MSE 690
Ethical conduct in research

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Responsible conduct of research

**THERE IS NO ONE BEST WAY TO UNDERTAKE** research, no universal method that applies to all scientific investigations. Accepted practices for the responsible conduct of research can and do vary from discipline to discipline and even from laboratory to laboratory. There are, however, some important shared values for the responsible conduct of research that bind all researchers together, such as:

- **Honesty** - conveying information truthfully and honoring commitments.
- **Accuracy** - reporting findings precisely and taking care to avoid errors.
- **Efficiency** - using resources wisely and avoiding waste.
- **Objectivity** - letting the facts speak for themselves and avoiding improper bias.

At the very least, responsible research is research that is built on a commitment to these and other important values that define what is meant by integrity in research. Rules of the Road, presents a brief overview of the different ways research responsibilities are defined, ranging from formal regulations to informal codes and common practices.
Research misconduct

DEFINITION OF RESEARCH MISCONDUCT

Research misconduct means fabrication, falsification, or plagiarism in proposing, performing, or reviewing research, or in reporting research results.

(a) **Fabrication** is making up data or results and recording or reporting them.

(b) **Falsification** is manipulating research materials, equipment, or processes, or changing or omitting data or results such that the research is not accurately represented in the research record.

(c) **Plagiarism** is the appropriation of another person’s ideas, processes, results, or words without giving appropriate credit.

(d) Research misconduct does not include honest error or differences of opinion.

http://ori.dhhs.gov/misconduct/definition_misconduct.shtml
Responsible conduct of research


The scientific research enterprise, like other human activities, is built on a foundation of trust. Scientists trust that the results reported by others are valid. Society trusts that the results of research reflect an honest attempt by scientists to describe the world accurately and without bias. The level of trust that has characterized science and its relationship with society has contributed to a period of unparalleled scientific productivity. But this trust will endure only if the scientific community devotes itself to exemplifying and transmitting the values associated with ethical scientific conduct.


Chemists Acknowledge Responsibilities To:

- **The Public.** Chemists have a professional responsibly to serve the public interest and welfare and to further knowledge of science.
- **The Science of Chemistry.** Chemists should seek to advance chemical science, understand the limitations of their knowledge, and respect the truth....
- **The Profession.** Chemists should remain current with developments in their field, share ideas and information, keep accurate and complete laboratory records, maintain integrity in all conduct and publications, and give due credit to the contributions of others. Conflicts of interest and scientific misconduct, such as fabrication, falsification, and plagiarism, are incompatible with this Code.
- **The Employer.** Chemists should promote and protect the legitimate interests of their employers, perform work honestly and competently, fulfill obligations, and safeguard proprietary information.
- **Employees.** Chemists, as employers, should treat subordinates with respect for their professionalism and concern for their well-being....
- **Students.** Chemists should regard the tutelage of students as a trust conferred by society for the promotion of the student’s learning and professional development
- **Associates.** Chemists should treat associates with respect, regardless of the level of their formal education, encourage them, learn with them, share ideas honestly, and give credit for their contributions.

http://www.iit.edu/departments/csep/PublicWWW/codes/coe/acs-chma.htm

From: www.citiprogram.org
Materials Research Society (MRS)
Policy on Publication Ethics and Responsibilities

Available at: www.mrs.org/s_mrs/doc.asp?CID=30&DID=201354

“The policy adopts and builds on the Statement of Ethics and Responsibilities of Authors Submitting to AIP Journals published by the American Institute of Physics”
“Each physicist is a citizen of the community of science. Each shares responsibility for the welfare of this community. Science is best advanced when there is mutual trust, based upon honest behavior, throughout the community. Acts of deception, or any other acts that deliberately compromise the advancement of science, are unacceptable. Honesty must be regarded as the cornerstone of ethics in science. Professional integrity in the formulation, conduct, and reporting of physics activities reflects not only on the reputations of individual physicists and their organizations, but also on the image and credibility of the physics profession as perceived by scientific colleagues, government and the public. It is important that the tradition of ethical behavior be carefully maintained and transmitted with enthusiasm to future generations.”

“The following are the minimal standards of ethical behavior relating to several critical aspects of the physics profession”
Research Results

“The results of research should be recorded and maintained in a form that allows analysis and review. Research data should be immediately available to scientific collaborators. Following publication, the data should be retained for a reasonable period in order to be available promptly and completely to responsible scientists.

... Fabrication of data or selective reporting of data with the intent to mislead or deceive is an egregious departure from the expected norms of scientific conduct, as is the theft of data or research results from others.”
Publication and Authorship Practices

“Authorship should be limited to those who have made a significant contribution to the concept, design, execution or interpretation of the research study. All those who have made significant contributions should be offered the opportunity to be listed as authors. Other individuals who have contributed to the study should be acknowledged, but not identified as authors. The sources of financial support for the project should be disclosed.

Plagiarism constitutes unethical scientific behavior and is never acceptable. Proper acknowledgement of the work of others used in a research project must always be given. Further, it is the obligation of each author to provide prompt retractions or corrections of errors in published works.”
Peer Review

“Peer review provides advice concerning research proposals, the publication of research results and career advancement of colleagues. It is an essential component of the scientific process.

Peer review can serve its intended function only if the members of the scientific community are prepared to provide thorough, fair and objective evaluations based on requisite expertise. Although peer review can be difficult and time-consuming, scientists have an obligation to participate in the process.

Privileged information or ideas that are obtained through peer review must be kept confidential and not used for competitive gain.

Reviewers should disclose conflicts of interest resulting from direct competitive, collaborative, or other relationships with any of the authors, and avoid cases in which such conflicts preclude an objective evaluation.”
Plagiarism

Although there is widespread agreement in the scientific community on including plagiarism as a major element of the PHS definition of scientific misconduct, there is some uncertainty about how the definition of plagiarism itself is applied in ORI cases.

As a general working definition, ORI considers plagiarism to include both the theft or misappropriation of intellectual property and the substantial unattributed textual copying of another’s work. It does not include authorship or credit disputes.

The theft or misappropriation of intellectual property includes the unauthorized use of ideas or unique methods obtained by a privileged communication, such as a grant or manuscript review.

Substantial unattributed textual copying of another’s work means the unattributed verbatim or nearly verbatim copying of sentences and paragraphs which materially mislead the ordinary reader regarding the contributions of the author. ORI generally does not pursue the limited use of identical or nearly identical phrases which describe a commonly-used methodology or previous research because ORI does not consider such use as substantially misleading to the reader or of great significance.

Many allegations of plagiarism involve disputes among former collaborators who participated jointly in the development or conduct of a research project, but who subsequently went their separate ways and made independent use of the jointly developed concepts, methods, descriptive language, or other product of the joint effort. The ownership of the intellectual property in many such situations is seldom clear, and the collaborative history among the scientists often supports a presumption of implied consent to use the products of the collaboration by any of the former collaborators.

For this reason, ORI considers many such disputes to be authorship or credit disputes rather than plagiarism. Such disputes are referred to PHS agencies and extramural institutions for resolution.
“To write well and avoid plagiarism, focus on insights, not grammar. Here are eight rules of thumb to follow:

1. Read the text.
2. Think about it. What did the authors say? How does it relate to the topic you are writing about?
3. Put it aside!
4. Using your own language and style (whatever it is), write out what you want to say.
5. Add proper citations by citing all ideas or information taken from another author. Check for accuracy.
6. Do not quote unless absolutely necessary. If you must quote, make sure the quote is exact, use quotation marks and cite.
7. Do not paraphrase. There are very few situations in scientific writing where it is necessary or appropriate. Note: A citation, such as Johal et al. (1995), gives credit for information and ideas. It is insufficient to give credit for writing!
8. …”
Determination of dopant of ceria system by density functional theory

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Abstract Oxides with the cubic fluorite structure, e.g., ceria (CeO₂), are known to be good solid electrolytes when they are doped with cations of lower valence than the host cations. The high ionic conductivity of doped ceria makes it an attractive electrolyte for solid oxide fuel cells, whose prospects as an environmentally friendly power source are very promising. In these electrolytes, the current is carried by oxygen ions that are transported by oxygen vacancies, present to compensate for the lower charge of the dopant cations. Ionic conductivity in ceria is closely related to oxygen-vacancy formation and migration properties. A clear physical picture of the connection between the choice of a dopant and the improvement of ionic conductivity in ceria is still lacking. Here we present quantum-mechanical first-principles study of the influence of different trivalent impurities on these properties. Our results reveal a remarkable correspondence between vacancy properties at the atomic level and the macroscopic ionic conductivity. The key parameters comprise migration barriers for bulk attractive electronic parts. In the optimal electrolyte, these parts should balance. This finding offers a simple and clear way to narrow the search for superior dopants and combinations of dopants. The ideal dopant should have an

Optimization of ionic conductivity in doped ceria

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Oxides with the cubic fluorite structure, e.g., ceria (CeO₂), are known to be good solid electrolytes when they are doped with cations of lower valence than the host cations. The high ionic conductivity of doped ceria makes it an attractive electrolyte for solid oxide fuel cells, whose prospects as an environmentally friendly power source are very promising. In these electrolytes, the current is carried by oxygen ions that are transported by oxygen vacancies, present to compensate for the lower charge of the dopant cations. Ionic conductivity in ceria is closely related to oxygen-vacancy formation and migration properties. A clear physical picture of the connection between the choice of a dopant and the improvement of ionic conductivity in ceria is still lacking. Here we present a quantum-mechanical first-principles study of the influence of different trivalent impurities on these properties. Our results reveal a remarkable correspondence between vacancy properties at the atomic level and the macroscopic ionic conductivity. The key parameters comprise migration barriers for bulk diffusion and vacancy-dopant interactions, associated by association (binding) energies of vacancy-dopant clusters. The interactions can be divided into repulsive elastic and attractive electronic parts. In the optimal electrolyte, these parts should balance. Factors that determine Eₐ would be very helpful for future development of advanced solid oxide fuel cells.

For pure ceria, whose ionic conductivity is not particularly high because of low concentration of oxygen vacancies, Eₐ is equal to the sum of the vacancy formation energy (Eᵥₐ) and the migration barrier (Eₘᵢᵣ). Ceria doped with lower valence cations contains intrinsic oxygen vacancies, which improve the conductivity. However, because of interactions, the dopants and vacancies form associates with a certain binding or association energy (Eₐₐ), which prevents the vacancies from being mobile (9–12). The number of mobile vacancies is determined by Eₘᵢᵣ in the same way as the concentration of vacancies in pure ceria is governed by Eᵥₐ. Hence, for doped ceria, Eₐ can be identified as the sum of Eᵥₐ and Eₘᵢᵣ. At sufficiently high temperature, most vacancies will be dissociated, and in this regime, the concentration of mobile vacancies is simply determined by the doping level. However, in this article, we are interested in properties at low or intermediate temperatures. The aim is to maximize the concentration of mobile vacancies, which means that the dopant and dopant concentration should be chosen to minimize Eₐₐ. In this strive, we focus on trivalent cations from the lanthanide series as dopants of ceria.
July 18, 2008

Purdue committee completes research misconduct investigation

Allegation A.2
Dr. Taleyarkhan with falsifying intent caused Mr. Adam Butt’s name to be added to the author bylines of the papers even though Mr. Butt was not a significant contributor to the experiments, the data analyses, or the writing of the manuscripts.

Conclusion
The Committee concluded that this allegation was supported by the evidence of the additional authorships and the additional publications knowing that Butt was not on the work. The Committee concluded that there had been falsification.

Allegation B.2
Dr. Taleyarkhan with falsifying intent stated in the opening paragraph of his paper in Physical Review Letters 96:034301 (2006) that “these observations [referring to Science 295:1868 (2002)] have now been independently confirmed.”

Conclusion
Based on the findings in this section and in the preceding sections, we find that Dr. Taleyarkhan’s claims of independent confirmation of his sonofusion results are simply not supported by the weight of the evidence of his extensive involvement in the NED and NURETH-11 research and publication. The direct assertion of independent confirmation in the PRL96 paper is falsification of the research record and thus is research misconduct.

Cleared of other allegations
MSE 690: Ethics Assignment

• Complete the course: “Responsible Conduct of Research” from CITI:
  • www.citiprogram.org

• You will have to register as a Purdue student and select “Physical Sciences”

• You do not need to perform the “Human Research” course

• All MSE 690 students and MSE postdoctoral scholars should perform the course before the end of the summer semester
  • Print your certificate and leave it with Mrs. Patti Finney in ARMS 2200
This is the email address we have for you: ale.strachan@gmail.com. If this is not correct, please edit or change your email address now.

You are affiliated with 1 participating institution(s) on the CITI website. You will have at least one grade book per institution to track your progress in meeting the institution’s coursework requirements (see below).

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Purdue University

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