Sample manuscript for *Journal of Physical and Chemical Reference Data*[a)]

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[2]*Corporation or Laboratory, Street address, Postal code, City, Country*

[3]*Department, University, City, State (spell out full name) Zip code, USA*

This is an abstract. It gives the reader an overview of the manuscript. In this sample article we provide instructions on how to prepare and submit your paper to *Journal of Physical and Chemical Reference Data*, a journal of the American Institute of Physics (AIP). Authors must follow the instructions given in this document. The AIP staff appreciates your effort to follow our style when preparing your manuscript.

Keywords: manuscript; sample; style

1. The Manuscript

Use this "sample manuscript" as a guide for preparing your article. This will ensure that your submission will be in the required format. Please read all of the following manuscript preparation instructions carefully and in their entirety. The manuscript must be in good scientific American English; this is the author's responsibility. All files MUST be submitted through our online electronic submission system at http://jpcrd.peerx-press.org.

1.1. Manuscript preparation

Articles must be prepared as either a Microsoft Word .doc/.docx file or a REVTeX/LaTeX file. The entire manuscript should be set up for 21.6 × 28 cm (8-1/2 × 11 in. or A4) pages with 2.54 cm (1 in.) margins all the way around. The font and the point size will be reset according to the journal's specifications, but authors most commonly use the Times Roman font and point size 12. The manuscript must begin with a title, names of all authors and their affiliations, and an abstract, followed by the body of the paper, tables and figures, if any, included, and the reference section. Consecutively number all tables (1, 2, 3, etc.) and figures (1, 2, 3, etc.), including those in an Appendix. Figures may be embedded in the text or not (author's choice). Figure captions must be included in the manuscript. Number all pages consecutively, beginning with 1.

[a)] This is an example of a footnote to the title if the paper was part of a conference: Contributed paper, published as part of the Proceedings of the 17th International Conference on Physics, Anytown, State, May 2010.

[b)] A. Author and B. Author contributed equally to this work.

[c)] This is an example of a footnote to an author's name: Author to whom correspondence should be addressed. Electronic mail: author@somewhere.org.

[d)] This research was performed while C. Author was at Anywhere National Laboratory, City, State, Postal code, Country.

1.2. Manuscript submission

All files MUST be submitted through the online system: http://jpcrd.peerx-press.org. Each version of the manuscript (the original and subsequent revisions) should be submitted with its own complete set of files: a cover letter (indicating the title, authors, and contact information), a complete article file, and separate figure files (see Sec. 11—Figures). When uploading a revised manuscript, also include a response/rebuttal letter (indicating the changes made to address the Editor's and Reviewers' comments).

2. Title

Make the title as concise as possible but informative enough to facilitate information retrieval. Only the most common acronyms and abbreviations are allowed in the title. Use acronyms with considerable moderation and always define at first use.

3. Abstract

Limit the abstract to less than 500 words. It must be self-contained (contain no footnotes or citations to references), adequate as an index (giving all subjects, major and minor, about which new information is given), and a concise summary (giving the conclusions and all results of general interest in the article). The abstract must be one paragraph and should not contain displayed mathematical equations or tabular material.

4. Key Words

Key words appear below the abstract. A maximum of 12 is allowed. They are listed in alphabetical order and separated by semicolons.

5. Authors' Names and Addresses

Authors' names should preferably be written in a standard form for all publications to facilitate indexing and to avoid ambiguities. Include the names and postal addresses of all institutions, followed by city, state, zip code, and USA if in the United States or by postal code, city, and country if not in the U.S. Please provide complete address(es). See the byline for this sample article for examples.

Authors with Chinese, Japanese, or Korean names may choose to have their names published in their own languages alongside the English versions of their names in the author list of their publications. For Chinese, authors may use either Simplified or Traditional characters. Chinese, Japanese, or Korean characters must be included within the author list of the manuscript when submitting or resubmitting. The manuscript must be prepared using Microsoft Word or using the CJK LaTeX package. Specific guidelines for each authoring tool are given at http://www.aip.org/pubservs/cjk_instructions.html.

6. Footnotes

Footnotes are generally unacceptable in AIP journals, with the exception of footnotes to the title or authors. All other information should be included in the reference section. Use a), b), c), etc., for footnotes to the title or authors. The following list shows some examples:

[a)] Contributed paper, published as part of the Proceedings of the 17th International Conference on Physics, Anytown, State, May, 2010. (footnote to title)

[b)] A. Author and B. Author contributed equally to this work.

[c)] Author to whom correspondence should be addressed. Electronic mail: author@somewhere.org.

[d)] This research was performed while C. Author was at Anywhere National Laboratory, City, State, Postal code, Country.

Footnotes should be used sparingly in the body of the paper. When absolutely necessary, a footnote should be indicated by a letter superscript and typed at the bottom of the manuscript page on which it appears. Footnotes should be numbered consecutively through the entire manuscript, starting with "a." For footnotes in Tables, see Sec. 12.

7. CONTENTS

Each article contains its own table of contents, titled "CONTENTS," flushed left, 10/12 times roman, heading numbers are aligned left, subheadings are indented, with dot leaders to bullets (which are later updated with page numbers), located before text begins. A list of Tables and/or a list of Figures is also included under the Contents listing. (Note: the CONTENT section is not a numbered section; we have only numbered it here to be consistent within our sample.)

8. Headings

Headings are mandatory in regular articles. Maintain a consistent heading style within the article. Numbered section headings are preferred in all AIP journals. Following is a list that shows the four different levels and style for each heading:

1. Principal Heading
1.1. Second level heading
1.1.1. Third level heading
1.1.1.1. Fourth level heading

9. Equations

Equations should be punctuated and aligned to bring out their structure, and numbered on the right. Mathematical operation signs indicating continuity of the expression should be placed at the left of the second and succeeding lines. Use (×) rather than a centered dot, except for scalar products of vectors. Use a solidus (/) instead of built-up fractions in running text, and in display wherever clarity would not be jeopardized. Use "exp" for complicated exponents.

$$I_D(\theta) = \frac{a}{2} + \sum_{n+1}^{2} (\cos 2n\theta + \sin 2n\theta). \quad (1)$$

$$B_i = \begin{pmatrix} 1 & 2 & \cdots & N \\ B_i(1) & B_i(2) & \cdots & B_i(N) \end{pmatrix}, \quad (2)$$

$$\begin{aligned} \langle \Phi_1 | \hat{H} | \Phi_2 \rangle &= \langle \Phi_1 | \hat{V}_{IJ} | \Phi_2 \rangle \\ &= \int d\mathbf{r}_1 \int d\mathbf{r}_2 \, \frac{\rho_J^{eg}(\mathbf{r}_1)\rho_I^{eg}(\mathbf{r}_2)}{r_{12}} \equiv V_{\text{Coul}} \end{aligned}, \quad (3)$$

$$c(T) = \exp\left(\frac{-E_d}{k_B T}\right). \quad (4)$$

Please note that you must use MathType or the Equation Editor 3.0 and NOT Microsoft Math Editor. When equations built with Microsoft's Editor are back-saved, they are converted to low-resolution graphics and are not usable.

10. Notation

Notation must be legible, clear, compact, and consistent with standard usage. Choose commonly used symbols from your discipline. All unusual symbols whose identity may not be obvious must be identified the first time they appear, and at all subsequent times when confusion might arise. If many symbols are used, particularly if their meaning is likely to be non-obvious, authors are encourages to include a separate "List of Symbols" section between the List of Figures and the main body of the paper. Even if a List of Symbols section is used, symbols should still be defined when first used. Superscripts are normally set directly over subscripts; authors should note where readability or the meaning requires a special order. Use appropriate symbols (for example from Word's Symbol font) rather than approximating them with other characters. For example, use the degree symbol, not a superscript letter "o," and use a "minus" sign for negative numbers (including exponents) instead of a hyphen.

11. Figures

Cite figures in text in numerical order of publication-ready illustrations. It is vital that you prepare your illustrations so that they are legible when reduced. Figures 1–6 show examples of various types of production-ready illustrations: color, line art, halftone, and combination (line art and halftone). Table 1 gives (a) general guidelines for preparing your illustrations and (b) guidelines for the preparation of electronic files.

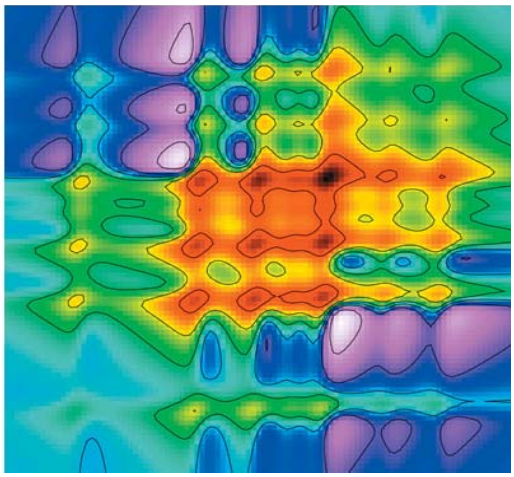

FIG. 1. (Color) This figure will appear in color in print and online. Figures should be created at 300 dpi and submitted at 300 dpi for the best presentation. Choose CMYK (cyan, magenta, yellow, black) for any figure that will appear in color in the print version.

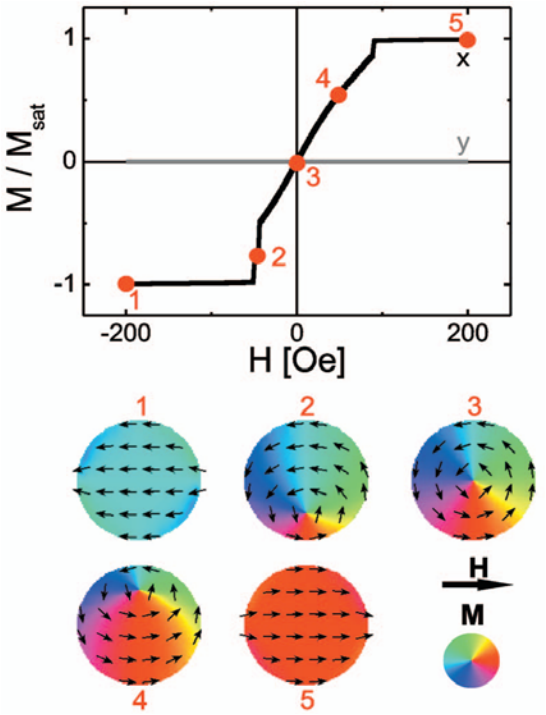

FIG. 2. (Color online) This figure will appear in color only in the online version only, not in the printed version. Figures should be created at 300 dpi and submitted at 300 dpi for the best presentation. Choose RGB (red, green, blue) for any figure that will appear in color only online.

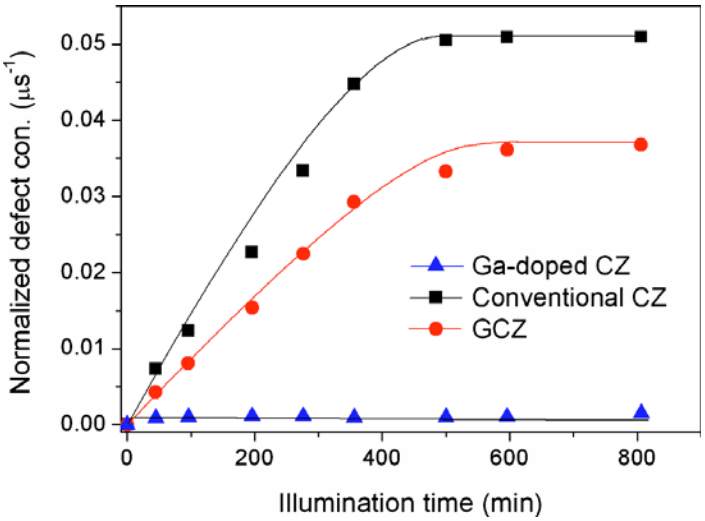

FIG. 3. This is a good example of information that is presented clearly. In the printed journal if this figure appears in black and white, the reader will be able to discern the "blue" triangles, the "red" circles, and the closed "black" squares. A description as well as the color is needed. If the caption simply discusses "the red and blue symbols," the reader of the print version would not understand because he/she would be seeing the figure without the color.

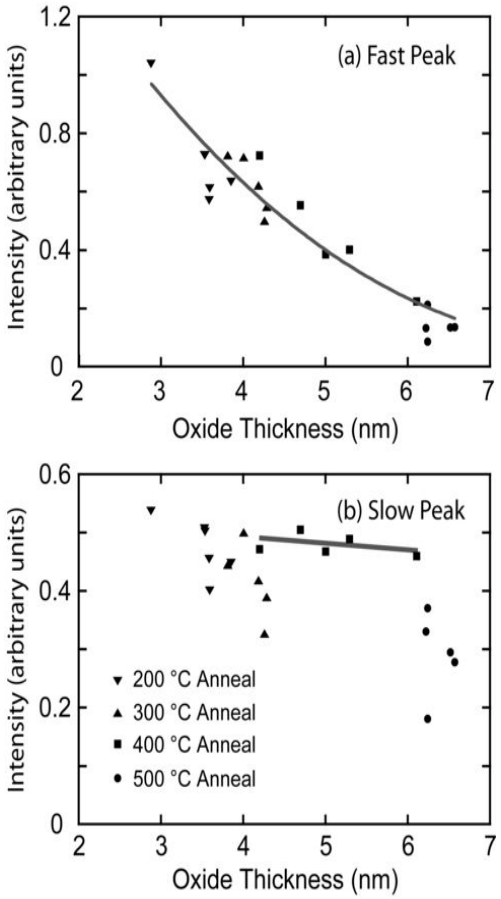

FIG. 4. This is an example of line art. Figures should be created at 600 dpi and submitted at 600 dpi for the best presentation. Save line art as black/white bitmap, not grayscale.

.

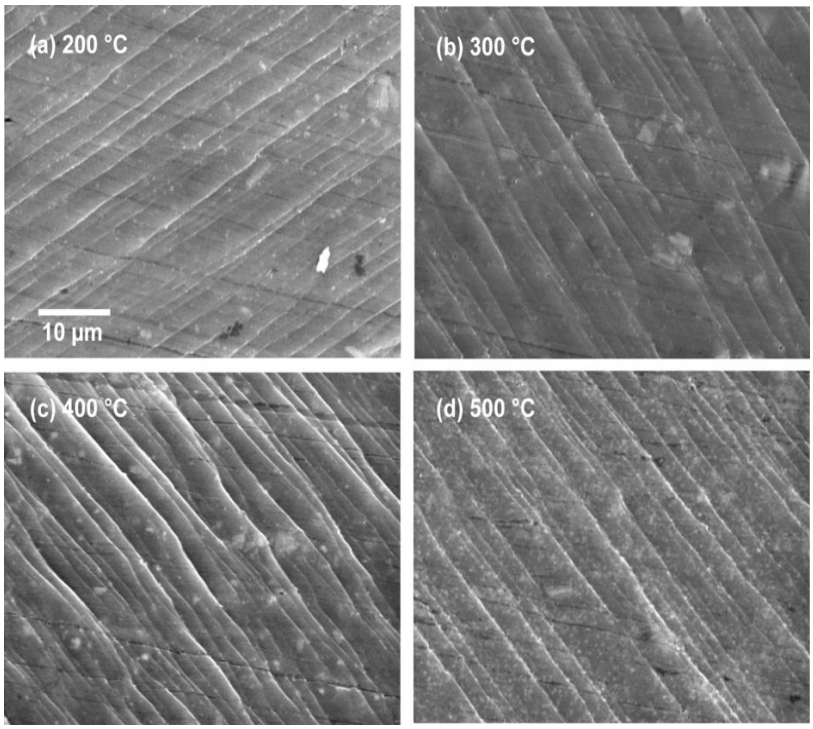

FIG. 5. This is an example of a halftone. Figures should be created at 300 dpi and submitted at 300 dpi for the best presentation.

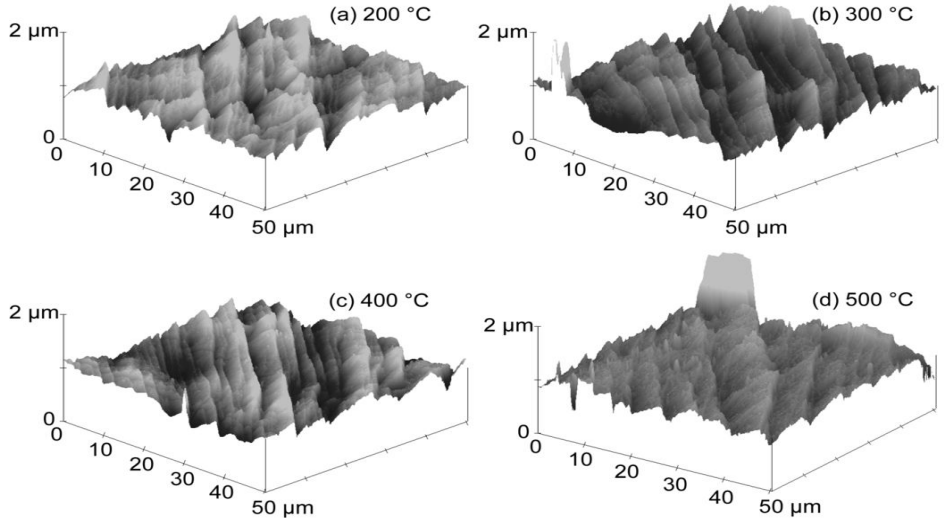

FIG. 6. This is an example of a combination figure (line art and halftone). Figures should be created at 600 dpi and submitted at 600 dpi for the best presentation.

TABLE 1. This table provides instructions on how to prepare figures.

(a) General guidelines for preparing illustrations

- Number figures in the order in which they appear in the text.
- Label all figure parts with (a), (b), etc. Each figure file should contain all parts of the figure. For example, if Fig.1 contains three parts [(a), (b), and (c)], then all parts should be combined in a single file for Fig. 1.
- Avoid any large disparity in size of lettering and labels used within one illustration.
- Prepare illustrations in the final published size, not oversized. The maximum published width for a one-column illustration is 8.5 cm (3-3/8 in.). The maximum width for a two-column figure is 17 cm (7.0 in.).
- In cases where reduction is required, avoid small open symbols that tend to fill in and avoid small lettering; ensure that, in the final published illustration, there is a minimum of 8-point type size (2.8 mm high; 1/8 in. high) for lettering and 0.5-point width for lines.
- Ensure that lettering and lines are dark enough, and thick enough, to reproduce clearly. Remember that fine lines tend to disappear upon reduction.
- The figures may be embedded in the manuscript in the approximate position and size you think is appropriate. **In addition, separate figure files must be provided (see below for accepted file formats) along with the manuscript.**

(b) Guidelines for preparation of electronic graphics files

- Acceptable formats for figures: Portable Document Files (PDF), Encapsulated PostScript Files (EPS), PostScript, or Tagged Image File format (TIF). EPS (using Arial or Times Roman fonts) is preferred graphic format when preparing illustrations. Microsoft Word (.doc or .docx) or JPEG (.jpg) files are **not** acceptable.
- More detailed information is given about figure preparation on the JPCRD website in the How to Prepare Illustrations under the Information for Contributors tab.
- Settings: Set the graphic for 600 dpi resolution for line art, 300 dpi for halftones, and 600 dpi for combinations (line art + halftone).
- Save line art as black/white bitmap, not grayscale.
- Save halftones and combinations as grayscale, not black/white bitmap.
- Click here for publication charge information.
- Submit color files at 300 dpi in one of the accepted file formats: PDF, EPS, PS, or TIF. No other type of color illustration is acceptable. When selecting a file mode, for print choose CMYK (cyan, magenta, yellow, black) and for color online choose RGB (red, green, blue).
- PDF files should be vector files.
- In the PDF illustration, resolution of any shaded or photographic images must be 600 pixels per inch (PPI).
- Within the PDF illustration, resolution of line art with no shading should be 1200 pixels per inch (PPI).
- All fonts must be **embedded** in the PDF.
- Select "High Quality Print" when creating a PDF through the application's print command.
- If usable color graphics files are received in time for the production process, authors will see color versions of those illustrations when viewing their author proofs. (The Corresponding Author will receive e-mail notification from AIP when the proof, as a PDF file, is available for downloading.)
- The author is responsible for obtaining permissions to reuse previously published material. Full credit lines are needed for figures that are used with permission. An example of the recommended format for crediting material from a journal article is: "Reprinted with permission from [FULL CITATION]. Copyright [PUBLICATION YEAR], American Institute of Physics." Full citation format is as follows: Author names, journal title, Vol. #, Issue #, Page # (or CID#), Year of publication. For example, the credit line would appear as: "Reprinted with permission from J. Chem. Phys. 128, 024365 (2008). Copyright 2008 American Institute of Physics. If you need help acquiring permissions from another publisher, use this form [CLICK HERE].

12. Tables

Separate tables (numbered in the order of their appearance in the text) should be used for all but the simplest tabular material. Tables must have captions that make the tables intelligible without reference to the text. The structure should be clear, with simple column headings giving all units. Unaltered computer output and notation should be uploaded as supplemental files. Table captions are positioned above the table and should be styled as "TABLE 1. This is a table caption." Capitalize the first word in the table headings and subheadings. References and footnotes within tables are designated by lowercase Roman letter superscripts and given at the end of the table. See Table 2 for an example of correct table styling.

TABLE 2. Bond distances for alkene molecules (atomic units).

No. C[a]	$RI,I+1$[b]	$SRI,I+1$[c]	$RI-1,I+RI,I+1$[d]	$SRI-1,I+RI,I+1$[e]
2	2.5255	…	…	…
4	2.6175	0.123	5.306	…
6	2.6314	0.0999	5.3025	0.0112
8	2.6368	0.0876	5.3009	0.0111
10	2.6396	0.0795	5.2999	0.0106
14	2.6424	0.0689	5.2989	0.0096
18	2.6437	0.0623	5.2982	0.0088
22	2.6443	0.0573	5.2973	0.008
26	2.6448	0.0536	5.2968	0.0074

[a]C is the number of carbon atoms.

[b]$RI,I+1$ is the distance between two neighboring carbon atoms, while $\langle RI,I+1 \rangle$ is the average of $RI,I+1$ for a given molecule.

[c]$SRI,I+1$ is the standard deviation of $RI,I+1$ within the given molecule.

13. Multimedia Files

Multimedia files can be included in the online version of published papers. All such files are peer reviewed. When published, these files can be viewed by clicking on a link from the figure caption, provided that the reader has a video player installed, such as Windows Media PlayerTM, Quick Time PlayerTM, or RealOne PlayerTM. Please see Information for Contributors on our website. Click on Guidelines for Multimedia. Please note the following important information when preparing your manuscript:

- Treat all multimedia files as figures, numbered in sequence as they are referred to in text. (Multimedia files will **not** have a numbering scheme separate from the figures.) For each multimedia file, provide a figure, which is a static representation of the multimedia file. Also provide an accompanying caption. At the end of the caption, include the phrase "(enhanced online)."
- All multimedia files must be cited in the text, referred to by their figure number.

14. Supplemental Material

Text material that may not be of interest to all readers, long data tables, multimedia, and computer programs may be deposited as supplementary materials. Information about depositing supplemental material may be found at the journal's Information for Contributors section on the website.

15. Acknowledgments

Typically, standard acknowledgments include financial support and technical assistance, and may include dedications, memorials, and awards. Check with the Editorial Office for suitability of an acknowledgment if there is any question. To indicate the author, use initials. For example, "B.A. wishes to thank A. Waldron for technical assistance. C.A. wishes to thank Anytown University for use of their equipment." Note: the Acknowledgment section is not a numbered section.

16. Appendix

Appendices are placed after the acknowledgments section and before the listing of references. Appendices must have a Level One heading as illustrated below. They do not follow the sequential heading numbering given in the rest of the paper. If there is only one appendix, then the heading is set as follows:

Appendix

If there is more than one appendix, the headings are set as:

Appendix A: Description

Appendix B: Description

Subheadings in an Appendix are labeled A.1, A.2, etc.

17. References

References must be numbered consecutively in order of first appearance in the text and should be listed at the end of the text material. Reference citations in text are rendered in several ways. For example:

Voitsenya *et al.*[4]

Kawa and Lin[8]

MOLPRO (Ref. 10)

The citation in the reference list must include the full list of authors. Do not list the first author followed by an abbreviation such as *et al*. See Table 3 for acceptable reference formats.

TABLE 3. This table provides instructions on how to prepare references.

Journal citations:

[1]C. B. Alcock, M. W. Chase, and V. P. Itkin, J. Phys. Chem. Ref. Data **23**, 385 (1994).

Books:

[2]A. A. Bondi, *Physical Properties of Molecular Crystals, Liquids, and Gases* (Wiley, New York, 1968).

Series:

[3]G. Neumann, in *Current Topics in Materials Science*, edited by E. Kaldis (North-Holland, Amsterdam, 1981), Vol. 7, Pt. 1, pp. 53–68.

Conference proceedings:

[4]J. G. Neumann and P. G. O'Shea, *Proceedings of the 2005 Particle Accelerator Conference*, Portland, OR, 12–16 May 2005 (Wiley, New York, 2005).

Conference proceedings cited in a journal:

[5]A. G. Agarwal, *Proceedings of the Fifth Low Temperature Conference*, Madison, WI, 1999 [Semiconductors **66**, 1238 (2001)].

Thesis / dissertation:

[6]S. M. Smith, Ph.D. thesis, Massachusetts Institute of Technology, 2003.

Reports:

[7]W. K. Fields, ECE Report No. XXX, 2005.

Patents:

[8]P. L. Balk, U.S. Patent No. 6,330,110 (3 February 2004).

E-prints:

[9]Y. M. Zalkins, e-print cond-mat/040426.

Private communication:

[10]O. M. Singh (private communication).

Supplemental material:

[11]See supplementary material at http://dx.doi.org/10.1063/1.3055594 for all the force fields used in this work, presented in table format.

Web sites:

[12]*NIST Chemistry Webbook*, edited by P. J. Linstrom and W. G. Mallard, http://webbook.nist.gov (accessed July 14, 2004). NIST Standard Reference Database Number 69 (National Institute of Standards and Technology, Gaithersburg, MD).