CHEMISTRY OF MATERIALS
Editorial
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Your Research Results Look Compelling, but Are They Reliable?

As we have described in an earlier issue of *Chemistry of Materials*, an experimental section that accurately captures the necessary details of your work to allow future researchers to reproduce your work is essential to the longevity of your paper.[1] If others can reproduce what you do, then your work will have a greater impact within your research area, well into the future. Irreproducible results lead to frustration, wasted resources (time, funds, materials), and questions from your peers regarding the quality of your work.

Your published work represents many months or years of time, thought, and effort. It is critical to convince future readers that the results you are presenting are reproducible, and that by following your experimental details, similar data can be obtained by a skilled worker in a safe manner. A future reader may decide that reproducing or building upon your work is too much of a risk, and hence this person may discard it—no one wants to waste time struggling to replicate published work. The ability to reproduce results is always important but becomes blatantly obvious when reporting device performance and the key material characteristics that make your paper exciting and unique. We have observed, throughout the scientific literature, a proliferation of device performance data lacking clear indication of reproducibility and statistics; if one experimental parameter is being changed within a device, can the reader truly ascertain that device 1 is better than device 2? We have also noticed important materials characterization central to the thesis of the paper presented without statistical data, such as a histogram to represent size distribution of the resulting nano/microparticle sizes, shapes, or other characteristics; is, for example, nanoparticle synthesis 1 truly producing a more monodisperse/smaller/better product than nanoparticle synthesis 2? Figure 1 shows a schematic representation of two parameters being compared—merely reporting the average values, or the best values, could be misleading if the differences are statistically insignificant. You do not want to leave the reader wondering if your reported device or materials results are, in fact, the very best of a series of ill-performing devices (also referred to as cherry picking), or if the spread of results is very large, or if only one device or sample was even made.[2] A lack of reported information, both with regards to data and experimental conditions, can only mean that any or all of these scenarios are possible and, hence, present a risk.

At *Chemistry of Materials*, in early 2014, we added some simple guidelines regarding device and materials reporting to our Information to Authors web page.[3] These guidelines are stated below, with additional explanation. In no way can we hope to cover every single scenario regarding a new material or device; instead we try to outline the spirit of what you, as authors, can do to convince your readers that your results are reproducible. Since authors will typically already have statistics and comments about materials/device reproducibility in hand at the time of writing their manuscript, we do not believe that requiring the reporting of such additional data will be an impediment to publishing. On the contrary, inclusion of this information will encourage future readers to take your work

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seriously and feel confident that they can use your results as the foundation for their own research programs.

As stated in our Information to Authors, authors are asked to include the following when writing their manuscript:

(i) The number of devices examined and the range of results. This can be conveyed in bar graphs (histograms) to represent data for a statistically meaningful number of samples or could be reported as a specific number of samples with an accompanying specified standard deviation. The journal will not accept a single result that appears to be the best obtained. It is important to emphasize typical results and the degree of variation so that reviewers and future readers can assess reproducibility, and hence the validity, of the work.[3]

For instance, in the following example, Wong and co-workers crystallized specific indene-C_{70} bisadducts and incorporated them into organic photovoltaic devices (OPVs).[4] As can be seen in Figure 2, the performance of the devices is provided with very clear statistics: the average performance metrics of 10 devices are shown, with standard deviations and an appropriate level of precision for each datum. Similar statistics should be provided for all other devices (for example, batteries, catalysts, thermoelectrics, etc). In the case when materials are very rare or difficult to obtain, a paper reports only a small number of devices; in circumstances such as these, authors should simply state the limitations and reasons and allow the readers to arrive at their own conclusions.

In the case of materials reporting, we would like to encourage similar statistical treatments. In a recent paper by Cossairt and co-workers, InP nanoparticles were prepared via two different routes, one using $P(SiMe_3)_3$ and another using a mixture of $P(SiPh_3)_3$ and $P(SiMe_3)_3$.[5] As shown in Figure 3, the authors measured over 300 nanoparticles to produce a histogram to represent the size distribution. The authors can claim, with little ambiguity, that the first method (Figure 3a) produces smaller, less disperse nanoparticles since the average size in Figure 3a is 2.6 ± 0.6 nm, whereas the second route (Figure 3b) yields an average size of 3.4 ± 1.0 nm. The representation of data in this paper reassures future readers as to the reproducibility of this work.

(ii) Sufficient experimental data to reproduce the results and enable valid comparisons with other work. Manuscripts that report devices must provide additional important characteristics beyond those above to enable comparison with

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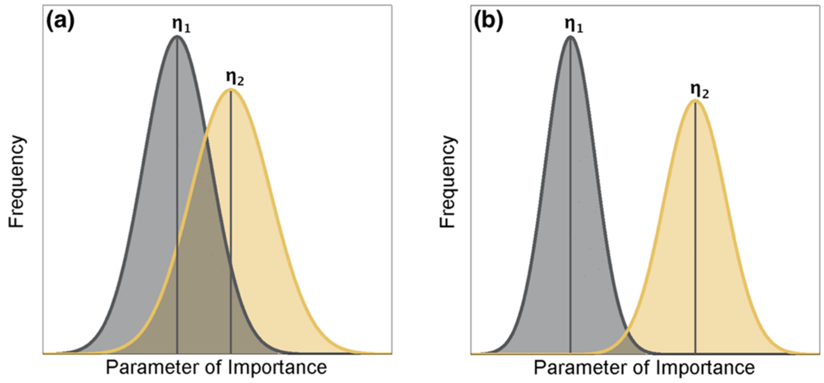


Figure 1. Is device or material 1 better than device or material 2? (a) Substantial overlap of the number of data points related to the parameter being measured (η_1 versus η_2) suggests that the two populations are not different within experimental error. Reporting only the mean (average) value would be misleading if they are not statistically distinguishable. (b) Populations of devices or materials that appear to be distinct within experimental error. Reporting of multiple devices either in tabular or histogram form is essential to support claims that your data/devices/materials are truly different. Figure adapted with permission from ref 2. Copyright 2013 American Chemical Society.

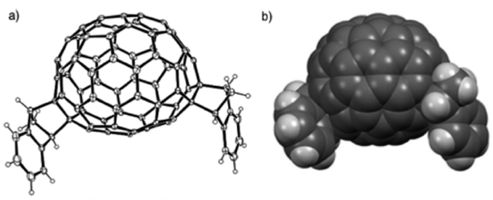


Table 1. Photovoltaic Performance of BHJ Devices Using P3HT and Various $IC_{70}BA$ Fractions in the Active Layer[a]

$IC_{70}BA$ fractions	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
mixture	0.82 ± 0.01	9.3 ± 0.3	62 ± 3	4.7 ± 0.35
1	0.80 ± 0.01	8.5 ± 0.2	56 ± 3	3.9 ± 0.20
2	0.84 ± 0.01	9.7 ± 0.4	65 ± 3	5.3 ± 0.40
±−1 (2.1)	0.86 ± 0.01	10.3 ± 0.2	67 ± 2	5.9 ± 0.25
2.2	0.84 ± 0.02	9.5 ± 0.2	60 ± 4	4.8 ± 0.30

[a]The data shown are the average values obtained from 10 devices with standard deviation.

Figure 2. Example showing helpful device statistics, in addition to the average values. The authors clearly state that the average values were calculated based upon 10 devices and that the ± values are the standard deviation, and they use an appropriate level of precision. Reproduced with permission from ref 4. Copyright 2014 American Chemical Society.

prior work by the authors or others. For example, efficiency depends on, but is not limited to, the area and architecture of a photovoltaic device; such parameters should be included in the manuscript, either in the main body or Supporting Information.[3]

A recent paper by Liu and Sun synthesized, characterized, and tested the performance of $Zn_xCo_{3-x}O_4$ nanoarrays for electrocatalytic water oxidation (oxygen evolution).[6] The authors provided a table (Table 2 in their paper, shown in Figure 4) that compared the activity of their catalyst to other published systems. We recognize that experimental conditions could be different between various groups (and even within individual papers and experiments), thus complicating a direct comparison, but some attempt to do so is valuable and very informative. Authors who describe their work in their manuscripts as "superior", "enhanced", or "improved" without providing context and comparative values and data do not do themselves a favor; future readers will not believe a claim of "superior" without substantiation.

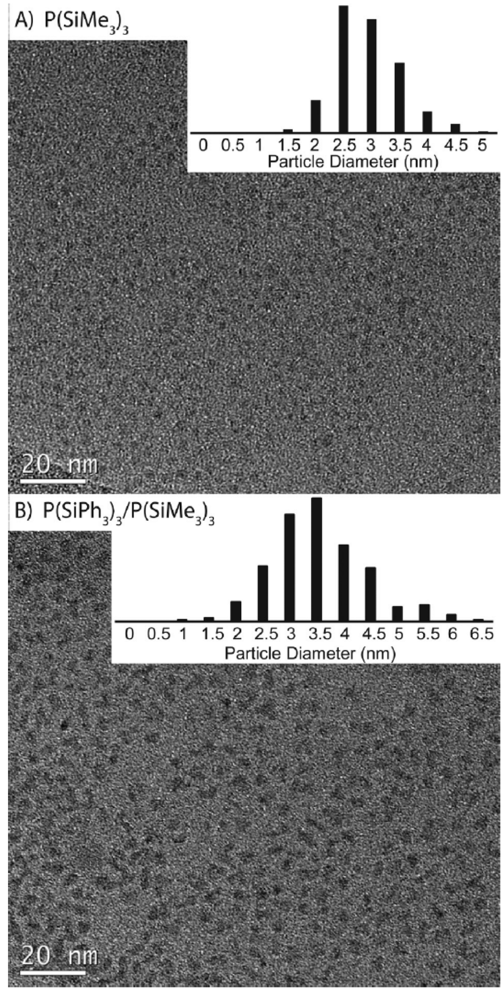


Figure 3. TEM data from ref 5. In this work, the authors compare two different experimental parameters for the synthesis of InP nanoparticles. With the histogram representation of over 300 nanoparticle sizing measurements in each, it is clear which set of conditions leads to small, less disperse nanoparticles (A is smaller and less disperse than B). Reprinted with permission from ref 5. Copyright 2014 American Chemical Society.

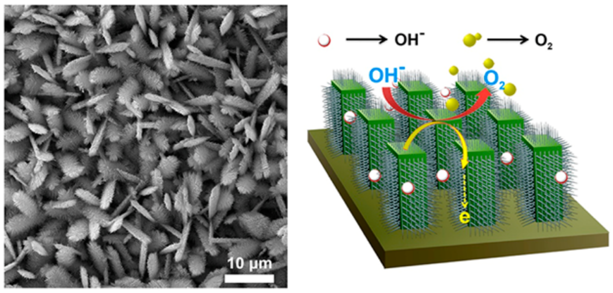


Table 2. Comparsion of OER Activities for Various Transition-Metal Oxides

type of material	overpotential (V) at I = 10 mA/cm^2	catalyst loading (mg/cm^2)	ref
nanostructured Mn(III) oxide[a]	0.54	NA	6
$Mn_3O_4/CoSe_2$[a]	0.45	~0.2	8
Co_3O_4/N-rmGO[b]	0.31	~1	16
Co-oxide[c]	0.57 (5 mA/cm^2)	NA	17
$NiFe(OH)_2$[d]	0.27 (0.5 A/cm^2, 80 °C)	NA	45
Ni–Fe oxides[e]	0.25 (0.4 A/cm^2, 40 °C)	~0.25	46
$Zn_xCo_{3-x}O_4$-3:1 RP arrays	0.32	~1	this work

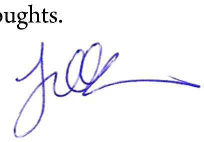
[a]Glassy carbon, 0.1 M KOH, 1600 rpm. [b]Ni foam, 1.0 M KOH. [c]Indium tin oxide, 0.1 M potassium phosphate. [d]Stainless steel mesh, 4.0 M KOH. [e]Ni foam, 1.0 M KOH.

Figure 4. Table from ref 6 that provides comparisons of the activity of the authors' oxygen evolution reaction catalysts versus others in the literature. Such a comparison provides context and helps to benchmark the field. Reprinted with permission from ref 6. Copyright 2014 American Chemical Society.

(iii) Careful attention must be given to significant figures of experimental results. The final result cannot exceed the precision of the measurement with the smallest number of significant figures.[3]

A good level of precision can be seen in the OPV data within Figure 2. The experimental variations that are convoluted within device fabrication and testing need to be considered carefully. For instance, a fill factor (FF) of 62 ± 3 seems reasonable; any number of decimal places after the 62 would be suspect. Future readers are human, and complacency or an apparent inability to determine the correct level of precision could lead to doubts about other scientific aspects of your work.

To summarize, we reiterate that this short editorial cannot cover all possible scenarios or situations. As both authors and editors, we at *Chemistry of Materials* want future readers to have confidence in the work we publish. Detailed statistical analyses may require a substantial amount of space in the main text of a paper, and so authors may wish to direct readers to the Supporting Information (SI), where detailed analyses can be thoroughly described. Through transparent reporting of the statistics, experimental details, and other parameters, authors can reassure future readers that the research described within your paper is reliable and reproducible. As always, we would like to hear your thoughts.



Jillian M. Buriak, Editor-in-Chief

AUTHOR INFORMATION

Notes

Views expressed in this editorial are those of the author and not necessarily the views of the ACS.

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