[redacted]

Od: [redacted]
Odesláno: středa 31. března 2021 15:46
Komu: [redacted]
Kopie: [redacted]
Předmět: Outcome of Review

Dear [redacted]

Our office investigated concerns regarding the Mossbauer spectroscopy data in the following *ACS Sustainable Chemistry and Engineering* articles:

A)- Iron-Oxide-Supported Ultrasmall ZnO Nanoparticles: Applications for Transesterification, Amidation, and O-Acylation Reactions: Gade, Vilas B.; Rathi, Anuj K.; Bhalekar, Sujit B.; *et al.* ACS SUSTAINABLE CHEMISTRY & ENGINEERING Volume: 5, Issue: 4, Pages: 3314-3320. Published: APR 2017. (https://doi.org/10.1021/acssuschemeng.6b03167)

B)- Zero-Valent Iron Nanoparticles Reduce Arsenites and Arsenates to As(0) Firmly Embedded in Core-Shell Superstructure: Challenging Strategy of Arsenic Treatment under Anoxic Conditions: Tucek, Jiri; Prucek, Robert; Kolarik, Jan; *et al.* ACS SUSTAINABLE CHEMISTRY & ENGINEERING Volume: 5, Issue: 4, Pages: 3027-3038. Published: APR 2017. (https://doi.org/10.1021/acssuschemeng.6b02698)

After reviewing the original data sets, the narrative descriptions of data processing methods employed, and the data processing methods applied in the generation of journal figures, we find no evidence to support claims of data manipulation. As such, the journal will not be pursuing retraction or correction of these articles, and the journal considers the case closed.

Sincerely,

[redacted]

Executive Editor: ACS Sustainable Chemistry & Engineering

[redacted]

Od: [redacted]
Odesláno: čtvrtek 8. dubna 2021 14:31
Komu: [redacted]
Kopie: [redacted]

Předmět: [Water Research, 2016/2018, Moessbauer spectra] scientific misconduct > My evaluation

Dear [redacted] and co-authors:

I have contacted you in January 2021 regarding concerns that were raised regarding potential scientific misconduct and potential data fabrication related to your two following publications published in Water Research:

> Kolarik, J., Prucek, R., Tucek, J., Filip, J., Sharma, V.K. and Zboril, R. (2018) Impact of inorganic ions and natural organic matter on arsenates removal by ferrate(VI): Understanding a complex effect of phosphates ions. Water Research 141, 357-365. 10.1016/j.watres.2018.05.024
> Kralchevska, R.P., Prucek, R., Kolarik, J., Tucek, J., Machala, L., Filip, J., Sharma, V.K. and Zboril, R. (2016) Remarkable efficiency of phosphate removal: Ferrate(VI)-induced in situ sorption on core-shell nanoparticles. Water Research 103, 83-91. 10.1016/j.watres.2016.07.021

Meanwhile, you have provided me with the raw data and information on data treatment. And I have invited four experts on Moessbauer spectroscopy to evaluate the raw data, data treatment, and the published Moessbauer spectra.

Based on input from these expert reviewers and my own evaluation I come to the following conclusions:

1. There is no indication of scientific misconduct and no indication of data fabrication. There is no reason for Water Research to retract the two published papers.

2. The Moessbauer spectra presented in the two Water Research papers are not providing the raw data but are showing only data after data treatment using the software MossWinn. This makes it difficult for readers to judge the extent of data treatment. The application of MossWinn and the underlying statistical approach are clearly noted in the Material and Methods. The reviewers I have contacted raised significant concerns related to the data treatment. These concerns are not about scientific misconduct but about the suitability of the chosen approach. The readers of Water Research should benefit from being able to review the raw data, from the critical comments raised by the reviewers, and the responses provided by the authors. To allow for this, I have invited the reviewers to provide a "Comment" that will be published in Water Research. Once the Comment has been accepted, I will ask you, the authors, to prepare a "Reply" that will be published in Water Research back-to-back with the Comments. Comments and Replies are paper types we have in Water Research for such a situation of scientific disagreement. In the Reply it will be important for the authors to include their raw data as SI so that readers can review and can ultimately use their own judgement.

Please let me know if you have comments.

Best regards,
[redacted]
Editor-in-Chief of Water Research

[redacted]

Od: [redacted]
Odesláno: pondělí 11. ledna 2021 16:08
Komu: [redacted]
Kopie: [redacted]
Předmět: [Water Research, 2018] scientific misconduct > Your perspective

Dear [redacted]
(cc to co-authors)

I am contacting you regarding your following publication published in Water Research:

> Kolarik, J., Prucek, R., Tucek, J., Filip, J., Sharma, V.K. and Zboril, R. (2018) Impact of inorganic ions and natural organic matter on arsenates removal by ferrate(VI): Understanding a complex effect of phosphates ions. Water Research 141, 357-365. 10.1016/j.watres.2018.05.024

I have been contacted by [redacted] informing me that Palacky University Olomouc has identified a problem of scientific misconduct related to Moessbauer spectra contributing to the above mentioned publication. [redacted] is asking me to have your above mentioned publication retracted from Water Research.

Before taking action, I would like to hear your perspective on this suggested scientific misconduct and how to best proceed. Please respond to this email by January 18, 2021.

Best regards,
[redacted]
Editor-in-Chief for Water Research and Water Research X.

ooo
[redacted]
[redacted]

Hi Dr. [redacted]

Yes - I corrected it as such. The statement should read as a mistake and not misconduct.

I hope this helps.

Best wishes,
[redacted]

[redacted]

ELSEVIER
230 Park Avenue
New York, NY 10169, USA
E: [redacted]
Office:
Mobile: [redacted]

On Jun 8, 2021, at 3:19 AM, [redacted] wrote:

*** External email: use caution ***

Dear Dr. [redacted]

I have been informed about the decision that was drawn regarding the article *Hana Kmentová, Devaki Nandan, Štěpán Kment, Alberto Naldoni, ManojB.Gawande, Zdeněk Hubička, Radek Zbořil. Catal.Today 328 (2019) 111-117,* which [redacted] forwarded to me.

I really appreciate highly professional and fair investigation from Elsevier side and that all the evidences such as raw data related to the study and relevant information provided by the authors were taken into account. As I mentioned in my last email, as a [redacted], I went through the raw data and other information that I demanded from the authors and according all the evidences I moved toward the statement of authors that the mistake in the article was unintended yet regrettable mistake. Based on the retraction notice I found that Elsevier finally came to the same conclusion and according my understanding the retraction was used to correct the errors, which is the decision that I fully agree with. I also very much appreciate that you agreed to link the retraction notice with a newly published paper, in which the authors are going to present data of the overall reinvestigation study. It will be the final step to fully correct the mistake in the Catalysis Today article.

In order to close the matter at the level of the Board of Directors of the Czech Advanced Technology and Research Institute, I would like to kindly ask you to

confirm me that the retraction of the article was indeed used according to the Elsevier policy to correct the error in the publication, and thus the allegation regarding the possible scientific misconduct of the authors was dismissed.

Thank you very much,
Yours Sincerely,

[redacted]

--

[redacted]

Palacky University Olomouc | Czech Republic
Czech Advanced Technology and Research Institute

[redacted]

Od: [redacted]
Date: pá 28. 8. 2020 v 13:48
Subject: Re: Nature Comm paper retraction
To: [redacted]

Dear [redacted], dear [redacted]

Thanks for the text. I have gone through and made two minor changes. Firstly I removed the reason why data was not available - it is best just to give the necessary facts (the data is no longer available). Secondly I removed 'some' form the second sentence.

Let me know what you think - if this is ok I will run it past our internal group, and you can contact all the co-authors.

With best wishes,
[redacted]

"The authors are retracting this Article because for Supplementary Fig. 6 and related discussion on the stability of the superparamagnetic iron nanoparticles, we no longer had the raw data to comply with the data storage policy of Nature Communications. Additionally, due to very low Mössbauer effect of superparamagnetic iron nanoparticles embedded in graphene oxide matrix and related low statistical quality of raw Mössbauer data, there is uncertainty in values of Mössbauer parameters derived from Figure 2, and we, the authors, therefore wish to retract this Article."

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[redacted]

Nature Research

Heidelberger Platz 3, 14197 Berlin, Germany
T: [redacted]

nature.com/ncomms/

@NatureComms
