ACS Catalysis

Editorial

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Preparing Your Manuscript for Submission to *ACS Catalysis*

In 2013, after the release of our first impact factor (IF) in June, the manuscript submission rate to *ACS Catalysis* doubled, remaining at the elevated rate for the remainder of the year and climbing even higher in 2014. With this increase in submissions came a concomitant increase in the standards for acceptance, both with regard to scientific and technical quality, as well as potential for impact in the field of catalysis. Thus, while manuscript submission numbers continue to rise, acceptance rates are falling, with many papers returned immediately after an initial assessment by the editor(s), and many others declined after external peer review. Anticipating another increase in submissions this summer after the release of our second IF (7.572), we expect acceptance rates to drop even further. To this end, we summarize here some recommendations that can increase the probability of having a manuscript selected for external review and, eventually, recommended for publication in *ACS Catalysis*.

Several measures of a successful paper are that it is widely read, inspires others, and then serves as the basis for follow-up work, where it is often cited. Consequently, there are a number of factors that are important to publication in *ACS Catalysis* that simultaneously will help the published work become more broadly appreciated in the catalysis community. Several of these are described below.

The first key question is how reliable or reproducible are the results? As Jillian Buriak, Editor-in-Chief of our sister journal, *Chemistry of Materials*, pointed out in a recent editorial,[1] "irreproducible results lead to frustration, wasted resources (time, funds, materials) and questions from your peers regarding the quality of your work." Many researchers will assess whether the results described in a paper they are reading are reliable on the basis of the way the work is presented, deciding quickly whether the work is sound enough to merit follow-up work. In this regard, there are several factors that often serve as the basis for such judgments and are important to both the trustworthiness of the results and their interpretation, as well as to successful publication in *ACS Catalysis*.

DATA REPRODUCIBILITY AND APPROPRIATE STATISTICS

The essence of the Buriak editorial[1] is the importance of establishing the reliability of the work and the presentation of the results, with proper statistics, to firmly support the conclusions. How many samples were studied? How reproducible are the results? What is the experimental uncertainty of the measurements? A single outstanding sample should never be the basis for a publication. Related to this issue is the number of significant figures reported for the quantitative data. Readers will undoubtedly assess the authors' knowledge of the reliability of their data on the basis of the authors' understanding of the accuracy of the instrumentation used or the measurements made. For example, when surface areas are reported for catalysts with five significant figures (e.g., 734.87 m^2/g), a reader immediately forms an impression that the author either did not pay attention to detail, or that he or she did not understand the accuracy of the methods used.[2] Similarly, if the selectivity of a catalytic reaction is measured three times with some variability — 97.8, 94.5, 96.2% — the final selectivity reported should not have three significant digits; in this example, a value of 96 ± 2% might be reported instead. Another example often relevant to mechanistic studies of catalysis is the reproducibility of the kinetic experiments: experimentally determined rates or rate constants should be reported with standard deviations that are the result of multiple experiments. Of course, the possible involvement of mass or heat transfer effects has to be excluded when measuring these catalytic rates. Finally, the reactant conversion and product selectivity data should satisfy the material balance.

CATALYST CHARACTERIZATION

Determining the structure of a catalyst that serves as the basis for a publication is crucially important, and characterization of the structure makes up a significant component of many submissions to *ACS Catalysis*.[3] Because of the nature of the catalytic process, trace species, such as an impurity phase or rare surface sites, can sometimes dominate a catalytic process, a problem that has been recognized in catalysis for over a century.

Characterization of a multicomponent solid (heterogeneous) catalyst generally includes phase (bulk) and surface compositions, textural properties (specific surface area, pore volume, and pore size distribution), size, and dispersion of the active metal (if any). Surface-sensitive probes including (selective) chemisorption are often required to define the chemical properties of a catalytic surface.

For molecular and supported molecular catalysts, standard characterization techniques include, but are not limited to, NMR spectroscopy, X-ray structure determination (or X-ray absorption spectroscopy, in the case of nonordered materials), IR or Raman spectroscopy, mass spectrometry, and in some cases, magnetic susceptibility data. For new catalysts, elemental analysis is the only unequivocal measure of purity, and in most cases these data should be reported. If it is not possible to acquire elemental analysis data, this should be explicitly stated, and representative NMR data should be displayed in the Supporting Information. In the Experimental Section (or Supporting Information), data from NMR spectroscopy, IR spectroscopy, and mass spectrometry should not simply be listed, but rather, the data should be interpreted for the reader. For example, to the extent possible, for NMR spectroscopy data, resonances should be given specific assignments to chemical species.

For biocatalysts, the purity of the enzymes should be determined by standard techniques such as sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), Western Blot, analytical gel filtration, reversed-phase HPLC, and mass spectrometry. In addition, the identity of the enzymes produced by recombinant DNA technologies should be

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determined by DNA sequencing. In some rare situations, enzymes isolated from native hosts are used as biocatalysts. In this case, the identity of the enzymes should be determined by protein sequencing and mass spectrometry.

In the case of computational studies, methods should be accurately described in a condensed way in the main paper and in more detail in the Supporting Information (SI). There, all details (method, parameters, structural models) should be given so that others may replicate the results. The most important relaxed structures should be given in XYZ coordinates (Å) in the SI as well.

COMPARISONS TO OTHER CATALYSTS

Many papers submitted to *ACS Catalysis* provide comparisons to previously reported catalysts. In most cases, general comparisons that describe one catalyst as "better" than another should be avoided. A catalyst can have a higher rate, or better selectivity, or a longer lifetime, and such descriptive terms should be applied to specific aspects of the catalyst, rather than to a general description of the molecule or material. When providing such direct and specific comparisons, explicit indication of reaction conditions should also be provided. Although comparisons to baseline catalysts can be useful when the comparison is done in a rigorous manner, such comparisons should not serve as the sole basis or reason for publication. Comparison should also be made to the state-of-the-art catalyst for a given reaction wherever possible. When such information is included in the manuscript, reviewers, editors, and readers typically have more confidence in the authors' knowledge of the field, and they are more likely to trust the authors' work.

Given the great variability in conditions under which catalysts are tested, and the variability of measures of "good" catalysts, use of subjective descriptors by the authors (e.g., superior, outstanding, excellent, exceptional, notable, etc.) should be avoided in the general sense,[4] unless a specific feature evaluated in the paper is being considered (e.g., enhanced or improved selectivity under the conditions employed). Universal metrics that are applicable and understood widely in catalysis such as turnover frequencies (TOFs) and turnover numbers (TONs) can be useful bases for comparison. For surface-catalyzed reactions by nonmetallic materials whose active sites are ill-defined, areal catalytic rates can also be used. However, in such cases, the conditions under which the measurements were made must be reported and carefully considered. One should also remember that TOFs should be based on rate measurements involving no mass or heat transfer effects. For batch systems, this should be an initial rate based on kinetic data at low conversions, whereas for flow systems, this should be from steady-state rate measurements, ideally at low conversions. TOFs or reaction rates should never be estimated in batch systems based on a single conversion/yield point taken at long times, and if they are, they should be regarded as site-time yields, because the TOF changes as a function of conditions in batch systems, such as degree of conversion of the reactant. Similarly, in flow conditions, TOFs should be estimated in a differential reactor at low reactant conversions. Evaluation of catalyst stability cannot be made at reactant conversions approaching 100% or thermodynamic equilibrium.

The comparison of catalysts under similar and appropriate conditions is also important. In this regard, Armor wrote a useful perspective on comparisons of new catalysts to industrial benchmark catalysts nearly a decade ago.[5,6] The tenets in this document remain true today, and this short article should be required reading for all catalysis researchers.

CLARITY AND PRECISION OF LANGUAGE

Too often, strong technical work is marred by poor paper composition, especially in cases where the authors are not native English speakers. Authors should ensure that the language is not a barrier to the reader and can consult services such as the ACS Chemworx English editing service (http://es.acschemworx.acs.org/en/) in cases where access to assistance from native speakers is not possible.

SUMMARY

As an editorial team, we are excited about the rapid development of *ACS Catalysis*, and we feel privileged to serve the catalysis community as editors. We are highly appreciative of the community's recognition of *ACS Catalysis* as a publication forum of growing importance. We hope the discussion above will shed some light on the decisions we make with regard to adjudicating papers and can help authors craft highly impactful papers that are more likely to be accepted for publication in the journal.

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AUTHOR INFORMATION

Notes

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

REFERENCES

(1) Buriak, J. M. *Chem. Mater.* **2014**, *26*, 2211−2213.
(2) As an example of too many significant figures, see average pore diameter assessment in Table 1 of: Wu, F. S.; Feng, Y.; Jones, C. W. *ACS Catal.* **2014**, *4*, 1365−1375.
(3) Potential exceptions to this requirement include papers focused on new molecular catalysts for organic synthesis, where novel reactivity is the focus of the work and detailed catalyst characterization is planned at a later stage.
(4) For example, in evaluating photocatalysts with popular dye degradation tests, one must realize that an array of catalysts can behave wholly different in different tests, depending on the nature of the dye and conditions used: Bae, S. Y.; Kim, S. J.; Lee, S. H.; Choi, W. Y. *Catal. Today* **2014**, *224*, 21−28.
(5) Armor, J. N. *Appl. Catal., A* **2005**, *282*, 1−4.
(6) Although ref 5 focuses on comparisons to industrial catalysts and *ACS Catalysis* more often publishes fundamental investigations of catalysis or papers describing new reactivity, the principles of the paper are important in any catalytic context.