Scientific Writing Workshop

November 29, 2021
IIT Gandhinagar

Attributes of a High-Quality Research Paper

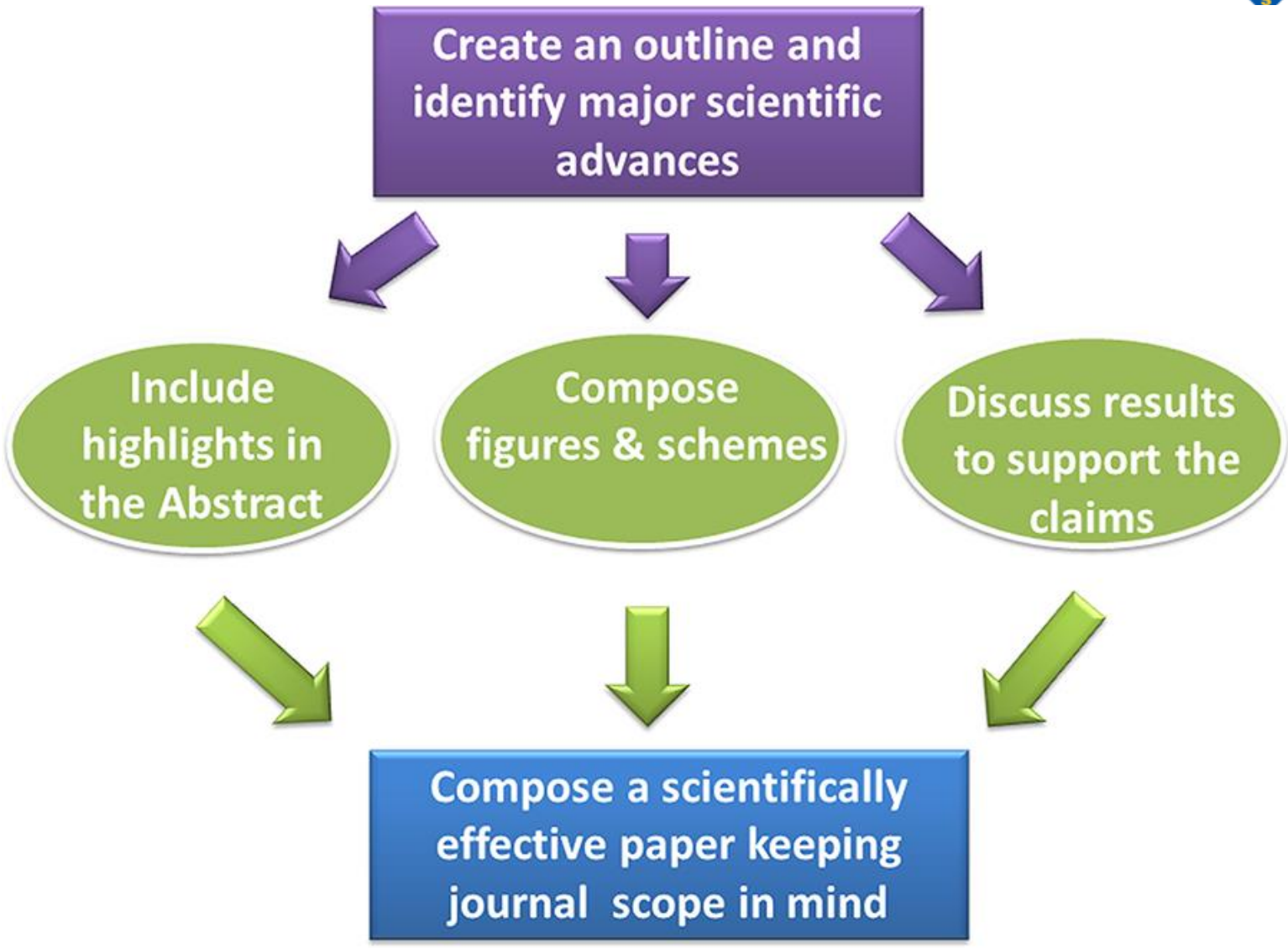
- **Not just a scientific report** of empirical observations but a **detailed analysis** of the data and in-depth mechanistic insights
- The title and abstract are **simple and attractive**
- The figures and schemes are **well drawn and self-explanatory**
- The Experimental/Methods section provides sufficient details so that **reproducible in another laboratory**
- **Compelling and exciting scientific story**

Tell a Story!

- Make sure the paper has a main theme and punchline
- Avoid “data dumping”
- Provide context to prior literature, and cite the original work in the reference section
- **Explain why the problem is important!**
- Share experimental details that would allow a reasonably educated person in your field to re-perform the experiments
- Analyze the data accurately and objectively
- Provide a strong conclusion, describing how your work moves the field forward, but be realistic

Image: https://jasonfurnell.wordpress.com/

Key Steps in Composing a Scientifically Effective Paper



J. Phys. Chem. Lett. 2013, 4, 1578

Anatomy of a Manuscript

Title

Abstract

Introduction

Graphics

Experimental Section

Results and Conclusion

References

Acknowledgement

What's in a Name?

- First thing that draws attention
- Shorter titles often make a greater impact

- ✓ Make sure that your title is grammatically sound
- ✓ Craft a compelling title – describe your results/findings in as few words as possible, in an evocative and exciting way

- ✗ "Study", "Investigation", or "Demonstration" reflects routine scientific work
- ✗ Avoid asking a question in the title – be clear on what is accomplished
- ✗ Manuscript titles should not make claims of priority, originality, convenience, effectiveness, or value

- **Don't use the words "convenient", "efficient", "elegant", "expedient", "facile", "first", "new", "novel", "practical", "simple", "unique", "unprecedented", and "versatile"**

http://pubs.acs.org/paragonplus/submission/joceah/joceah_authguide.pdf

Attract Readers with a Strong Title

"We strongly believe that the science should speak for itself and that the use of adjectives that sound too self-promoting can have adverse impact."

FUNCTIONALITY

- **Attract potential audience**
- **Aid retrieval and indexing**

CONTENT **

- **Simple**
- **Effective**
- **Accurate**

Overly Long Title:
Synthesis, Electrochemistry, Spectroscopic Characterization, and X-ray Crystal Structures of Ni(III) Complexes that can be Isolated and Promote Carbon–Carbon Bond-Forming Reductive Elimination

Shortened Title:
Carbon–Carbon Bond-Forming Reductive Elimination from Isolated Nickel(III) Complexes

* ***Chem. Mater.*** **2014, 26, 334**
** ***J. Phys. Chem. Lett.*** **2013, 4, 1578**

ACS Editors' Choice

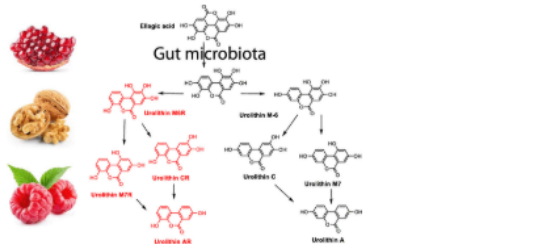
Identification of Novel Urolithin Metabolites in Human Feces and Urine after the Intake of a Pomegranate Extract

Rocío García-Villalba, María V. Selma, Juan C. Espín and Francisco A. Tomás-Barberán*

J. Agric. Food Chem. 2019 67, 40, 11099-11107 **(Article)** ACS Editors' Choice
Publication Date (Web): September 8, 2019
ACS Editors' Choice Date: September 28, 2019

Abstract | Full Text | PDF

ABSTRACT



JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY

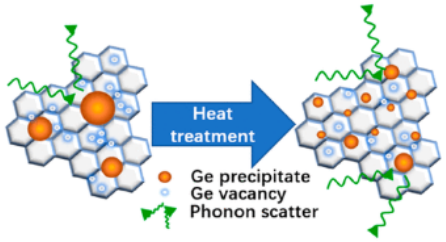
Realizing High Thermoelectric Performance in GeTe through Optimizing Ge Vacancies and Manipulating Ge Precipitates

Yang Jin, Yu Xiao, Dongyang Wang, Zhiwei Huang, Yuting Qiu* and Li-Dong Zhao*

ACS Appl. Energy Mater. 2019 2, 10, 7594-7601 **(Article)** ACS Editors' Choice
Publication Date (Web): September 9, 2019
ACS Editors' Choice Date: September 27, 2019

Abstract | Full Text | PDF

ABSTRACT



ACS APPLIED ENERGY MATERIALS

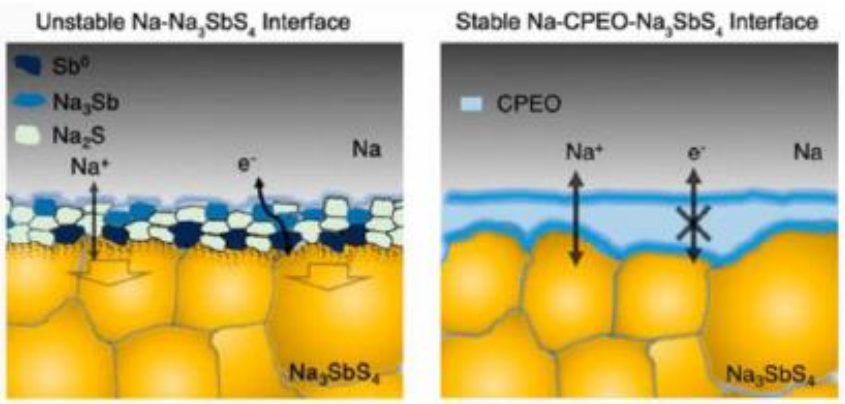
Table of Content (ToC)

- Typically the first glimpse a potential reader has of your published paper
- A good ToC image must, simultaneously:
  - Resonate with the title (to provide synergistic support)
  - Instantly provide a sense of what is to be learned
- Ensure that everything in the ToC image is comprehensible and lucid, and yet exciting
- A common mistake is simply to cut and paste a figure/reaction scheme from the paper to use as the ToC

Design Good TOC Graphics

- Recommended Reading: “Table of Contents Images: Science and Beauty = Clarity”, *Chem. Mater.*, 2016, **28** (6), pp 1589–1590, DOI: 10.1021/acs.chemmater.6b00928
- Excessive use of cartoon images in any of the graphics are unadvised, the image should look professional.
- No logos from universities, government associations, or companies!

A



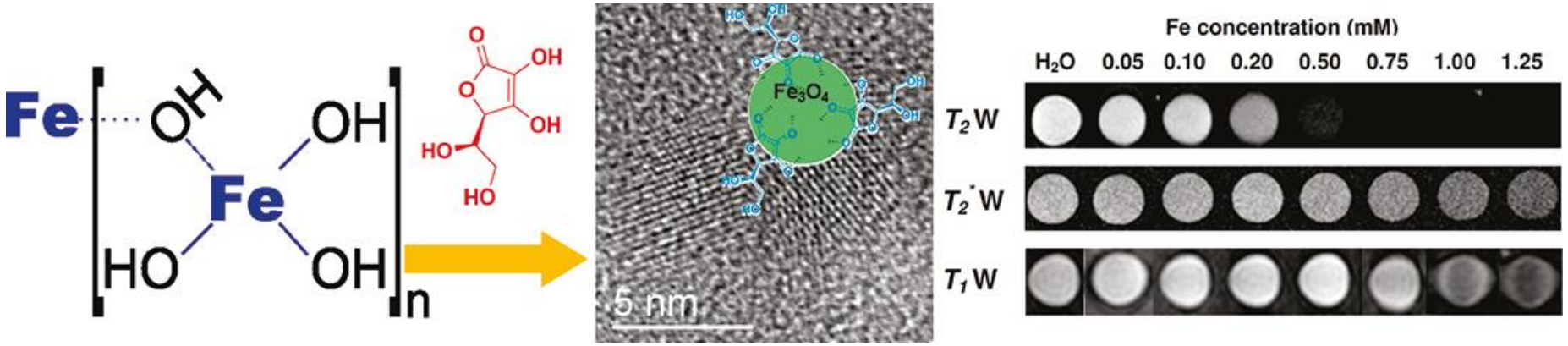
Good Example

B

Not so Good Example

Example

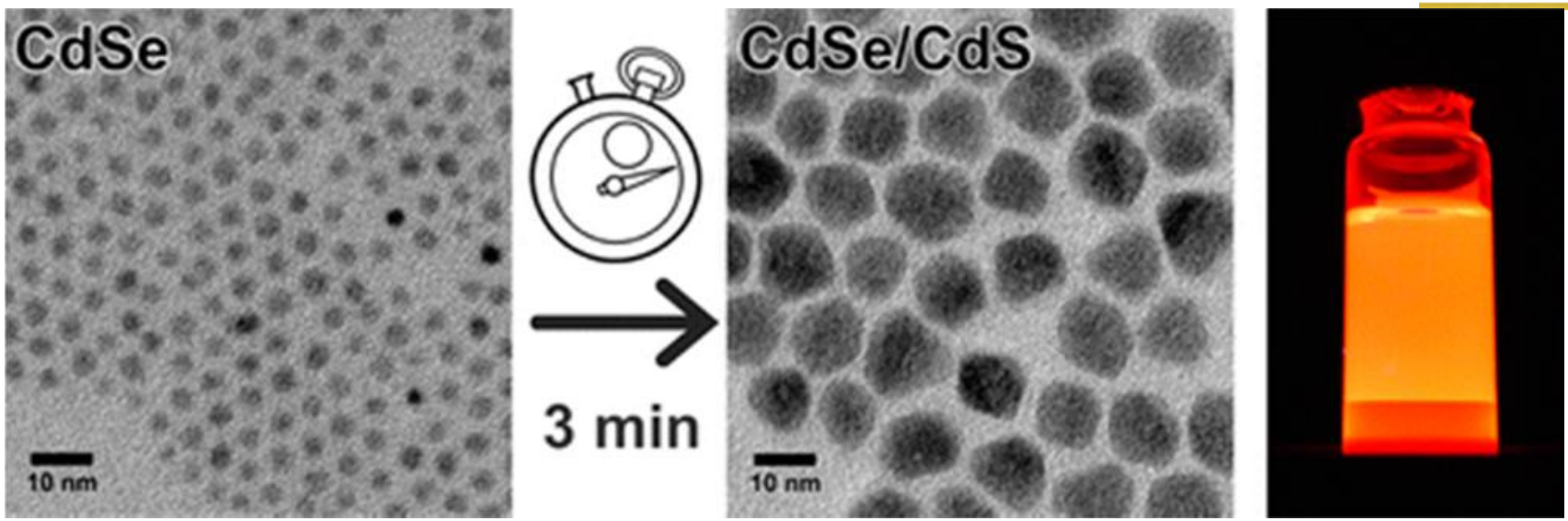
Water-Soluble Superparamagnetic Magnetite Nanoparticles with Biocompatible Coating for Enhanced Magnetic Resonance Imaging



- ✓ The ToC image here quickly outlines a synthesis of iron oxide nanoparticles, with the reagents clearly displayed.
- ✓ The subsequent use of the magnetite nanoparticles in MRI is obvious from the gray scale plot on the right, and so the ToC suggests a complete body of work.

ACS Nano 2011, 5, 6315
ACS Nano 2011, 5, 7687

“Flash” Synthesis of CdSe/CdS Core−Shell Quantum Dots”

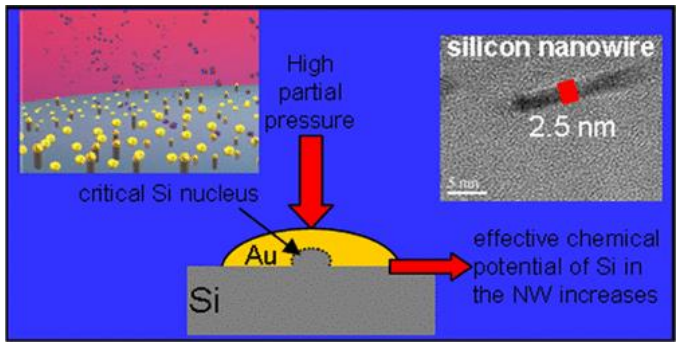


- The title here projects that the concept of speed with respect to nanoparticle synthesis is the obvious focus of the paper.
- The use of the word “Flash” ties in well with the stopwatch in the ToC image, and hence makes the point that the nanocrystal synthesis is fast.
- The glowing vial suggests that the quality of the resulting nanoparticles is not compromised.

Chem. Mater. 2014, 26, 1289

Think!
Are these suitable for TOC representation?

A



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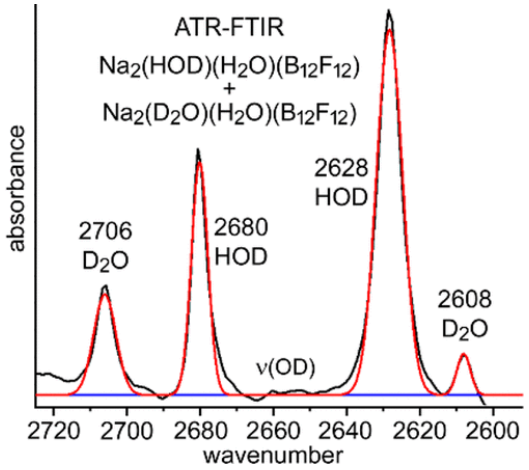

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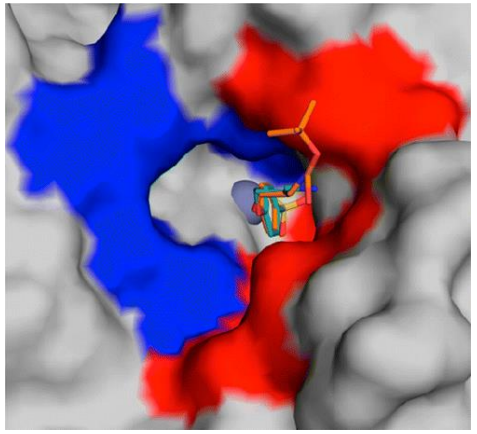

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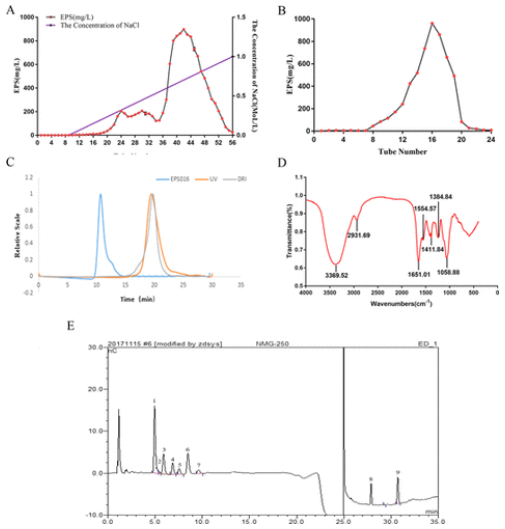


Abstract

- A summary of the work being discussed in the paper
- Written in such a way that any reader who is not familiar with the topic will be able to understand and appreciate the main points of the study
- Avoid 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

Abstract

*Extra effort should be taken to compose an effective and concise abstract!**

FUNCTIONALITY

- Allow readers to **determine paper scope**
- Aid **retrieval and indexing**

CONTENT

Any reader who is not familiar with the topic will be able to understand and appreciate the main points

- **Concise**
- **Self-contained/Separately**
- **Informative**
- **DO NOT** supplement or evaluate the conclusions
- **DO NOT** cite references, tables, figures

* ***J. Phys. Chem. Lett*. 2013, 4, 1578**

Interface stability in solid-state batteries

Development of high conductivity solid-state electrolytes for lithium ion batteries has proceeded rapidly in recent years, but incorporating these new materials into high-performing batteries has proven difficult. Interfacial resistance is now the limiting factor in many systems, but the exact mechanisms of this resistance have not been fully explained - in part because experimental evaluation of the interface can be very difficult In this work, we develop a computational methodology to examine the thermodynamics of formation of resistive interfacial phases . The predicted interfacial phase formation is well correlated with experimental interfacial observations and battery performance. We calculate that thiophosphate electrolytes have especially high reactivity with high voltage cathodes and a narrow electrochemical stability window. We also find that a number of known electrolytes are not inherently stable but react in situ with the electrode to form passivating but ionically conducting barrier layers As a reference for experimentalists, we tabulate the stability and expected decomposition products for a wide range of electrolyte, coating, and electrode materials including a number of high-performing combinations that have not yet been attempted experimentally

Background

Methodology

Major conclusions

Closing remark

Chem. Mater., 2016, 28, 266

High-Quality $(CH_3NH_3)_3Bi_2I_9$ Film-Based Solar Cells: Pushing Efficiency up to 1.64%

Bismuth-based solar cells have exhibited some advantages over lead perovskite solar cells for nontoxicity and superior stability, which are currently two main concerns in the photovoltaic community. As for the perovskite-related compound $(CH_3NH_3)_3Bi_2I_9$ applied for solar cells, the conversion efficiency is severely restricted by the unsatisfactory photoactive film quality. Herein we report a novel two-step approach— high-vacuum BiI_3 deposition and low-vacuum homogeneous transformation of BiI_3 to $(CH_3NH_3)_3Bi_2I_9$—for highly compact, pinhole-free, large-grained films, which are characterized with absorption coefficient, trap density of states, and charge diffusion length comparable to those of some lead perovskite analogues. Accordingly, the solar cells have realized a record power conversion of efficiency of 1.64% and also a high external quantum efficiency approaching 60%. Our work demonstrates the potential of $(CH_3NH_3)_3Bi_2I_9$ for highly efficient and long-term stable solar cells *

Briefly state the problem/purpose of the research

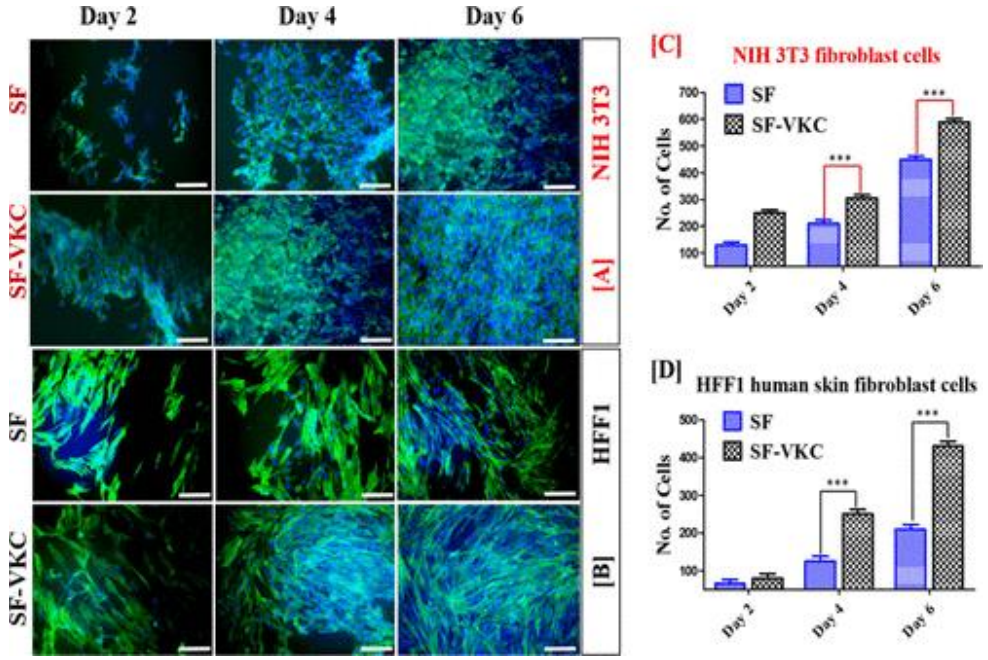
A couple of sentences indicating the methodology and key observations (scope of the study)

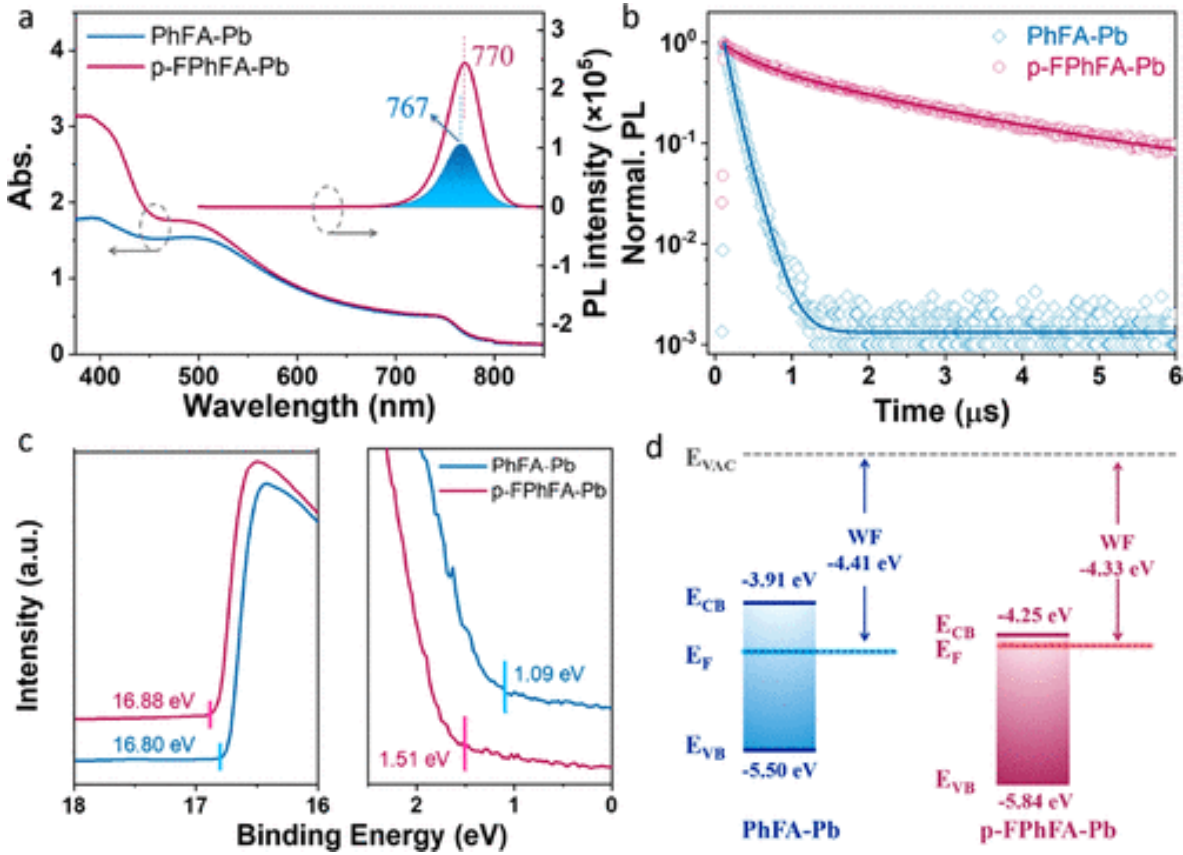
Point out major conclusions

End with a sentence summarizing the implication of the study in a broader context (e.g., possible applications) that highlights importance of the work

Draw Graphics with Care

- Be clear and precise, simple but informative
- Graphics should complement the text and support your story
- Use **color**!
- Graphics must be original, unpublished artwork, created by an author



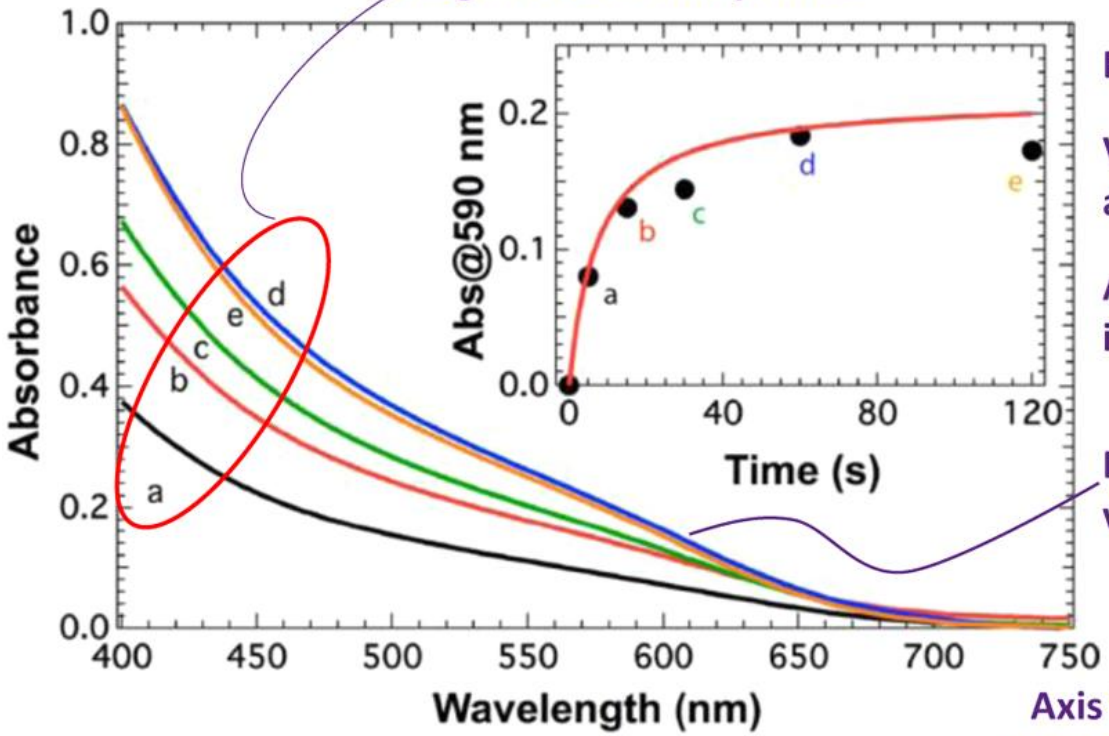


Accuracy of data presentation

Aesthetics of the figure

Visible Major and Minor Ticks

Legends to identify traces



Bold Axis Line

Visible Major and minor Tics

Analyzed data in the inset

Distinguishable, vibrant colors

Axis Title with units (Bold and Larger Font)

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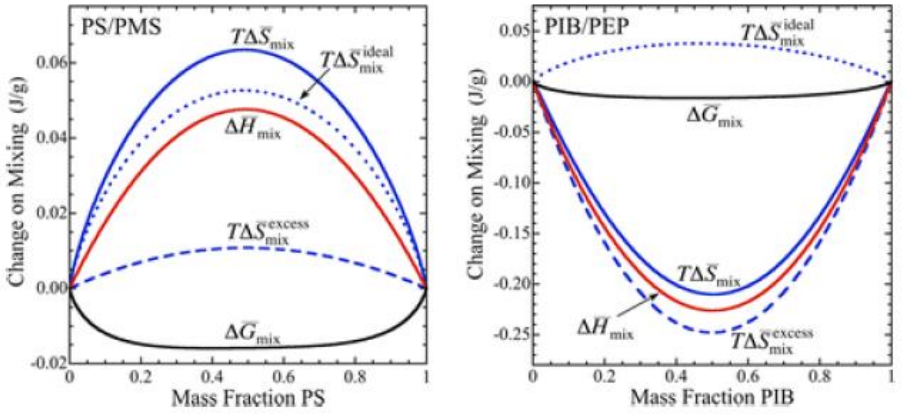

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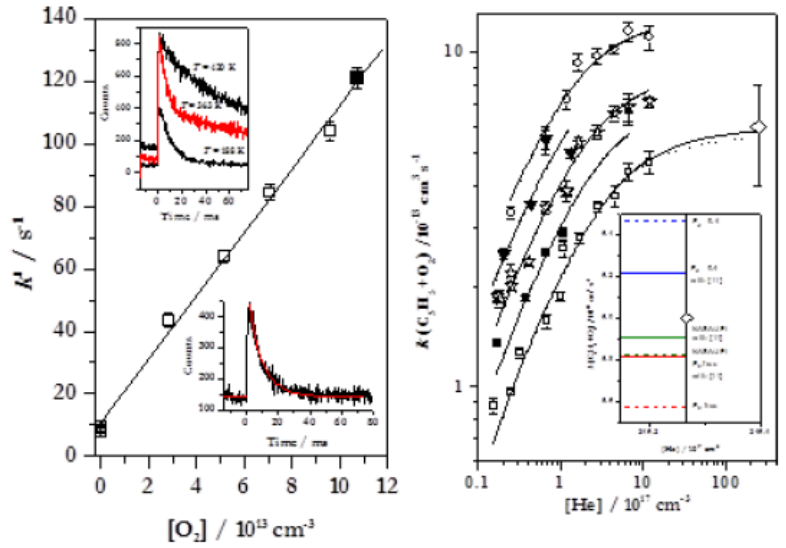

J. Phys. Chem. Lett. 2014, 5, 2118

Prepare High Quality Graphics/Figures

- Be sure to check the PDF file you are about to upload to the submission system!
- You do not want your paper to look like this:

nm. Fig 13-C revealed small cavities on the surface due to surface tension or low concentrations of nanomaterials during calcination.

Figure 13. AFM images: a) Topography of N:Ni:TiO_2(O) film, b)3D topography of the surface roughness, c) 3D topographic images of the magnification for showing hole, cavities and roughnes5.

Atomic force microscopic analysis of N:Ni:TiO_2(E) film. Fig14-A, particles are distributed homogeneously across the surface, which reduces surface roughness and there are lots of white spots on it. It is related to prolonging the coating time causes NP agglomerate. The square cross-sectional roughness of the film is 2.336 nm. The total surface roughness (Sq) is 4.91 nm. Fig 14-B shows the longitudinal line at the glazed tile surface. This mode creates two awful conditions: 1- shortage of nanomaterials that penetrate into the valleys and due to the calcination, burned down and lost amounts of NP. 2- stop the NP in that part make them agglomeration in the surface.

Figure 14. AFM image: a) Topography of N:Ni:TiO_2(E) film, b)3D topography of the surface roughness.

Atomic force microscopic analysis of N:Ni:TiO_2(P) film. Fig 15-A and B, the particles are dispersed in a surface but particles so greater than others one. Their size measured ~1.81 µm. The surface roughness (Ra) is 12.29 nm and the square cross-sectional roughness of the film is 90.18 nm. The total surface roughness is (Sq) equal, 57.43 nm. This mode indicated particles and roughness depended on the coating time. As suggested, the fixed price and wasting the extra nanomaterials on the surface, on the other hand, it destroyed the tile's aesthetic.

Figure 15. AFM images: a) Topography of N:Ni:TiO_2(P) film, b)3D topography of the surface roughness.

Consequently, by the prolonging the coating time the NS growth and the surface got rough.

2. Ultra violet-diffuse reflectance spectra (UV-DRS) analysis

Fig 16 shows the absorption spectra of all synthesized PCs which P25 TiO_2 white powder and bare TiO_2 as a reference in a wide spectral range, it covered UV and visible region i.e., 1.45 to 3.54 eV (350–850 nm). The band gap can be calculated using E_g=hc/λ. In this

15

Construct a Well-written Cover Letter

*"Cover Letter is a statement of why the paper is **appropriate** for the journal*"*

FUNCTIONALITY

- Interest the editor enough to read your paper carefully and choose to send it out for peer review
- A chance for authors to persuade the editors of the significance of their work in a less formal manner

CONTENT

- Highlight your **most important** findings
- State **impact** to the community
- **DO NOT** copy Abstract!
- **DO NOT** simply state that your manuscript is "of interest to the field" or "novel." Address **specific aspects** of the journal's Aims & Scope statement

*** *ACS Nano* 2010, 4, 2487**
http://www.business2community.com/communications/avoid-embarrassing-marketing-gaffes-communicate-effectively-0897764

Dear **Professor Bertozzi**,

Address the Editor-in-Chief or Associate Editor directly & correctly. Pay attention to Transfer or Resubmission

We wish to submit our manuscript "**TITLE**" for publication in ***ACS Central Science.***

Include the title of the manuscript and mention the journal name
Pay attention to Transfer or Resubmission

We describe a new, non-natural enzyme-catalyzed reaction, aziridination of olefins via intermolecular nitrene transfer. **We discovered** that a variant of cytochrome P450BM3 used in **our previous studies** of intermolecular sulfimidation also catalyzes aziridination. **We were able to improve this activity** more than 50-fold and the enantioselectivity of enzyme-catalyzed aziridination was improved to 99% ee for a range of styrenyl substrates.

Highlight the results/main findings of your work

This work should be of interest to the broad audience that *ACS Central Science* wishes to reach. It touches on evolution—how new enzyme activities can appear and be improved through evolution—as well as inorganic catalysis, biocatalysis, and chemical synthesis.

Explain why the work is appropriate for the journal's readership, why it is important/ urgent, be specific

Permission from Professor Frances Arnold received

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Assessing Significance & Technical Quality

Assessing Presentation & Readiness

Writing Your Review

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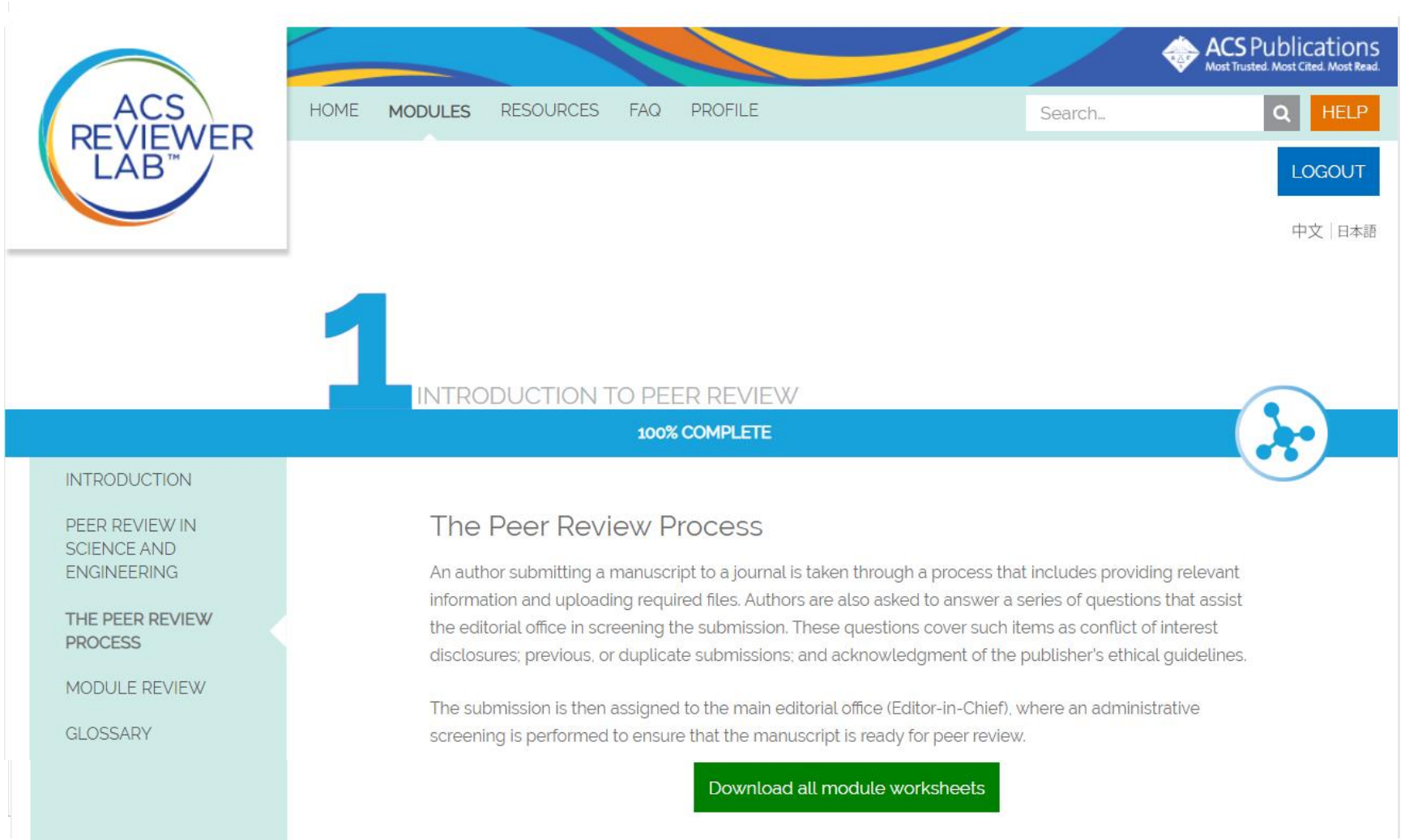
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The Peer Review Process
An author submitting a manuscript to a journal is taken through a process that includes providing relevant information and uploading required files. Authors are also asked to answer a series of questions that assist the editorial office in screening the submission. These questions cover such items as conflict of interest disclosures; previous, or duplicate submissions; and acknowledgment of the publisher's ethical guidelines.
The submission is then assigned to the main editorial office (Editor-in-Chief), where an administrative screening is performed to ensure that the manuscript is ready for peer review.
Download all module worksheets

Congrats You are a Reviewer Now!

Ethics & Plagiarism

10 Tips for Ethical Authorship

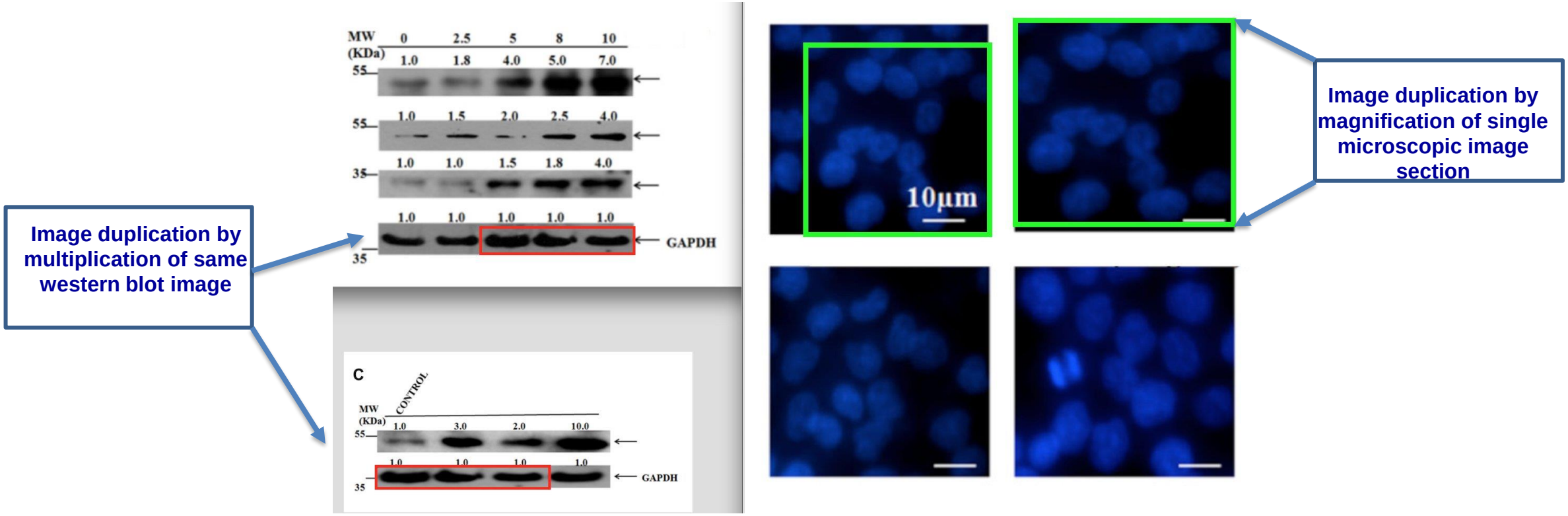
https://axial.acs.org/2017/07/31/10-tips-ethical-authorship/

Most Common Ethical Violations

- **Self-plagiarism** – reusing your own content
- **Prior publication** – journals have policies about what they consider to be published content
- **Concurrent submissions** – submitting the same manuscript to multiple journals at the same time
- **Data fabrication or falsification** – deliberately or unintentionally changing the data to fit the conclusions

Most common types of image duplications

- Western blot images
- Microscopic images



Source: Science Chronicle https://journosdiary.com/2018/07/10/elisabeth-bik-image-duplications/

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A [2]Rotaxane-Based Circularly Polarized Luminescence Switch

Arthur H. G. David, Raquel Casares, Juan M. Cuerva*, Araceli G. Campaña and Victor Blanco*

Cite this: *J. Am. Chem. Soc.* 2019, XXXX, XXX, XXX-XXX
Publication Date: October 22, 2019
https://doi.org/10.1021/jacs.9b07143

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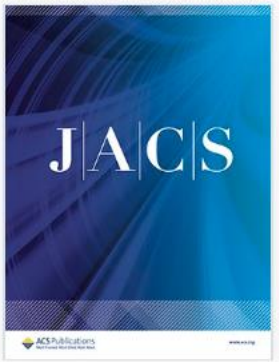

Journal of the American Chemical Society

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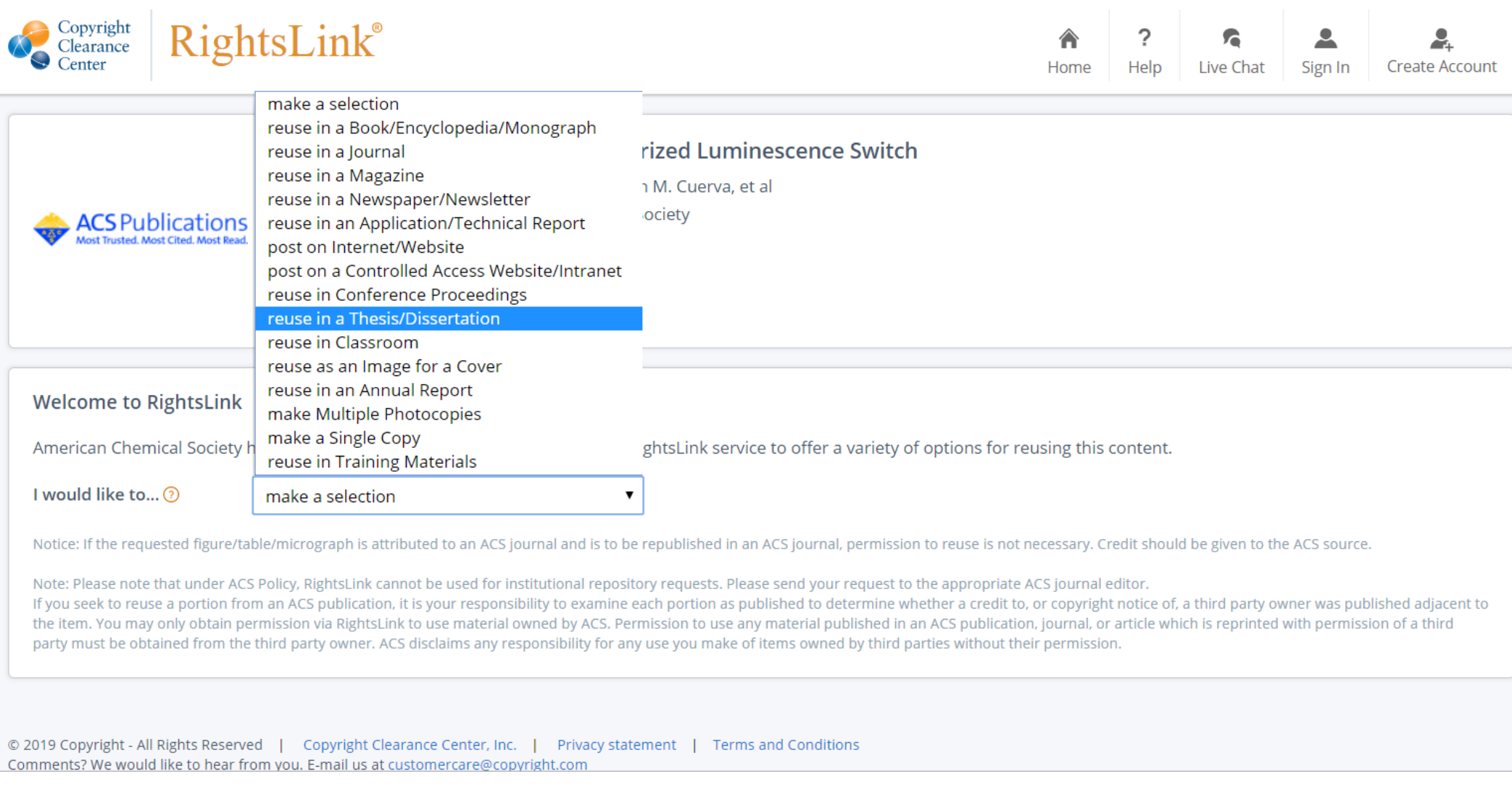
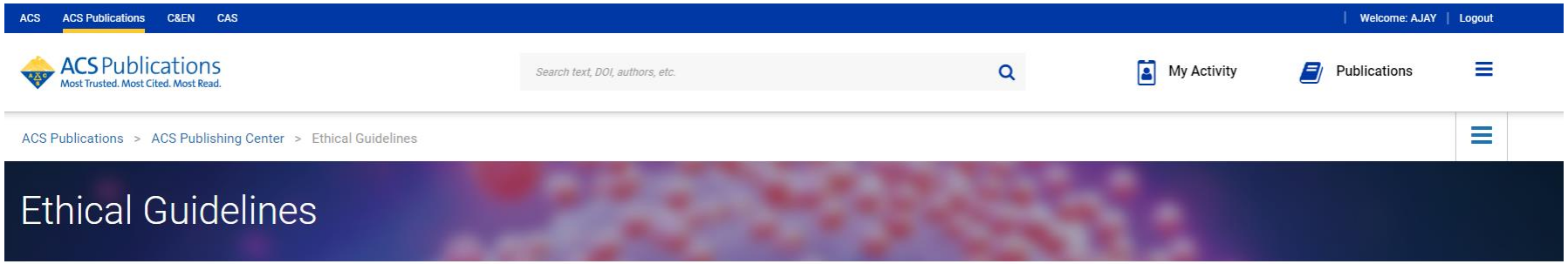


Ethical Guidelines at ACS



Ethical Guidelines to Publication of Chemical Research

The Editors of journals published by the American Chemical Society provide a set of ethical guidelines for persons engaged in the publication of chemical research, specifically, for editors, authors, and manuscript reviewers. These guidelines were developed by the Editors of the journals published by the Publications Division of the ACS and are reviewed regularly to ensure their clarity.

The ACS Journals' Ethical Guidelines are offered from a conviction that the observance of high ethical standards is so vital to the whole scientific enterprise that a definition of those standards should be brought to the attention of all concerned.

Special Notes for Authors

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https://pubs.acs.org/page/policy/ethics/index.html

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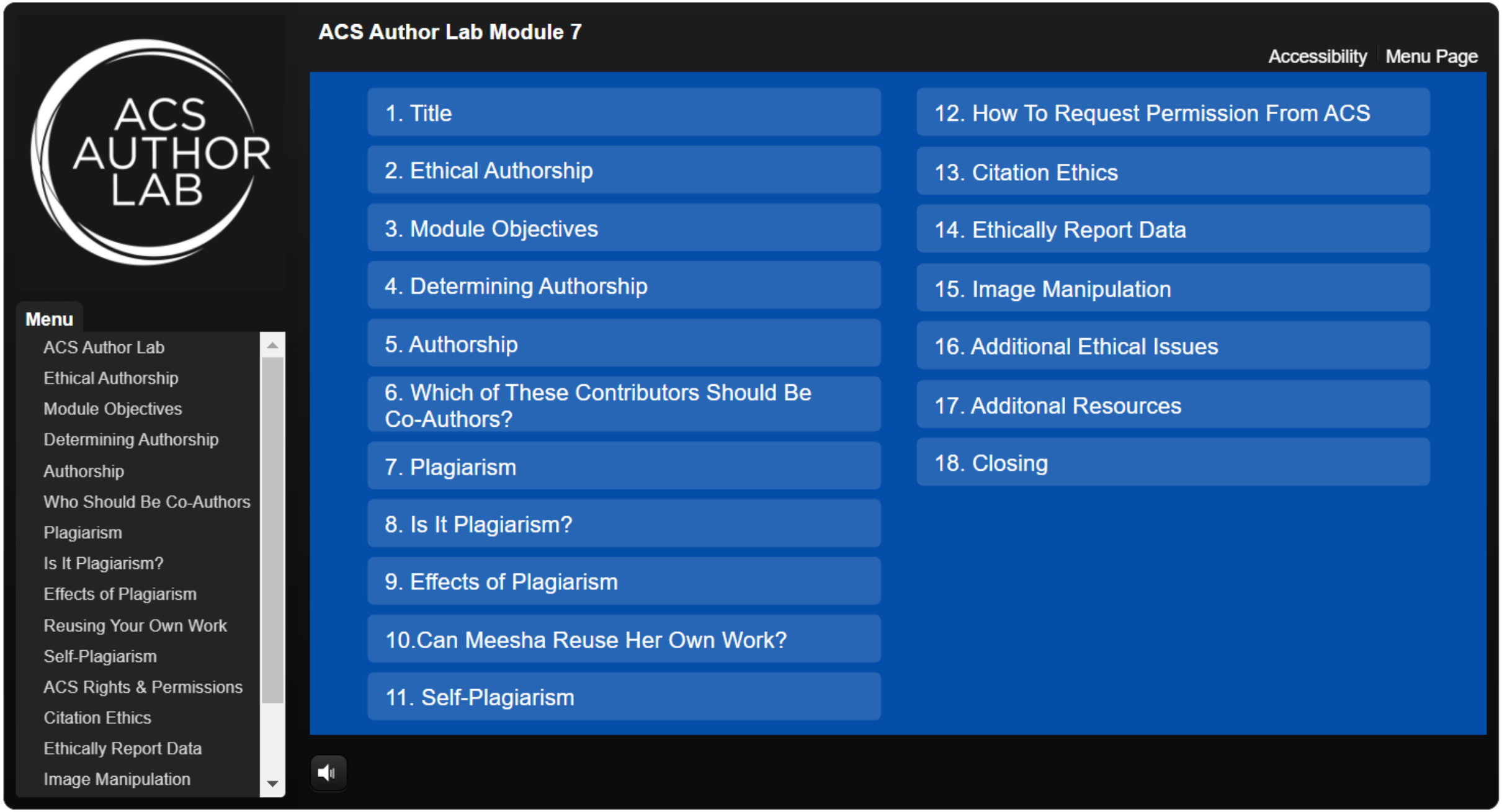
- ❑ Navigate the Revision Process
- ❑ Adhere to Ethical Guidelines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5. Authorship
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14. Ethically Report Data
15. Image Manipulation
16. Additional Ethical Issues
17. Additonal Resources
18. Closing

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- Authorship
- Who Should Be Co-Authors
- Plagiarism
- Is It Plagiarism?
- Effects of Plagiarism
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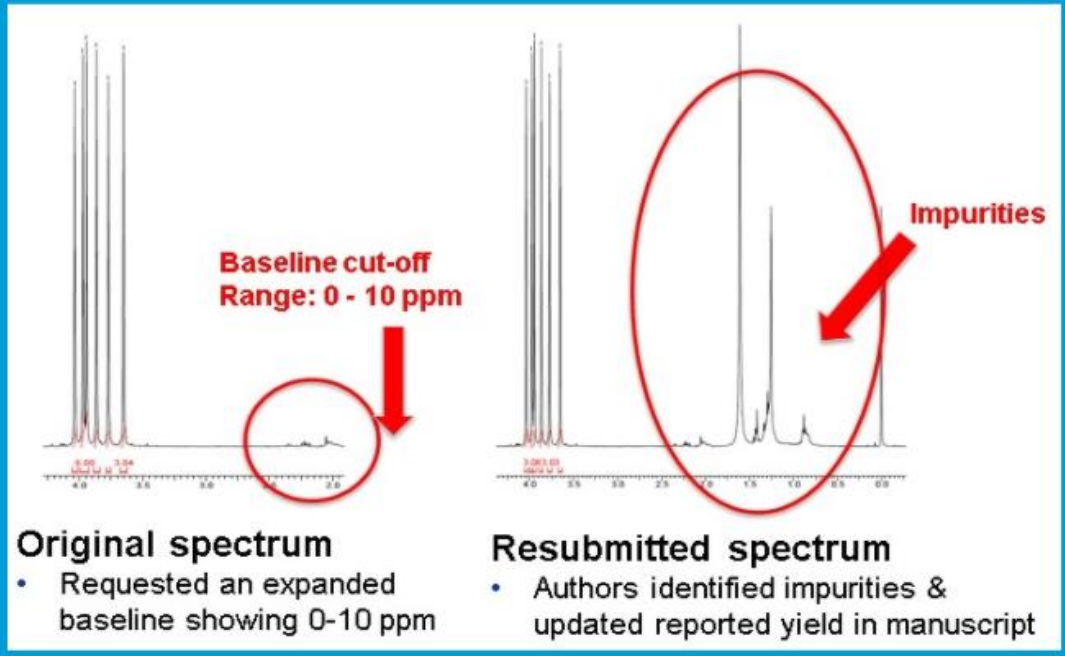
- Image Manipulation
- Additional Ethical Issues
- Additional Resources
- Closing

Image Manipulation



Original spectrum
- Requested an expanded baseline showing 0-10 ppm

Resubmitted spectrum
- Authors identified impurities & updated reported yield in manuscript

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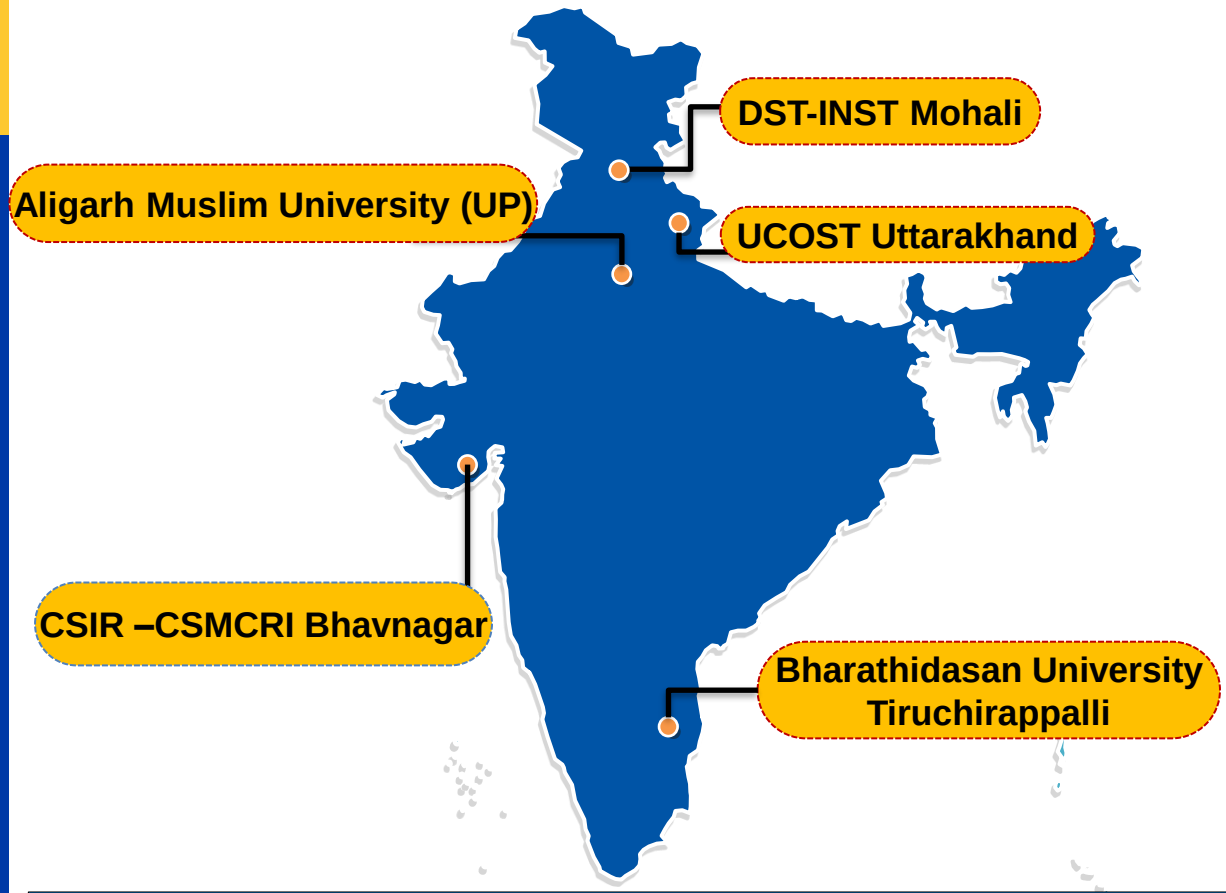

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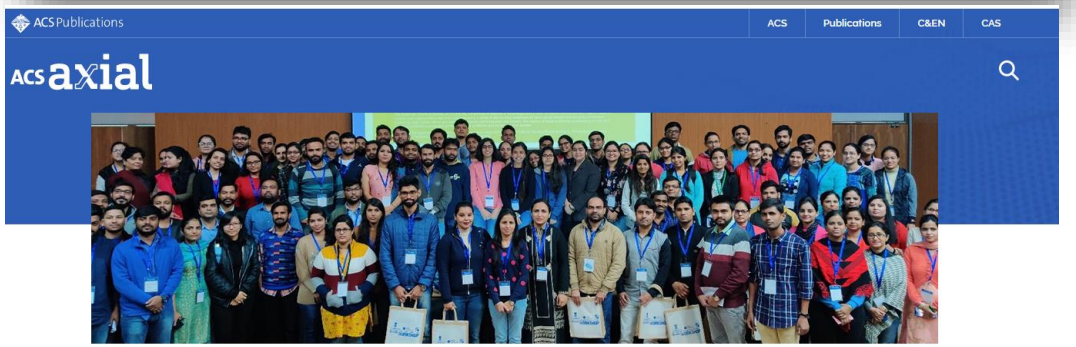

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