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Literature Perspectives on Reproducibility Issues

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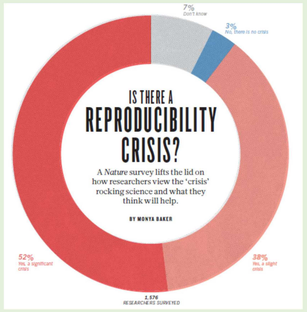
Is there a crisis?

Nature report of 1,576 Researchers surveyed in 2016

90% Indicated there was a reproducibility crisis in science

3% Said no crises

7% Didn't know



Baker, Nature 533 (2016) 452

My grant is too small, I ….

Why is this an issue now? What is new or different?

Scientists Aim To Pull Peer Review Out Of The 17th Century

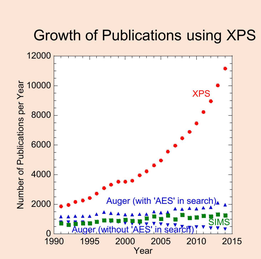
Richard Harris NPR February 24, 2018 Weekend Edition Saturday

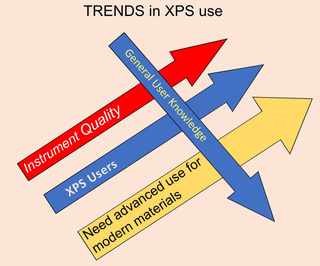
The technology that drives science forward is forever accelerating, but the same can't be said for science communication. The basic process still holds many vestiges from its early days — that is the 17th century.

- "…**peer review that is both necessary and antiquated**. The fate of that paper rests on just two or three scientists. Imagine how this would feel if the matter in question were a consumer product."
- "…pen refill reviews on Amazon are more informative that what the current peer review system offers on scientific work costing millions of dollars."
- "If the only thing Amazon ever published were reviews of the first three people who bought a product, then we'd have a very ineffective system for knowing what was good and bad," says Michael Eisen, a Howard Hughes Medical Institute (HHMI) investigator at University of California, Berkeley.

Does it impact surface analysis?

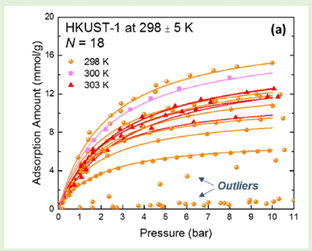
Number of XPS users increase while expertise decreases





From Cedric Powell NIST

Isotherm measurements in metal–organic frameworks (MOFs) are not very reproducible!



"In the limited examples for which enough data exist to assess the existence of outliers, approximately **20% of isotherms** in the literature were classified as **outliers."**

- Often only **one measurement** was made
- "**Error bars** are **not standard** in this field."

"Scientific progress is severely impeded if experimental measurements are not reproducible. **Materials chemistry** and related fields commonly report new materials with **limited attention paid to reproducibility."**

Jongwoo Park, Joshua D. Howe, and David S. Sholl, Chemistry of Materials 2017

Systemic drivers of non-reproducibility.

Multidisciplinary and multimethod nature of modern science
- Expertise limitations and/or lack or resources to address all critical areas and methods
- Insufficient cooperative/collaborative research

Increased complexity of systems, science questions and tools applied
- Limitations to research design
- Need for increasingly large range of analysis tools
- Large amounts of data and "black box" data analysis
- Publication, peer review, and record taking/reporting limitations
- Over reliance on "purchased" supplies without characterization or understanding

High competition for limited resources
- Grant sizes have not increased and are hard to get
- Hyper competitive research environment

Baer and Gilmore, JVSTA Nov/Dec

The 7 biggest problems facing science, according to 270 academic scientists

7 Problems and how to fix them:
- Academia has a huge money problem
- Too many studies are poorly designed
- Replicating results is crucial — and rare
- Peer review is broken
- Too much science is locked behind paywalls
- Science is poorly communicated
- Life as a young academic is incredibly stressful

Conclusion:
- Science has challenges, but is not doomed

By Julia Belluz, Brad Plumer, and Brian Resnick (2016)
https://www.vox.com/2016/7/14/12016710/science-challeges-research-funding-peer-review-process

What were they thinking?

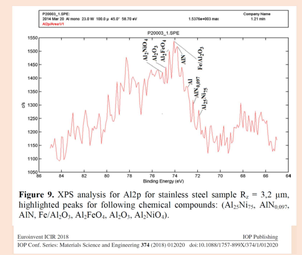
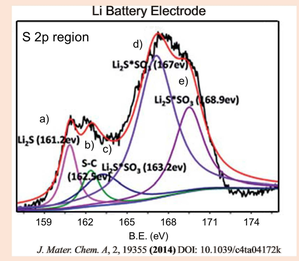


Figure 9. XPS analysis for Al2p for stainless steel sample R_z = 3,2 µm, highlighted peaks for following chemical compounds: (Al_2Ni_3, $AlN_{0.007}$, AlN, Fe/Al_2O_3, Al_2FeO_4, Al_2O_3, Al_2NiO_4).

Eurointerad ICBI 2018 — IOP Publishing
IOP Conf. Series: Materials Science and Engineering **374** (2018) 012020 doi:10.1088/1757-899X/374/1/012020



J. Mater. Chem. A, 2, 19355 **(2014)** DOI: 10.1039/c4ta04172k

C&E News Editorial: Reproducibility Issues

Richard Harris Nov 2017 C&E News [95 (2017) 2]

Conversations about the "**reproducibility crisis**" in science often focus on preclinical medical research and social psychology experiments.

Judging by the problems that drive reproducibility issues, **problems exist everywhere**.

Multiple layers of causes:
- First is that scientists put too much faith in the ingredients they use.
- Another huge area of trouble is experimental design and statistical analysis.
- A root cause is that scientists are human beings, and we tend to see what we want (or expect) to see
- Another common driver in science is the hypercompetitive world of academia.

So what's a careful scientist to do?
- First and foremost, be aware of the conditions around you that may increase the risk of irreproducible results, behavior. Also take heart. This reproducibility "crisis" isn't really a crisis at all.
- These are not new problems. We need to recognize that a problem exists before we can seek solutions.

Data - Dealing with, curating, delivery and provenance of data is a common issue

Multiple types of **data, metadata and large-data issues** and access appear in reproducibility discussions

Software often stands between the raw data and the user
- Numbers are processed and data sets are combined automatically, often with proprietary software (Sené, et al. *Nature,* 547 (2107)397-399, 2017).
- Research Data Alliance (https://www.rd-alliance.org/about-rda)

Tracking **provenance for research data** is vital to science and scholarship, important to sharing and exchanging data:
- Where did it come from? Who modified it? Is this copy the same as the copy I deposited? In what way is it the same? How do I resolve discrepancies or anomalies?
- Focuses on the comparison and evaluation of models for data provenance.
- It is concerned with questions of data origins, maintenance of identity through the data lifecycle, and how we account for data modification.

The FAIR (Findable Accessible Inter-operable & Re-useable) data management principles include not only data, but **algorithms, tools, and workflows** that led to that data. (Wilkinson *et al, Scientific Data,* 3 (2015)160018)

XPS problems recognized, solutions offered

Practical Guides for X-Ray Photoelectron Spectroscopy (XPS): Initial Questions
Submitted to JVSTA: Baer, Artyushkova, Brundle, Castle, Gaskell, Grans, Haasch, Linford, Powell, Shard, Sherwood and Smentkowski.

Over the past three decades, the use of X-ray photoelectron spectroscopy (XPS) has grown and it is now the most commonly applied method of surface analysis. XPS has become essential for many types of research, expanding from chemistry and materials science into many other areas including those associated with environmental, atmospheric, and biological systems. It was recognized about 20 years ago that, as XPS matured, the reliable use of XPS would likely be constrained by the availability of XPS experts and expertise among the many users of the technique. To a significant degree, this concern has become reality. It is clear to experienced XPS users that in many publications where XPS use is reported, the information is limited in some way and that too often the XPS data reported are incomplete or misinterpreted.

You want me to do what?

Requests to "please perform surface analysis on these samples" are common in many laboratories. When that is the only information provided, it is somewhat like getting into a taxi and asking the driver to take you someplace without saying where. Most meaningful surface analysis measurements are conducted with specific questions in mind.

Practical Guides for X-Ray Photoelectron Spectroscopy (XPS): Initial Questions

Nano-object reproducibility difficulties are increasingly recognized

From journal articles

"Common **pitfalls** in nanotechnology…,"

"The characterization **bottleneck**,"

"Discriminating the states of matter in metallic nanoparticle **transformations**: **What are we missing**?

"Core–shell nanoparticles as prodrugs: Possible cytotoxicological and biomedical **impacts of batch-to-batch inconsistencies"**

From editorials and commentaries

"The **problem** with determining atomic structure at the nanoscale,"

"**Where are we heading** in nanotechnology environmental health and safety and materials characterization?"

"Identification and avoidance of potential **artifacts and misinterpretations** in nanomaterial ecotoxicity measurements"

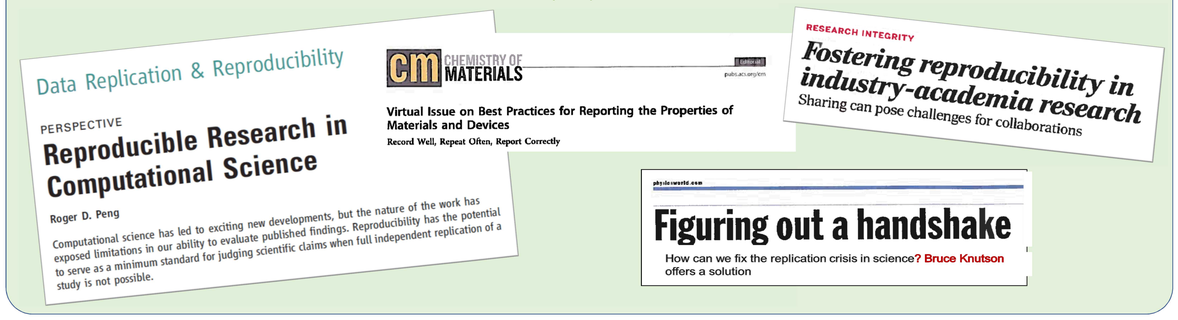
Scientific news articles

"Particle **size matters**"

"Tiny traits cause **big headaches**…."

ISO Standard 20579-4

Problems widely reported in the literature



DARPA sponsoring research into reproducibility

DARPA DEFENSE ADVANCED RESEARCH PROJECTS AGENCY

Systematizing Confidence in Open Research and Evidence (SCORE)
Dr. Adam Russell

The Scientific Paper is Obsolete: Here's what's next

James Somers, The Atlantic April 5, 2018 https://www.theatlantic.com/science/archive/2018/04/the-scientific-paper-is-obsolete/556676/ 6/5/2018

The Atlantic
The Scientific Paper Is Obsolete
Here's what's next.

THE SCIENTIFIC PAPER—the actual form of it—was one of the enabling inventions of modernity.
- Before it was developed in the 1600s, results were communicated privately in letters, ephemerally in lectures, or all at once in books.
- There was no public forum for *incremental* advances.
- By making room for reports of single experiments or minor technical advances, **journals made the chaos of science accretive.**

Papers today are longer than ever and full of jargon and symbols.
- They depend on chains of computer programs that generate data, and clean up data, and plot data, and run statistical models on data.
- These programs tend to be both so sloppily written and so central to the results that it's contributed to a replication crisis.
- Put another way, papers fail to perform their most basic task: to report what you've actually discovered, clearly enough that someone else can discover it for themselves.

Responding to the growing issue of research reproducibility

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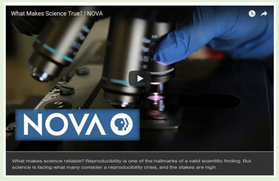
An increasing number of studies, surveys, and editorials highlight experimental and computational reproducibility and replication issues that appear to pervade most areas of modern science. This perspective examines some of the multiple and complex causes of what has been called a "reproducibility crisis," which can impact materials, interface/(bio)interphase, and vacuum sciences. Reproducibility issues are not new to science, but they are now appearing in new forms requiring innovative solutions. Drivers include the increasingly multidiscipline, multimethod nature of much advanced science, increased complexity of the problems and systems being addressed, and the large amounts and multiple types of experimental and computational data being collected and analyzed in many studies. Sustained efforts are needed to address the causes of reproducibility problems that can hinder the rate of scientific progress and lower public and political regard for science. The initial efforts of the American Vacuum Society to raise awareness of a new generation of reproducibility challenges and provide tools to help address them serve as examples of mitigating actions that can be undertaken. *Published by the AVS.* https://doi.org/10.1116/1.5049141

J. Vac. Sci. Technol. A 36(6), Nov/Dec 2018

The National Academies of SCIENCES ENGINEERING MEDICINE
BOARD ON BEHAVIORAL, COGNITIVE, AND SENSORY SCIENCES
Division of Behavioral and Social Sciences and Education

National Academies Study: Reproducibility and Replication in Science. As the result of a mandate from Congress, the National Academies will explore the issues of reproducibility and replication in scientific and engineering research. Report in 2018/2019

Watch the PBS NOVA episode on data reproducibility using the QR code below:



https://youtu.be/NGFO0kdbZmk

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