Fw: <Review> - Research misconduct

Georgia Tech Open Records Office <openrecords@gatech.edu>
Wed 10/13/2021 7:41 AM
To: Virgil, Franchesca <fvirgil6@gatech.edu>

Office of Institute Communications
Open Records Division
***Georgia** Institute of **Tech**nology*
openrecords@gatech.edu

Georgia Tech

From: Grover, Martha A <mg200@gatech.edu>
Sent: Wednesday, October 13, 2021 6:08 AM
To: Georgia Tech Open Records Office <openrecords@gatech.edu>
Subject: FW: <Review> - Research misconduct

Dear Francesca,
Here is the email record regarding No. 092131.
Sincerely,
Martha

From: Michael Casiato [redacted]
Date: Thursday, July 23, 2020 at 3:21 PM
To: Martha Grover <martha.grover@chbe.gatech.edu>
Cc: Dennis Hess <dennis.hess@chbe.gatech.edu>, "Williams, Rhea" <R_Williams@acs.org>, EIC Office Industrial & Engineering Chemistry Research <eic@iecr.acs.org>
Subject: Re: <Review> - Research misconduct

Dr. Williams - please proceed at your convenience.

Kind regards,

Michael

On Thu, Jul 23, 2020 at 2:17 PM Grover, Martha A <martha.grover@chbe.gatech.edu> wrote:

> I agree, it is fine to move forward.
> Thank you,
> Martha
>
> **From:** Dennis Hess <dennis.hess@chbe.gatech.edu>
> **Date:** Thursday, July 23, 2020 at 3:14 PM
> **To:** Michael Casiato [redacted] "Williams, Rhea" <R_Williams@acs.org>
> **Cc:** EIC Office Industrial & Engineering Chemistry Research <eic@iecr.acs.org>, Martha

Grover <martha.grover@chbe.gatech.edu>
Subject: Re: <Review> - Research misconduct

Dear Michael,

I see no reason to re-contact the other co-authors, since no substantive changes have been made to the statement, and the co-authors approved the previous statement.

Regards,
Dennis

From: Michael Casciato <[redacted]
Sent: Thursday, July 23, 2020 3:11 PM
To: Williams, Rhea <R_Williams@acs.org>
Cc: EIC Office Industrial & Engineering Chemistry Research <eic@iecr.acs.org>; Grover, Martha A <martha.grover@chbe.gatech.edu>; Hess, Dennis W <dennis.hess@chbe.gatech.edu>
Subject: Re: <Review> - Research misconduct

Dr. Williams,

I have received responses from Dr. Grover and Dr. Hess that they support these minor updates to the language, and I support them as well.

I do not see the changes you made as material or substantive, so I do not think we need to go back to all of the co-authors on these papers for their approval.

However, if you, Dr. Grover, or Dr. Hess would like me to contact them for confirmation, please let me know.

Regards,

Michael

On Wed, Jul 22, 2020 at 9:22 PM Williams, Rhea <R_Williams@acs.org> wrote:

> Dear Michael,
>
> Thank you for submitting the three retraction statements to I&EC Research.
>
> Prior to acceptance of the retraction notices, we are providing this group with an opportunity to review the three edited versions below. ACS staff and the Editor have reviewed the text for clarity and consistency with other retractions. For example, presuming all co-authors are supportive of each retraction, the individual list of names became unnecessary.
>
> Please review the three statements by no later than Monday, July 27.
>
> Sincerely,
> Rhea
>
> ie-2020-03481x
> **Retraction of "Optimization of a Carbon Dioxide-Assisted Nanoparticle Deposition Process Using Sequential Experimental Design with Adaptive Design Space"**
> dx.doi.org/10.1021/ie2028574 ***Ind. Eng. Chem. Res.*** 2012, 51, 4363–4370
> The authors retract this article following the voluntary admission of Michael J. Casciato that this article contained data that he had fabricated.
> Nanoparticle synthesis experiments were carried out, and while some of the experimental data were legitimate, a subset of the experimental data reported in this paper related to nanoparticle synthesis

were either falsified or fabricated. The modeling approaches, algorithms, and model outputs described are valid and were implemented, but they were applied to these data that were improperly manipulated. As such, the article is being retracted.
The original article was published on February 23, 2012 and retracted on [date – to be filled in by ACS production].

ie-2020-03482c
Retraction of "Synthesis of Optically Active ZnS-Carbon Nanotube Nanocomposites in Supercritical Carbon Dioxide via a Single Source Diethyldithiocarbamate Precursor"
dx.doi.org/10.1021/ie301553g ***Ind. Eng. Chem. Res.*** 2012, 51, 11710−11716
The authors retract this article following the voluntary admission of Michael J. Casciato that this article contained data that he had fabricated.
The scanning electron microscope (SEM) and X-ray diffraction (XRD) data in this paper were legitimate; however, the histogram data for particle size were falsified. The UV/Vis and photoluminescence data were fabricated. As such, the article is being retracted.
The original article was published on August 14, 2012 and retracted on [date – to be filled in by ACS production].

ie-2020-034839
Retraction of "Initial Experimental Design Methodology Incorporating Expert Conjecture, Prior Data, and Engineering Models for Deposition of Iridium Nanoparticles in Supercritical Carbon Dioxide"
dx.doi.org/10.1021/ie400996g ***Ind. Eng. Chem. Res.*** 2013, 52, 9645−9653
The authors retract this article following the voluntary admission of Michael J. Casciato that this article contained data that he had fabricated.
Synthesis experiments were conducted and some of the nanoparticle size data were estimated based on photos of nanoparticles on the substrates. Other nanoparticle size data were falsified or fabricated. The modeling approaches, algorithms, and model outputs described are valid and were implemented, but they were applied to these data that were improperly manipulated. The data related to expert opinion were collected and are legitimate. However, based on the falsified and fabricated portion of the work, the article is being retracted.
The original article was published on June 19, 2013 and retracted on [date – to be filled in by ACS production].

Rhea M. Williams, Ph.D.
Senior Managing Editor, ACS Publications Division
Global Journals Development I American Chemical Society
1155 16th St. NW I Washington, DC 20036
R_Williams@acs.org I T 202-306-3363 I http://pubs.acs.org

From: Michael Casciato [redacted]
Sent: Wednesday, July 15, 2020 2:39 PM
To: EIC Office Industrial & Engineering Chemistry Research <eic@iecr.acs.org>
Cc: Grover, Martha A <martha.grover@chbe.gatech.edu>; Hess, Dennis W <dennis.hess@chbe.gatech.edu>; Williams, Rhea <R_Williams@acs.org>
Subject: [EXT] Re: <Review> - Research misconduct

[Actual Sender is [redacted]]
Dr. Savage,

I have submitted all three of the retraction letters to the ACS Paragon Plus portal after review and approval from my co-authors.

The retraction letters were submitted as Additions/Corrections as you had requested.

The IDs for the retraction letters are:

ie-2020-03481x

ie-2020-03482c
ie-2020-034839

Please advise if there are any issues with the submissions that require my attention/correction.

Kind regards,

Michael

On Wed, Jul 8, 2020 at 4:33 PM Michael Casciato <[redacted]> wrote:

> Dr. Savage,
>
> Thank you for your feedback. I am aligned with your proposed path forward and will proceed as you suggest.
>
> I will draft letters and share with my co-authors, and once they have confirmed support I will proceed to submit them to the ACS Paragon Plus portal.
>
> I can commit to submitting all of the statements before July 31, 2020.
>
> Thank you again for your consideration with this unpleasantness, and apologies again for what I have done, as well as for generating additional work for you and your staff.
>
> Kind regards,
>
> Michael
>
> On Wed, Jul 8, 2020 at 8:44 AM EIC Office Industrial & Engineering Chemistry Research <eic@iecr.acs.org> wrote:
>
> > Dear Dr. Casciato:
> >
> > Thank you for your message of June 22 and admission of research misconduct. I appreciate the courage that is required to make that admission. Since some of the published data in the three *I&EC Research* articles are fabricated, I believe retraction of those articles is the appropriate path to take. For each article, I ask that you work with your co-authors to draft a retraction statement for each and then submit them individually as an Addition/Correction manuscript type in ACS Paragon Plus with all of the original co-authors appropriately listed on each submission. The retraction statement for each article should provide the reason for retraction (falsification or fabrication of data) and perhaps comment on how that data affects the main conclusions in the article. My office will review the text after it is submitted. Please try to submit the retraction statements by no later than July 31, 2020.
> >
> > You had mentioned a fourth article in your email message. Since there are no known ethical concerns with that article, there is no need to consider it any further.
> >
> > Sincerely,
> >
> > Phillip E Savage
> > Editor-in-Chief
> > I&EC Research
> > eic@iecr.acs.org
> >
> > **From:** Michael Casciato <[redacted]
> > **Sent:** Monday, June 29, 2020 2:44 PM
> > **To:** EIC Office Industrial & Engineering Chemistry Research <eic@iecr.acs.org>
> > **Cc:** Grover, Martha A <martha.grover@chbe.gatech.edu>; Hess, Dennis W <dennis.hess@chbe.gatech.edu>
> > **Subject:** Re: <Review> - Research misconduct

Nikki,

Thank you for your response; I will await feedback on how to proceed.

Kind regards,

Michael

On Mon, Jun 29, 2020 at 8:48 AM EIC Office Industrial & Engineering Chemistry Research <eic@iecr.acs.org> wrote:

> Dear Michael,
>
> Thank you for this information, which I have shared with the EIC and Managing Editor. We hope to get back to you with next steps soon.
>
> Sincerely,
>
> Nikki Lazenby
> for Dr Phillip Savage
> Editor-in-Chief
> I&EC Research
> eic@iecr.acs.org
>
> **From:** Michael Casciato <[redacted]>
> **Sent:** Monday, June 22, 2020 1:00 PM
> **To:** EIC Office Industrial & Engineering Chemistry Research <eic@iecr.acs.org>
> **Cc:** Grover, Martha A <martha.grover@chbe.gatech.edu>; Hess, Dennis W <dennis.hess@chbe.gatech.edu>
> **Subject:** <Review> - Research misconduct
>
> Dr. Savage,
>
> I am writing to inform you that I committed research misconduct with respect to several pieces of data in papers that I published in **Industrial Engineering & Chemistry Research (IECR)** while I was a graduate student.
>
> The papers in which I committed research misconduct were:
>
> - *Synthesis of Optically Active ZnS-Carbon Nanotube Nanocomposites in Supercritical Carbon Dioxide via a Single Source Diethyldithiocarbamate Precursor* (dx.doi.org/10.1021/ie301553g | **Ind. Eng. Chem. Res.** 2012, 51, 11710–11716)
> - *Initial Experimental Design Methodology Incorporating Expert Conjecture, Prior Data, and Engineering Models for Deposition of Iridium Nanoparticles in Supercritical Carbon Dioxide* (dx.doi.org/10.1021/ie400996g | **Ind. Eng. Chem. Res.** 2013, 52, 9645–9653)
> - *Optimization of a Carbon Dioxide-Assisted Nanoparticle Deposition Process Using Sequential Experimental Design with Adaptive Design Space* (dx.doi.org/10.1021/ie2028574 | **Ind. Eng. Chem. Res.** 2012, 51, 4363–4370)
>
> I am writing now to share this information with you, apologize for my actions, and request your guidance on how you would like to proceed with these publications.
>
> All of my co-authors on these three papers have been informed that I am contacting you with this note, and I have copied my thesis advisors as well, who have been counseling me on how to proceed as I rectify the mistakes I have made.

Please know that I committed these acts on my own. Nobody coerced me or suggested this action to me, and nobody else collaborated with me. None of my co-authors or thesis advisors were aware of this behavior.

I am coming forward now of my own volition to correct the record, borne out of a desire to fix the mistakes that I made.

I was not compelled in any way whatsoever by any other person, party, investigator or researcher, laboratory or organization, or any other body to disclose my unethical behavior. Furthermore, nobody discovered flaws, errors, or issues with the work I completed and drove me to this disclosure.

Please accept my sincere apologies for what I did, and please advise how you would like to proceed.

Summary of data in publications referenced and legitimacy of each piece of data:

- *Synthesis of Optically Active ZnS-Carbon Nanotube Nanocomposites in Supercritical Carbon Dioxide via a Single Source Diethyldithiocarbamate Precursor* (dx.doi.org/10.1021/ie301553g | **Ind. Eng. Chem. Res.** 2012, 51, 11710–11716)
  - **Figure 1**: I conducted the synthesis experiments on my experimental apparatus and I collected these data on the SEM. This figure is legitimate.
  - **Figure 2**: I conducted the synthesis experiments on my experimental apparatus and I collected these data on the TEM. This figure is legitimate.
  - **Figure 3**: I tried to get the image processing algorithm I had developed in MATLAB (and used for data reported in other publications) to work for these images, but was not successful. I eyeballed these data based on SEM photos and made up the histograms shown here. I would classify this figure as partially fabricated based on the data collected by SEM.
  - **Figure 4**: I conducted the synthesis experiments on my experimental apparatus and I collected these data on the XRD machine. This figure is legitimate.
  - **Figure 5**: I conducted the synthesis experiments on my experimental apparatus and I tried to collect these data. However, I was not successful in collecting the UV/vis data on the UV/vis machine. I made up the data to make them match up to literature reported data. I would classify this figure as fabricated based on literature data (citation 7 in the publication).
  - **Figure 6**: These data are accurate based on the data reported in Figure 5.
  - **Figure 7**: I conducted the synthesis experiments on my experimental apparatus and I tried to collect these data. However, I was not successful in collecting the photoluminescence data on the photoluminescence experimental apparatus. I made up the data to make them match up to literature reported data. I would classify this figure as fabricated based on literature data (citation 17 in the publication).
  - **Figure 8**: I generated this figure myself based on references cited.
  - **Table 2**: I calculated the values reported based on data presented in Figures 6 and 7, as described above. I would classify this table as fabricated based on the data presented in Figures 6 and 7.

- *Optimization of a Carbon Dioxide-Assisted Nanoparticle Deposition Process Using Sequential Experimental Design with Adaptive Design Space* (dx.doi.org/10.1021/ie2028574 | **Ind. Eng. Chem. Res.** 2012, 51, 4363–4370)
  - I built and ran the MATLAB programs that were required for modeling in this paper using all of the formulae, equations, and algorithms described in this work; none of those aspects of this were fabricated or falsified.

- **Figure 1**: This is just a flow diagram, but the key point I want to point out is that I built all of the MATLAB models and ran all of the algorithms myself for this paper, and I did not fabricate or falsify any of the algorithm or model outputs.
- **Table 1**: Data at 60 °C and 120 °C taken from Table 1 and Table 2 of J Nanopart Res (2012) 14:836 DOI 10.1007/s11051-012-0836-2. I can't recall precisely if I did experiments for data points at 90 °C and 150 °C (not in the *Journal of Nanoparticle Research* paper), if I adjusted data for these experiments, or if I made up data for these experiments.
- **Figure 2**: I conducted synthesis experiments to produce the silver nanoparticles deposited on the substrates described here, and I conducted the SEM analysis described for this figure.
- **Table 2**: I built and ran the algorithms and models described here in MATLAB; these are real and legitimate outputs of the model algorithm based on the data provided as described above.
- **Figure 3**: I generated this legitimate plot and algorithm/model output based off of data in Table 1 using the MATLAB program that I wrote.
- **Figure 4**: I generated this legitimate plot and algorithm/model output based off of data in Table 1 using the MATLAB program that I wrote.
- **Figure 5**: I generated this legitimate plot and algorithm/model output based off of data in Table 1 using the MATLAB program that I wrote.
- **Table 3**: I conducted synthesis experiments to produce the silver nanoparticles deposited on the substrates described here, and I conducted the SEM analysis and image analysis described for this figure. However, I also believe I made up some of these data. I do not recall precisely which were real and which were not. If I had to guess, I would say the replicates were made up. I would classify this as partially fabricated data.
- **Table 4**: I built and ran the algorithms and models described here in MATLAB; these are real and legitimate outputs of the model algorithm based on the data provided as described above.
- **Figure 6**: I generated this legitimate plot and algorithm/model output based off of data in Table 1 using the MATLAB program that I wrote.

▪ *Initial Experimental Design Methodology Incorporating Expert Conjecture, Prior Data, and Engineering Models for Deposition of Iridium Nanoparticles in Supercritical Carbon Dioxide* (dx.doi.org/10.1021/ie400996g | **Ind. Eng. Chem. Res.** 2013, 52, 9645–9653)

- I built and ran the MATLAB models using all of the formulae, equations, and algorithms described in this work; none of those aspects of this were fabricated or falsified.
- **Figure 1**: Plot was generated correctly from data cited in the *Journal of Nanoparticle Research* and IECR papers described in this document. As described in that section of this document, some of those data were real, some were adjusted, and some were made up.
- **Table 1**: These data are real and legitimate – I distributed these surveys and collected responses, and I reported the results without alteration here.
- **Table 2**: These data are real and legitimate – I distributed these surveys and collected responses, and I reported the results without alteration here.
- **Table 3**: These data are real and legitimate – I distributed these surveys and collected responses, and I reported the results without alteration here.
- **Table 4**: These data are real and legitimate – I built and ran the algorithm as described in the Methodology section, and the outputs were the results of the algorithm, reported without any alteration.

- **Table 5**: These data are real and legitimate – I built and ran the algorithm as described in the Methodology section, and the outputs were the results of the algorithm, reported without any alteration.
- **Figure 2**: I constructed this legitimate plot. It is an Arrhenius plot, and it shows the individual and unified models given the parameters that were provided in Table 4 and Table 5 from the algorithms implemented.
- **Figure 3**: I constructed this legitimate plot. I ran the algorithm and model to generate this plot. It shows the design points as a function of the tuning parameter gamma.
- **Figure 4**: I conducted the synthesis experiment to produce the iridium coated Si wafer substrate, and I conducted the image analysis on the SEM. This is a legitimate image of iridium nanoparticles as deposited on the Si wafer surface as described in the paper.
- **Table 6**: I conducted the synthesis experiment to produce the iridium coated Si wafer substrate, and I conducted the image analysis on the SEM. However, I also made up data to interpolate for some of these experiments. I do not recall precisely which were real and which were made up. I would classify this table as partially fabricated.
- **Figure 5**: I constructed this plot based off of the reported data in Table 6.
- **Figure 6**: I ran the model and algorithms that generated the L metric and confidence interval for this plot, based off of data from Table 6.

Additionally, I would point out that I am an author on one additional paper in **IECR** (**Ind. Eng. Chem. Res**. 2018, 57, 42, 13932–13939) that I worked on and published while working for Royal Dutch Shell, my current employer.

This paper does not contain any research misconduct, fabrication, or falsification, and I am fourth author on this paper.

I realize that my word does not carry value with you given the other admissions in this communication, but I did want to highlight this information to you as well for full transparency on my interactions with your journal.

If you plan to contact the co-authors on this particular paper (**Ind. Eng. Chem. Res**. 2018, 57, 42, 13932–13939), I would like to ask if you can please advise me so I can contact them first and advise on the context of this situation with both my co-authors and my managers at Shell. I have been managing this situation so far with my thesis advisors, but if you plan to contact my co-authors, I would prefer first contact be made by me.

Again, please accept my apologies for my behavior.

Thank you for your attention in this matter; I look forward to your response with guidance on how to proceed.

Regards,

Michael J. Casciato