ACS Catalysis and the Scope of Papers Sought in Three Catalysis Subdisciplines: Biocatalysis and Enzymology, Molecular Catalysis for Organic Synthesis, and Heterogeneous Photocatalysis

As a comprehensive catalysis journal, jointly “owned” by the vast array of researchers studying molecules and materials that catalyze reactions, the scope of ACS Catalysis is understandably quite broad. In this regard, the editorial team has stated that the journal seeks the top echelon of papers in all fields of catalysis; more specifically, we seek the papers that the editors and reviewers deem to be the top 10% of papers in catalysis, as measured by innovation, impact, depth of understanding, and other key factors. Over the last century, the study of catalysis has evolved in numerous subdisciplines, each with its own expectations for papers published within its subdomain. In respecting these traditions, laid out by generations of scientists working to advance catalysis, the editors at ACS Catalysis have chosen not to write a formal description of the journal scope that applies to all areas of catalysis beyond the top 10% metric described above. Instead, periodically over the years, we have sought to define and refine the expectations for various subdisciplines in catalysis, in parallel with publication of guidelines and tips for successful publication in ACS Catalysis through editorials or perspective articles. With the steady growth of ACS Catalysis, the expectations and standards for publication have evolved, and today, a very small fraction of submitted papers are accepted for publication.

In this editorial, we seek to clarify the scope of papers that best fit the journal in three key subdisciplines of catalysis where submissions and publications are growing rapidly—(i) biocatalysis and enzymology, (ii) molecular catalysis in organic synthesis, and (iii) heterogeneous photocatalysis. The journal remains a comprehensive title, covering all areas of catalysis, and discussions clarifying the scope in other subareas may appear in future editorials.

- **BIOCATALYSIS AND ENZYMOLOGY**

Biocatalysis is broadly defined as the use of enzymes or whole cells as catalysts for synthetic chemistry. Largely because of the inherent high selectivity and mild and environmentally friendly reaction conditions, biocatalysis has been widely considered one of the three main pillars for catalytic asymmetric synthesis (e.g., metal catalysis, organocatalysis, and biocatalysis). The editors encourage submissions on a broad range of topics ranging from enzymology to biocatalyst discovery, characterization, and engineering to various practical applications, with an emphasis on the fundamental and molecular level understanding of the catalytic processes.

- **Enzymology**. The journal seeks submissions reporting mechanistic studies of enzyme catalysis using either experimental or computational approaches. These studies belong to the traditional field of enzymology and have been commonly communicated in biochemistry or biophysics journals. However, in cases where the enzymes investigated have either demonstrated or potential application as biocatalysts in practical processes of synthetic utility, submissions to ACS Catalysis are strongly encouraged. It should be noted that for computational enzymology investigations, results from computer simulations should generally be supported by experimental data.

- **Development of Biocatalysts or Biocatalytic Processes**. The journal also seeks submissions reporting the discovery, characterization, and engineering of enzymes and their applications. New methodologies, both experimental and computational, for generating enzymes with new or improved properties are encouraged. Examples include but are not limited to directed evolution, rational/semirational design, computational protein design, and enzyme immobilization. Because the focus of the journal is on catalysis, it is important to report the catalytic performance of the naturally occurring or engineered enzymes in terms of catalytic efficiency under kinetically relevant conditions, selectivity (stereo-, chemo-, and regio-), stability, and substrate specificity. Examples of practical applications include but are not limited to synthesis of small molecules, polymers, and biological macromolecules (e.g., peptides, proteins, and nucleic acids), biofuel cells, biosensors, biodegradation, and bio remediation.

The journal is also interested in submissions reporting cascade catalytic systems involving multiple enzymes. Of particular interest are those submissions reporting hybrid catalytic systems combining biocatalysts with nonbiological catalysts such as metal catalysts, organocatalysts and photocatalysts, as a few examples. Often these hybrid catalytic processes are conducted in one-pot, or a single reaction vessel, to explore the potential synergies or interference among the different types of catalysts, possibly simplifying catalytic processing. We encourage authors to include information on the kinetic aspects of the cascade reaction.

Submissions reporting whole-cell based biocatalysis are also encouraged. However, the focus should be on catalysis rather than the engineering of the cells. The latter may be more appropriate for journals in the areas of metabolic engineering and synthetic biology.

Finally, we encourage submissions reporting the generation of artificial enzymes based on either proteins or nucleic acids. Particularly, we are interested in artificial enzymes with unusual activity. Manuscripts reporting either methodology development, mechanistic studies, or applications will be considered.

- **MOLECULAR CATALYSIS IN ORGANIC SYNTHESIS**

ACS Catalysis seeks to publish contributions that convey impactful new fundamental discoveries, which can include the development of new catalysts and synthetic methods, elucidation of catalytic mechanisms, utilization of new methods for the preparation of known molecules, development of

Published: July 1, 2016
catalysts to prepare new classes of compounds, as well as improvements of synthetic methods (e.g., enhanced selectivity, improved yields, etc.).

**Development of Catalysts or Catalytic Processes.** We encourage submissions on the development of new catalysts, which includes ligand design for metal-based catalysts and conceptually novel catalysis and catalytic systems that enable new reactivity and/or selectivity for executing organic transformations. Because the performance and potential of new catalysts are often evaluated in a known reaction manifold, it is important to demonstrate meaningful advantages over previously reported catalysts and processes in terms of the nature of the catalysts, efficiency, selectivity (chemo-, regio-, and stereo-), and substrate scope.

**Reaction Discovery and Development.** Submissions on the development of new catalytic transformations are encouraged. This encompasses catalyst-controlled unprecedented modes of bond connection or cleavage that find potential synthetic utility. While the ultimate usefulness of new processes can be difficult to gauge, there should be some indication of potential impact. While it is important to demonstrate substrate scope, this can be balanced with the inherent novelty of the reaction. We also appreciate contributions that exemplify the strategic use of known catalysts or catalytic systems for delivering a viable solution to challenging synthetic problems such as an intrinsically difficult bond construction or a hitherto unattainable selectivity.

**Mechanistic Studies.** The journal also covers research focused on mechanistic understanding of catalytic reactions. A criterion to be fulfilled is to provide new insight into how catalytic reactions proceed while providing rationale for the observed reactivity and selectivity. This approach can be bolstered by computational analysis with a set of reliable complementary experimental data, and the importance of the elucidation can be assessed by its general implications.

**Catalytic Rates and TOFs.** In heterogeneous catalysis and in molecular catalysis papers that address molecules produced on a large scale, characterization of catalytic performance with rates such as turnover frequencies (TOFs) under kinetically controlled conditions is expected, whereas solely describing the catalyst performance with product yields at extended times is inappropriate. In contrast, for papers addressing synthesis of high value products, such as those typically explored in the organic chemistry community, characterization of catalyst performance with reaction rates is less important, and the traditional metrics used in this community—catalyst loading, reaction time, and product yield—are most important.

We anticipate that the appropriate combination of these elements will strengthen manuscripts. On the other hand, we are reluctant to consider papers that describe the extension of substrate scope of already reported catalysts or catalytic systems, unless such extension is likely to be broad in impact. Likewise, descriptions of applications of known catalytic reactions to the synthesis of specific and limited classes of organic molecules are discouraged, unless there are significant new insights relevant to catalysis or the process developed represents a novel route to access the given molecular architecture of high value. Similarly, subjective descriptions of new catalysts or pathways as “green” are inappropriate justification for publication unless substantial discussion and analysis of this aspect is also included. Manuscripts that primarily describe substrate expansion based on previously published studies or a straightforward extension of a known reaction to related substrates/functionality, without presenting new mechanistic insights, will likely be declined without external peer review.

Finally, we underscore the importance of characterization data. The experimental procedures should be precisely described such that other researchers are able to reproduce the results. In addition, all new compounds, including substrates, products of catalytic reactions and catalysts, should be fully characterized on the basis of standard techniques. In particular, new compounds should be characterized by a reasonable combination of elemental analysis (which should be routinely acquired and reported for new compounds), NMR spectroscopy, mass spectrometry, as well as other data (e.g., HPLC traces, UV–vis, IR spectroscopy). To the extent possible, resonances from NMR data should be assigned to a specific chemical functionality.

Computational-only studies that elucidate new knowledge are welcome, as long as they are sufficiently tied to experimental results to lend credibility to the results of the computational modeling. These computational studies should provide trends and catalytic insights, not only numerical results on a specific system. Computational methods should be described, either in the article or the Supporting Information, with sufficient detail to allow reproduction of the results. If the full details of the computations are in the Supporting Information, a very short description giving the essential aspects should still be included in the article. The coordinates of all calculated structures should be given as Supporting Information (preferably as a single file in xyz format).

### HETEROGENEOUS PHOTOCATALYSIS

Photocatalysis is one of the most appealing application-driven research fields in catalysis, as it represents a sustainable strategy for carrying out chemical transformations. Broadly speaking, the term photocatalysis implies that a chemical catalytic transformation is driven by a light flux on a photocatalyst. Photocatalysis plays a central role in many important technologies, including sustainable energy conversion (e.g., the production of solar fuels), environmental pollution abatement, as well as the synthesis of useful molecules. As in other areas of catalysis, the journal seeks to publish cutting-edge scientific advances in photocatalysis, with the judgment of suitability for the journal taking into account the relevance, the novelty, and the quality of the presentation of the work.

**Water Splitting and Carbon Dioxide Upgrading.** The journal seeks papers reporting critical advancements in the photocatalysis of water splitting and carbon dioxide reduction using UV–visible light. This includes papers studying the half-reactions associated with these two photocatalytic conversion processes.

**Environmental Photocatalysis.** The field of environmental applications of photocatalysts, such as removal of water or air contaminants, has enjoyed a very prolific decade of research, contributing to the fast rate of development of new systems in this field. The number of catalysts reported annually in this research area is so high that meeting the novelty and impact of criteria of ACS Catalysis has become challenging in recent years. Manuscripts that are unable to clearly describe a breakthrough that significantly advances the state-of-the-art will likely be declined without external peer review.

**Photocatalytic Synthesis.** Synthesis of relevant molecules, for example, in medicinal or pharmaceutical research, represents a core area of importance in catalytic chemistry.
Advances in synthetic photocatalysis, such as replacing standard conditions for carrying out reactions (e.g., high-temperature reactions) with milder or more sustainable photocatalytic protocols, is an area of great interest to the journal.

Photocatalysis Studies Using Probe Molecule Degradation. The field of photocatalysis has witnessed significant increases in the number of published papers reporting claims of new photocatalytic phenomena using test reactions involving photocatalytic decomposition of probe molecules. Because the results from these reactions can often not be compared across different types of catalysts or different reaction conditions, these test reactions are increasingly viewed as being of limited fundamental value. To this end, ACS Catalysis typically only considers these papers in cases where the authors have made clear that new fundamental phenomena are reported.

Standardization of Reporting Data. One of the important shortcomings currently plaguing the field of heterogeneous photocatalysis is a lack of uniformity in reporting activities or other essential parameters. ACS Catalysis is committed to using consistent metrics for the evaluation of photocatalysts. Many papers generally refer to “high” or “superior efficiency” for a photocatalyst without providing a detailed description of the conditions or the experimental setups, creating reader confusion or misleading comparisons. Given the large diversity of the investigated materials, which are becoming more complex and sophisticated with each passing year, finding a unique set of parameters for evaluation of all catalysts is very difficult. However, efforts should be made to harmonize data by following general guidelines that set the route to a correct performance assessment of the specific photocatalyst. Beyond full material characterization, including catalyst textual properties, knowledge of essential information such as (i) the catalyst loading, (ii) catalyst stability and reaction reproducibility, (iii) wavelength of irradiation (or range of wavelengths), (iv) power of irradiation, (v) substrate concentration, (vi) nature and concentration of any sacrificial donor used, and (vii) apparent quantum efficiency should inevitably be mentioned. Moreover, the catalyst testing apparatus should be clearly described.

Authors should seek to comprehensively characterize their results such that misleading claims are not made. For instance, papers purportedly describing photocatalysis by titania catalysts often make use of an essential cocatalyst (e.g., platinum), which is often not clearly indicated in the discussion. Also, if a new “superior” material is reported, it should have clear advantages with respect to state-of-the-art materials in terms of the photocatalytic performance or some other metric (a commonly cited example is cost). However, if cost is the target, then the authors need to clearly describe the context in which a poorer performing but less costly material can be more useful than a better performing material. For example, if a material shows a considerably poorer performance compared to a very expensive state-of-the-art material (e.g., platinum), then a significantly larger amount of that material (and therefore larger reactors) is required to achieve equivalent performance. This can add significant cost to the process even if the catalyst is cheaper; thus, in general, it is difficult to make a definitive case that the low cost material is a significant practical advance. Nonetheless, this specific example does not preclude the importance of fundamental scientific insights about the low-cost or earth-abundant material that might make the study well-suited for publication in the journal. As in all areas of catalysis, for publication in ACS Catalysis, comparison to the state-of-the-art catalyst(s) for the given reaction is critical, while comparisons to a poorly performing material are not usually relevant.

Some helpful recommendations were recently given by IUPAC, where many of the problems related to reporting of photocatalytic performance were carefully addressed, and the definitions of important concepts such as photonic yield, quantum yield, turnover frequencies, and turnover numbers have been clearly described. The authors of new work in photocatalysis are strongly encouraged to consult this useful reference.

Closing Thoughts

As noted above, the editorial team of ACS Catalysis believes that the journal is jointly “owned” by the global catalysis community. Together, as editors, authors, and reviewers, we act as stewards for the journal, upholding the expectation of excellence in catalysis research as the key criterion for publication in the journal. Given this shared vision for the journal, we are understandably unable to consider all submissions for publication, and, as a result, a significant fraction of submissions are declined after editorial review. Focusing on the top 10% of papers in catalysis, the journal seeks contributions in all areas while concentrating on primarily publishing manuscripts that offer fundamental, molecular-level insights into a catalytic process, new catalytic processes, or substantially improved catalytic performance over the state-of-the-art. It is our hope that the discipline specific discussions of scope will help authors and reviewers understand what types of contributions are most likely to be accepted in the journal, providing useful guidance on the preparation and review of papers for the journal.

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