

Information for Authors of Papers

(Revised September 2010)

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Manuscripts must be submitted via the ACS Paragon Plus Environment (<http://paragonplus.acs.org/login>). Complete instructions and an overview of the electronic online (Web) submission process are available through the secure ACS Paragon Plus Web site. Authors must also submit all revisions of manuscripts via the ACS Paragon Plus Environment. The web submission site employs state-of-the-art security mechanisms to ensure that all electronically submitted papers are secure. These same security mechanisms are also utilized throughout the peer-review process, permitting access only to editors and reviewers who are assigned to a particular paper.

Authors whose manuscripts are published in the Journal will be expected to review manuscripts submitted by other researchers from time to time.

All manuscripts must be accompanied by a **cover letter** that contains **clear and precise** information about the submission. 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 and Authors
- Corresponding Author's name (surname in all capital letters), address, telephone number, fax number, and e-mail address
- manuscript type (Article, Feature Article, Review Article, Comment, special issue (if applicable), or Addition/Correction)
- designation of the Journal's subject category that best fits the manuscript (see list under Journal Scope in these instructions) [Note that the Editors reserve the right to reassign

manuscripts to different Journal sections. The Journal's subject category designated in the cover letter must match the entry given in Paragon Plus.]

- explanation of the manuscript's significance, including its originality and its contribution to new knowledge in the field
- notice if manuscript contains a dedication statement
- list of graphics to be published in color
- list of at least three recommended Reviewers for the manuscript; include the address, telephone number, fax number, and e-mail addresses for each suggested Reviewer
- submission history, if previously submitted to another ACS journal, and response to any reviews obtained [This helps to speed up the review process.]

When submitting manuscripts in Paragon Plus, Authors should do the following:

- list all authors on the manuscript correctly with current and accurate e-mail addresses for each. It is important to provide correct e-mail addresses for coauthors, because Paragon Plus will notify these authors that the manuscript has been submitted. Entering inaccurate or fictitious e-mail addresses is inadvisable, because it may delay the review process for the manuscript.
- provide copies of unpublished work [Not citing prior work in press by the same Authors can constitute an ethical violation.]
- make sure that coauthors are aware of the submission [See Ethics section for details.]
- if the manuscript is written in Microsoft Word, turn off the "Track Changes" feature before uploading into Paragon Plus
- check that the manuscript type and Journal's subject category match with what was given in the cover letter
- answer custom question about prior submission history
- make sure that the references are formatted correctly
- include Table of Contents Graphics image

Submission of hardcopy manuscripts is no longer allowed.

JOURNAL SCOPE

The Journal of Physical Chemistry A/B/C is devoted to reporting new and original experimental and theoretical basic research of interest to physical chemists, biophysical chemists, and chemical physicists. Manuscripts that are essentially reporting data, applications of data, or reviews of the literature are, in general, not suitable for publication in *JPC A/B/C*. An important criterion for acceptance is that the paper provides **new physical insight**.

The Journal of Physical Chemistry A/B/C is divided into the following sections:

JPC A (Dynamics, Kinetics, Environmental Chemistry, Spectroscopy, Structure, Theory)

- A1 Dynamics, Clusters, Excited States
- A2 Kinetics, Spectroscopy
- A3 Atmospheric, Environmental and Green Chemistry
- A4 Molecular Structure, Quantum Chemistry, General Theory

JPC B (Soft Condensed Matter and Biophysical Chemistry)

- B1 Macromolecules, Soft Matter
- B2 Surfactants, Membranes
- B3 Statistical Mechanics, Thermodynamics, Medium Effects
- B4 Biophysical Chemistry

JPC C (Nanomaterials, Interfaces, Hard Matter)

- C1 Nanoparticles and Nanostructures
- C2 Surfaces, Interfaces, Catalysis
- C3 Electron Transport, Optical and Electronic Devices, Hard Matter
- C4 Energy Conversion and Storage

MANUSCRIPT TYPES

Please note that all Letters should be submitted to
The Journal of Physical Chemistry Letters.

Articles should report original research that is expected to have a definable impact on the advancement of science and technology. Manuscripts should cover their subjects 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.

Feature Articles are usually published by invitation; however, Authors in important active research fields of interest to physical chemists are encouraged to propose such articles.

Two-page proposals should be sent to the Managing Editor (d_minton@acs.org) for consideration. 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. Feature Articles are limited to ~8 printed pages (equivalent to ~40 pages of manuscript with figures, tables, references, and double-space-typed text). A brief biography for each Author of the Feature Article should be included. A TOC graphic is required for use in the Web edition of the journal.

Review Articles are on active and rapidly changing fields. They are ~8 pages long (~40 typed pages). Authors are encouraged to submit two-page proposals to the Managing Editor (d_minton@acs.org) for consideration. A brief biography for each Author of the Review Article should be included. A TOC graphic is required for use in the Web edition of the journal.

Comments are significant remarks on work previously published (usually 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 the Comments are concerned with the work of other Authors, the Editors will generally permit these Authors to reply if approved by the Reviewers.

Additions and Corrections are Authors' corrections to published manuscripts and are limited to the length required to correct the errors.

Special Issues are published throughout the year. These issues can be a Memorial, a Festschrift, or a collection of papers from a Symposium. *JPC A/B/C* also publishes mini-issues, which are placed at the front of an issue (followed by regular journal content). Suggestions for special issue or mini-issue topics may be directed to the Managing Editor (d_minton@acs.org). As a general guideline, full special issues contain at least 25 Articles and mini-issues have 12–16 Articles.

ETHICS

Multiple Reporting of Research. It is improper for an Author to submit manuscripts describing essentially the same research to more than one journal.

Plagiarism. The Editors of *JPC A/B/C* will not tolerate plagiarism. This includes the verbatim copying of previously published work from other Authors and by the same Author. Please contact the Editors if there are questions about avoiding plagiarism.

Coauthorship. The submitting Author must obtain consent of coauthorship from all Coauthors listed prior to submitting the manuscript and include as Coauthors all individuals who made significant scientific contributions to the work. Any disagreement between the Corresponding Author and Coauthor(s) after submission will cause review of the manuscript to cease. Removal or addition of Coauthor(s) after submission of the manuscript requires confirmation in writing by the respective Coauthor(s).

The complete document “Ethical Guidelines to Publication of Chemical Research” is available via <http://pubs.acs.org/ethics>.

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 Journals, poorly written or formatted, fragmentary and marginally incremental, or lacking in significance.

All manuscripts submitted are reviewed and handled by the Editor-in-Chief or assigned to one of the Senior Editors. The Senior Editor and local 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 manuscripts to the publications office.

The Editors request the scientific advice of Reviewers who are active in the area of research 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 not only on the scientific content but also on the manuscript’s suitability for *JPC A/B/C*. 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 rebuttal if deemed necessary. The rebuttal 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 within 3 months will be inactivated by the Editor. When a manuscript is inactivated, it will no longer be available on your Paragon Plus home page. When this occurs, the revised manuscript must be resubmitted as a new submission. The cover letter should indicate the previous JP number as well as respond to the comments of the Reviewers. The manuscript will be processed as a revision with a new JP 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 examines 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 to detail how the Author responded to the Reviewers’ comments. The dates of receipt of the original and the revised manuscripts will both appear in publication.

ASAP PUBLICATION

Accepted manuscripts will be published on the “Articles ASAP” page on the Journal Web site as soon as page proofs are corrected and all author concerns are resolved. Publication on the Web usually occurs within 4 working days of receipt of page proof corrections, and this can be anywhere from 3 to 5 weeks in advance of the cover date of the issue. **Manuscripts assigned to a special issue often remain published ASAP for several months.** Authors should take this schedule into account when planning intellectual and patent activities related to a manuscript. The actual date on which an accepted paper is published on the Web is recorded on the Web version of the manuscript and on the first page of the PDF version.

MANUSCRIPT PREPARATION

Manuscript Format

Manuscripts must be prepared using accepted word-processing software, and all parts must be double-spaced. All pages must be numbered consecutively starting with the title page and including tables and figures. A standard font, in a size of 12 points or greater, must be used. Templates and instructions for software, including Tex/LaTex, are available on the Web.

Standard American English usage is required. Authors who are not familiar with standard American English are urged to seek assistance; deficiencies in grammar may be a serious hindrance during the review process. For more information, Authors may visit the [Language Editing Services](#) listed under the Publishing Tools tab of the Author & Reviewer Resource Center.

The ACS Style Guide (3rd ed., 2006; ISBN 13:9780841239999) is available from <http://pubs.acs.org/page/books/index.html>. The Third Edition is the definitive source for all information needed to write, review, submit, and edit scholarly and scientific manuscripts. Refer to a current issue of the Journals for general style.

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

- Title, Authorship, and Affiliations (single page)
- Author Biographies (Feature Articles & Review Articles)

- Abstract and Keywords (single page)
- Introduction
- Experimental Methods
- Results
- Discussion
- Conclusions
- Acknowledgment/Dedication
- Supporting Information Description
- References
- Tables
- Figure Captions
- Figures
- Table of Contents Image
- (Supporting Information: Separate files, includes proposed cover art image)

Title

The title should be specific and informative. Keywords in the title assist in effective literature retrieval. The title, authorship, and institutional affiliations should be included on a single page.

Authorship

Be consistent in authorship designation on the manuscript and on all correspondence. First name, middle initial, and last name are needed 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, fax number, and e-mail address of this correspondent.

Author Biographies

Feature Articles and Review Articles 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 are 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.

Abstract

The abstract should be a clear, concise, one paragraph summary (100–150 words). It should be informative rather than descriptive, giving scope, purpose, experimental approach, significant results, and major conclusions. Avoid the use of reference citations. Abbreviations and acronyms should be defined upon first usage. Authors' abstracts are used directly for *Chemical Abstracts*. Follow the recommended format when preparing the abstract. Representative abstracts are [shown below in the Appendix](#).

Keywords

Identify four to six keywords to assist in indexing your paper, and list these on a separate line beginning with “Keywords” on the abstract page. Do not use words contained in the title.

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 Methods

General Information. Complicated chemical equations, schemes, and structures should be supplied as furnished artwork, ready for publication. Schemes and charts should be numbered consecutively with Arabic numbers. Mathematical expressions and chemical formulas with unavailable symbols and letters should be clearly identified. Capital, lowercase, and Greek letters should be easily discernible or identified if ambiguity might result. Complicated superscripts and subscripts should be avoided. Fractional exponents should be used instead of root signs.

Authors should consult a current copy of the Journal and [The ACS Style Guide](#) for examples of style and general recommendations. See also: Mills, I.; et al. *Quantities, Units and Symbols in Physical Chemistry*, 2nd ed.; Blackwell Scientific Publications: Oxford, U.K., 1993.

Hazards. Any unusual hazards in the chemicals, equipment, or procedures used in an investigation should be clearly identified.

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 they contribute to the scientific objectives indicated in the Introduction.

Conclusions

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

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.

Dedications are not generally recommended and must reference scientific contributions without being overtly personal. Statements deemed inappropriately personal will be removed by the Journal office staff. If a dedication is included in a manuscript, the Author needs to notify the Journal office in the cover letter. In the case of a Dedication for a Special Issue, the Author should refrain from starting the Dedication with “Dedicated to the honoree on the occasion of ...” or “Dedicated to the memory of (the honoree),” because publishing the issue is itself in honor of the particular individual.

Supporting Information Paragraph

A paragraph must be included that indicates the nature of any material provided as Supporting Information and the means by which the interested Reader may obtain it. This is required even if the Supporting Information is described in the text of the manuscript. The following format should be used:

Supporting Information Available: Full description of the material. This material is available free of charge via the Internet at <http://pubs.acs.org>.

References

References to the literature should be numbered in one consecutive series by order of appearance in the text, with the text citations presented as unparenthesized superscript Arabic numbers. Authors should consult [The ACS Style Guide](#) for the appropriate style to use in citations of journal papers, books, and other publications. References will be linked to various electronic sources (e.g., the corresponding abstract from Chemical Abstracts Service, full text from other American Chemical Society Journals, etc.); therefore, the accuracy of references is critical. Authors are responsible for the accuracy of the references.

Unnecessarily long lists of references, including excessive self-citation, are to be avoided; however, authors must provide references to all relevant publications in which portions of the present work have appeared. [Citation of recent papers published in physical chemistry and chemical physics journals that highlight the significance of work to the general readership is encouraged.](#)

Journal references should contain author names, abbreviated journal title, year, volume, and pages (first–last). An example is provided below.

Habenicht, B. F.; Prezhdo, O. V. *J. Phys. Chem. C* **2009**, *113*, 14067–14070.

Book references should contain author names, book title (written in title case), publisher, city, and year. An example is provided below.

Datta, S. *Electronic Transport in Mesoscopic Systems*: Cambridge University Press: Cambridge, 1995.

In literature references, journal abbreviations should be those used by Chemical Abstracts Service [see *Chemical Abstracts Service Source Index (CASSI) 1907–2004*]. For references to *JPC A/B/C*, part A, B, or C must be specified for papers published in 1997 forward.

Additional data and peripheral discussion should be placed in the Supporting Information (SI) rather than in references. Supplementary references may be placed in SI. Submitted papers should not depend on unpublished material, and excessive reference to material in press or reports not readily found in research libraries is discouraged. If pertinent references are in press or unpublished for any reason, upload copies of the references as Supporting Information for Review Only to enable Reviewers to evaluate the manuscript. Papers accepted for publication are cited as “in press”; the DOI should be given if the paper is published online.

Tables

Tables should be numbered consecutively with Arabic numbers. Each table must have a brief title that describes its 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 as narrative, when many numbers must be presented, or when more meaningful interrelationships 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.

Column headings should be lowercase, except for symbols and proper names. Define nonstandard abbreviations in footnotes. Footnotes in tables should be given letter designations and be cited in the table by italic superscript letters. The sequence of letters should proceed by line rather than by column. If a reference is cited both in the text and in a table, a lettered footnote that refers to the numbered reference in the text should be inserted in the table.

In setting up tables, Authors should keep in mind the area of the Journal's page (17.8 cm × 25.0 cm) and the column width (8.5 cm) and should make tables conform to the limitations of these dimensions.

Figure Captions

A caption giving the figure number and a brief description, preferably only one or two sentences, must be included for each figure.

Figures

All figures must be mentioned in the text in consecutive order and must be numbered with Arabic numbers. If symbols are used, it is preferable to place a key in the artwork itself, not in the caption. Ensure that any symbols and abbreviations used in the text agree with those in the figures. Remove all color from graphics, except those graphics to be considered for publication in color. See more detailed information on submission of graphics under [Artwork](#) below.

Table of Contents (TOC) Image

A TOC graphic is required for Articles, Feature Articles, and Review Articles. TOC graphics will appear only in the Web edition of the journal. The illustration should capture the Reader's attention and, in conjunction with the manuscript title, should give the Reader a quick visual impression of the essence of the paper without providing specific results. The graphic should be in the form of a structure, graphical image, photograph, reaction scheme, or equation. The Author must submit the graphic in the actual size to be used for the TOC, fitting in an area 1.375 in. high and 3.5 in. wide (3.6 cm × 8.9 cm). Larger images will be reduced to fit within those dimensions. The type size of labels and other symbols within the graphic must be legible. Tables and spectra are not acceptable. Provide the TOC graphic upon submission of the paper as the last page of the manuscript.

ARTWORK

General Considerations

All graphics must be created in digital format. Although tif, jpg, and pdf formats are preferred, a list of all graphic file options may be found on the Web site.

In general, graphics should be copied from the graphics program window and pasted directly into the manuscript. The Author should make sure that the graphic is at the appropriate resolution (see below) before copying and pasting. The graphics should be resized in the graphics program and then pasted into the manuscript. The Author should not resize graphics after they are pasted into Word. This is true regardless of the graphic format (cds, tif, eps, pdf, etc.).

Quality

The quality of the graphics in the Journal depends on the quality of the originals provided by the Author. Figures cannot be modified or enhanced by the Journal production staff. Images produced from continuous-tone graphics such as photographs should have high contrast.

Resolution

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

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 on the Journal page. For efficient use of Journal space, single column graphics are preferred.

	single (preferred)	double
width		
minimum		10.5 cm (4.13 in.)
maximum	8.25 cm (3.25 in.)	17.78 cm (7 in.)
maximum depth	24 cm (9.5 in.)	24 cm (9.5 in.)

For best results, **submit graphics in the actual size at which they should appear in the published version.** Original graphics that do not need to be reduced to fit a single or double column will yield the best quality. Lettering should be no smaller than 4.5 points in the final published format. Helvetica or Arial fonts work well for lettering. Lines should be no thinner than 0.5 point. Lettering and lines should be of uniform density and the lines unbroken. If the submitted artwork must be reduced, larger lettering and thicker lines should be used so that, when reduced, the artwork meets the above mentioned criteria.

Avoid using complex textures and shading to achieve a three-dimensional effect. Parallel or cross-hatched lines should be used to fill enclosed areas with a pattern.

Color

The use of color to enhance the clarity of complex structures, figures, spectra, schemes, etc. is encouraged. Color reproduction of graphics will be provided **at no cost to the Author.** For manuscripts containing color, a surcharge is added to the standard cost of paper reprints. Graphics intended to appear in black and white or grayscale should not be submitted in color.

Chemical Structures

Structures should be produced with the use of a drawing program such as ChemDraw. Authors using the current versions of ChemDraw will find the necessary parameters incorporated into this program ("ACS Document 1996"). Authors using older versions of ChemDraw should use the following settings:

(1) As drawing settings select:

chain angle	120°
bond spacing	18% of width

fixed length	14.4 pt (0.508 cm, 0.2 in.)
bold width	2.0 pt (0.071 cm, 0.0278 in.)
line width	0.6 pt (0.021 cm, 0.0084 in.)
margin width	1.6 pt (0.056 cm, 0.0222 in.)
hash spacing	2.5 pt (0.088 cm, 0.0347 in.)

(2) As text settings select:

font	Arial/Helvetica
size	10 pt

(3) Under the preferences choose:

Units	points
Tolerances	5 pixels

(4) Under page setup choose:

Paper	US Letter
Scale	100%

(5) Use the ChemDraw ruler or appropriate margin settings to create charts, equations, and schemes with maximum widths of 8.25 cm (one-column format) or 17.8 cm (two-column format). If the foregoing drawing-setting lengths and widths are selected in centimeters rather than in points or inches, the ChemDraw ruler will be calibrated in centimeters.

(6) Copy and paste the graphics into the manuscript text file at the appropriate locations. Do not use the “insert” function.

Authors using other drawing packages should set the program parameters to match the above values as closely as possible.

Schemes

Sequences of reactions are called schemes. Schemes may have brief titles describing their contents and footnotes, if needed, for further detail. Schemes should be numbered with Arabic numbers in consecutive order.

Charts

Groups of structures that do not show reactions are called charts and should be numbered consecutively with Arabic numbers. Charts may have brief titles describing their contents and footnotes, if needed, for further detail.

Cover Art

Cover art images may be submitted with any type of manuscript, although publication preference will be given to Feature Articles, Review Articles, Special Issues, Articles that review very favorably, and manuscripts by Authors who review regularly for the journal. All Authors are encouraged to submit images for consideration as cover art. Cover images must capture the importance and excitement of the science discussed within the manuscript while also being “eye-catching” and aesthetically appealing. Submitted images are judged by the Managing Editor and Senior Editors. Cover images approved for publication may be modified by the ACS graphic artist with the Author giving final approval of the image. Images to be considered for the cover must be approximately 6 in. by 6 in. with a minimum of 300 dpi resolution (1800 × 1800 pixels,

~10 MB in file size). Do not reduce the image size or resolution when downloading it into Paragon Plus. Preferred image files are eps, tif, jpg, and png (not pdf). Cover art files should be submitted as Supporting Information. Images chosen for the cover will be published at **no cost to the author**.

Web-Enhanced Objects

The Journal encourages the submission of Web-enhanced objects (WEOs) for the presentation of graphical results that go beyond conventional print publication capabilities, including 3D rotatable figures, animations, spectra, video, and sound. Links to WEOs will appear in the Web HTML version of the paper. Files suitable for this form of publication should be viewable with commonly available Internet plug-ins (e.g., Chime) or helper applications (Rasmol, Mercury, etc.). Authors should submit WEOs via the Paragon Plus Web site as part of their submissions and clearly indicate to the Editor that the material is WEO material. Descriptions of WEOs should be noted in the appropriate places within the graphic caption or text of the paper, noting the type of file and format. Example: "A 3D rotatable image in xyz format is available." For more information, go to <http://pubs.acs.org/page/4authors/submission/weo.html>.

SUPPORTING INFORMATION

Extensive tables, graphs, spectra, calculations, detailed experimental methodology, and other material beyond a modest content in the published paper may be included as Supporting Information (SI) for Publication. SI is uploaded as separate files (file designation Supporting Information for Publication) at the time the manuscript is submitted. SI will be made available free of charge on the Web and can be accessed separately on the Web by Readers. The manuscript title and authors' names and affiliations should be provided on the first page of SI. All pages should be numbered consecutively starting with page S1. The list of supported file types for SI can be found at <http://pubs.acs.org/page/4authors/submission/software.html>. Zip compression may be used on large files prepared in the acceptable formats to speed transfer time. Files prepared in any other software must be provided in .pdf format.

Figures and tables that will appear in the published article are to be inserted **directly in the main body of the manuscript, and not included in the Supporting Information**.

GENERAL INFORMATION

Guidelines for Theory Papers

To be appropriate for publication in *JPC A/B/C*, theory papers must satisfy at least one of the following criteria:

1. provide significant new physical insight into an experimentally relevant system or process
2. present a new theoretical or computational methodology of general interest

Manuscripts that report the results of electronic structure calculations should follow the guidelines in J. E. Boggs (*Pure Appl. Chem.* **1998**, *70*, No. 4, 1015–1018). Manuscripts that present force field parameters and other potential energy surface information should follow the guidelines in D. J. Raber and W. C. Guida (*Pure Appl. Chem.* **1998**, *70*, No. 10, 2047–2049). Both sets of guidelines can be viewed online at <http://www.iupac.org/reports/1998/index.html>.

Guidelines for X-ray data

Authors are required to provide crystallographic data as Supporting Information in crystallographic information file (CIF) format.

Nomenclature

Registered trademark names should be capitalized whenever used. Trade and trivial names should not be capitalized. Usually the chemical name or composition should be given in parentheses or in a reference at the first occurrence of such a name. Nomenclature should conform with current American usage. Insofar as possible, Authors should use systematic names similar to those used by Chemical Abstracts Service and the International Union of Pure and Applied Chemistry.

Chemical Abstracts (CA) nomenclature rules are described in Appendix IV of the *Chemical Abstracts Index Guide*. For CA nomenclature advice, consult the Manager of Nomenclature Services, Chemical Abstracts Service, P.O. Box 3012, Columbus, OH 43210-0012. A name generation service is available for a fee through CAS Client Services, 2540 Olentangy River Road, P.O. Box 3343, Columbus, OH 43210-0334; phone, (614) 447-3870; fax, (614) 447-3747; or e-mail, answers@cas.org.

PARAGON PLUS TIPS

- Word documents and pdfs should contain everything, including figures, but not Supporting Information.
- Manuscripts will be deactivated if a revision is not returned three months from the date of request. Once deactivated, it will no longer appear on your Paragon Plus home page and the revision must be uploaded as a new manuscript.
- Do not use inaccurate or fictitious e-mail addresses because it may delay the review process for the manuscript.
- Contact the Help Desk (support@services.acs.org) for problems or questions concerning Paragon Plus or its use. Hours: 12 a.m. (midnight) to 8 p.m. EST/EDT Monday through Friday (excluding holidays). Phone: 1-800-227-9919 or 202-872-4357.

REVISIONS AND RESUBMISSIONS

For revisions:

- Clearly identify the manuscript as a revision; reference the manuscript number in the cover letter.
- Include an itemized list of changes, with a response to each comment made by the Editor and by each Reviewer.
- Be aware that the manuscript may be sent for additional review.
- Return revision within three months of request date or manuscript will be deactivated.

For resubmissions:

- Clearly identify the manuscript as a resubmission; reference the previous manuscript number in the cover letter.
- Include an itemized list of changes, with a response to each comment made by the Editor and by each Reviewer.

JOURNAL PUBLISHING AGREEMENT

ACS provides an **electronic Journal Publishing Agreement (eJPA)** that can be completed inside the ACS Paragon Plus Environment by the Author handling the peer review. The eJPA will be available on the **My Authoring Activity** of the Author's Home page once the manuscript has been assigned to an Editor. ACS also offers a PDF version of the form that can be completed and uploaded to ACS Paragon Plus during the manuscript submission or faxed after submission to the Assigned Editor. If the Corresponding Author cannot or should not complete either the electronic form or the PDF version for any reason, another Author should complete and sign the PDF version of the form. Note that only the Corresponding Author may complete the electronic version of the form. Forms and instructions are available at <http://pubs.acs.org/page/copyright/journals/index.html>.

To get permission to reproduce material (tables, figures, graphs, photographs, artwork), write or contact the copyright holder, giving complete information, to receive permission in writing. Most often the copyright holder is the publisher. Ask for the person who handles copyright permissions. Permission should be in writing and dated. For permission request information for papers published in ACS Journals, see <http://pubs.acs.org/page/copyright/permissions.html>.

Provide letter (email is fine) from author(s) of personal communications granting you permission to cite unpublished work.

PROOFS AND REPRINTS

Proofs

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Appendix: Examples of Abstracts

One or two sentences providing background on the problem.

Two or three sentences summarizing the methodology and results.

A concluding sentence highlighting the significance of the study.

Nitrogen oxides, including nitrogen dioxide and nitric acid, react with mineral dust particles in the atmosphere to yield adsorbed nitrate. Although nitrate ion is a well-known chromophore in natural waters, little is known about the surface photochemistry of nitrate adsorbed on mineral particles. In this study, nitrate adsorbed on aluminum oxide, a model system for mineral dust aerosol, is irradiated with broadband light ($\lambda < 300$ nm) as a function of relative humidity (RH) in the presence of molecular oxygen. Upon irradiation, the nitrate ion readily undergoes photolysis to yield nitrogen-containing gas-phase products including NO_2 , NO , and N_2O , with NO being the major product. The relative ratio and product yields of these gas-phase products change with RH, with N_2O production being highest at the higher relative humidities. Furthermore, an efficient dark reaction readily converts the major NO product into NO_2 during post-irradiation. Photochemical processes on mineral dust aerosol surfaces have the potential to impact the chemical balance of the atmosphere, yet little is known about these processes. In this study, the impact that adsorbed nitrate photochemistry may have on the renoxification of the atmosphere is discussed. (*J. Phys. Chem. A* **2009**, *113*, 7818–7825).

Polymerfullerene bilayer heterostructures are suited to study excitonic processes in conjugated polymers. Excitons are efficiently quenched at the polymerfullerene interface, whereas the polymervacuum interface is often considered as an exciton-reflecting interface. Here, we report about efficient exciton quenching close to the polymervacuum interface of spin-coated MDMO-PPV (poly[2-methoxy-5-(2'-ethyl-hexyloxy)-*p*-phenylenevinylene]) films. The quenching efficiency is estimated to be as high as that of the polymerfullerene interface. This efficient quenching is consistent with enhanced intermolecular interactions close to the polymervacuum interface due to the formation of a “skin layer” during the spin-coating procedure. In the skin layer, the polymer density is higher; that is, the intermolecular distances are shorter than in the rest of the film. The effect of exciton quenching at the polymervacuum interface should be taken into account when the thickness of the polymer film is on the order of the exciton diffusion length; in particular, in the determination of the exciton diffusion length. (*J. Phys. Chem. B* **2009**, *113*, 9104–9109).

Nanostructured metallic architectures have unique and highly attractive properties, including large optical field enhancements resulting in strong light scattering and absorption. Modification of prefabricated nanostructures by simple galvanic displacement (GD) allows for the design of new nanomaterials with enhanced optical properties. In this paper, we have studied the optical properties of two families of Ag fractals before and after GD in a Au(III) solution. The new nanomaterials showed significantly improved optical enhancing properties that allowed for straightforward and highly reproducible single-molecule detection by surface-enhanced resonance Raman scattering (SERRS). (*J. Phys. Chem. C* **2009**, *113*, 12897–12900).