* **2020**, 142, 11613–11628.

Example of an in-press journal reference:

Ham, J. S.; Park, B.; Son, M.; Roque, J. B.; Jurczyk, J.; Yeung, C. S.; Baik, M.-H.; Sarpong, R. C–H/C–C Functionalization Approach to N-Fused Heterocycles from Saturated Azacycles. *J. Am. Chem. Soc.* **2020**, DOI: 10.1021/jacs.0c04278.

Example of a reference to a book with no editors:

Desiraju, G. R.; Vittal, J. J.; Ramanan, A. *Crystal Engineering: A Textbook*. World Scientific Publishing Co Pte Ltd: Singapore, 2011.

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ACS Physical Chemistry Au applies ACS Research Data Policy **Level 1**, meaning the journal encourages all authors to publicly share all the data underlying the results reported in the paper, preferably via archiving in an appropriate public repository. Authors are also encouraged to provide a <u>Data Availability Statement</u> describing the public availability of the data supporting the article's conclusions. Publicly available data sets should be <u>cited appropriately</u>.

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Data Requirements

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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.

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 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.
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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.

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

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Appendix 1: PREPARING FOR SUBMISSION

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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 <u>Table of Contents/Abstract Graphics</u> for specifications.

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Figures

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

Charts

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

Tables

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

Schemes

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

Chemical Structures

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

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