

## Best Practices for Reporting on Heterogeneous Photocatalysis

Heterogeneous photocatalysis is of broad interest in materials chemistry and materials science, particularly with the rapid growth of research attention being directed toward energy-related applications, pollution mitigation, and other related areas of environmental impact.<sup>1</sup> A literature survey reveals more than 9000 papers with the word photocatalyst or photocatalysis in the title published during the last ten years (Source: Web of Science, July 3, 2014), with the number of papers published each year increasing significantly since 2005. The materials and physical chemistry journals of the American Chemical Society receive a significant number of papers in the area of photocatalysis.

As editors of *Chemistry of Materials*, *ACS Applied Materials & Interfaces*, and *The Journal of Physical Chemistry Letters*, we have written this Editorial to draw the attention of authors, reviewers, and readers to the importance of uniform guidelines for the analysis and characterization of new and modified heterogeneous photocatalyst materials. These best practices for photocatalysis characterization and efficiency reporting are not new to the photocatalyst community; indeed, they have been repeatedly discussed within the research community over many years.<sup>2–5</sup> Nonetheless, we as editors continue to receive papers for consideration that report on poorly characterized photocatalysts and make exaggerated claims, such as "highly efficient," "superior efficiency," or "improved efficiency," without properly disclosing the conditions and experimental procedures used to characterize the catalyst materials and determine the photocatalytic efficiencies. As a result, the major conclusions of the papers are oftentimes not supported by the experimental results, and comparisons with prior literature near impossible, which raises suspicions that the paper may be unreliable. These papers may suffer the consequence of poor review, or worse, being declined without external review.

The challenge in attempting to provide a list of requirements for publication of a new or modified photocatalyst is that the diversity of materials is high, and thus delineating a one-size-fits-all template is not realistic. We hope, however, to outline the essentials that could serve as a starting point for any paper that describes photocatalytic performance. At a minimum, the following points should be addressed by each paper that discloses the performance of new or modified photocatalyst materials:

**Photocatalyst Characterization.** New (nano)materials should be properly and fully characterized, including X-ray diffraction analysis, electron microscopy, X-ray photoelectron spectroscopy, effective surface area determination (BET measurements), light absorption characteristics (including diffuse reflectance spectroscopy, or if soluble or in thin-film form, UV–visible spectroscopy), and other techniques that may be relevant to the material(s) in question. If recording an emission spectrum, it is important to identify the origin of emission by taking an accompanying excitation spectrum. (Caution: Organic impurities often contribute to blue emission under UV excitation.)

**Reporting of Photocatalytic Efficiencies.** The conditions under which the efficiency of a photocatalyst is determined must be carefully and thoroughly defined including the following: Catalyst loading (or area and thickness if a film), the source and wavelength of light used for illumination (if monochromatic), or the wavelength distribution of light (if broadband), the optical irradiance at the sample ( $\text{mW cm}^{-2}$ ) or total optical power impinging on the sample if liquid ( $\text{mW mL}^{-1}$ ), and the substrate concentration. Studies should also include measurement of the apparent quantum efficiency,<sup>3,6</sup> defined as

$$\varphi_x = \frac{\mp(d[x]dt)}{d[h\nu]_{\text{inc}}/dt}$$

where  $d[x]/dt$  is the rate of change of the concentration of the reactant (or product) and  $d[h\nu]_{\text{inc}}/dt$  is the total optical power impinging on the sample. Note that the apparent quantum efficiency does not take into account the fraction of light absorbed by the photocatalyst, and therefore is in fact a lower limit on the true quantum yield. Statistics and error analysis should be included in any quantitative study to provide insight into the spread of experimental error to ensure that sample-to-sample differences are not, in fact, greater than claimed improvements observed between the materials being compared. Because authors are not limited with respect to the size of the Supporting Information, photographs of experimental apparatus, light profiles, and other helpful pieces of information would be valuable to future readers.

Where photoelectrochemical experiments are carried out, authors should report whether the experiments involved a three-electrode or two-electrode configuration (half-cell or full-cell, respectively), the bias potential, and for three-cell configuration, the reference electrode used.<sup>7</sup>

**Product Analysis and Reaction Mechanism.** Where a defined reaction is studied, analytical data for the amount of reactant used (e.g., for dye decomposition, or hole/electron scavengers) and/or product formed (e.g., hydrogen or oxygen) should be included. Efforts should be made to establish the photocatalytic degradation mechanism. Dyes such as methylene blue and Rhodamine B undergo irreversible transformation in visible light via a variety of different mechanisms.<sup>8</sup> These include OH radical induced oxidation, photosensitized degradation, photoinduced electron transfer with other coexisting species in the medium, and singlet oxygen generation. Comparison of dye degradation rate alone is not enough to point out the superiority of the photocatalyst. Comparing the photocatalytic activity with standards such as phenols should be useful.

**Sacrificial Donors.** The claims of efficiency enhancements made in the presence of sacrificial donors need to be assessed carefully. While sacrificial donors such as sulfide/polysulfide, EDTA, triethylamine, or methanol provide stability to the semiconductor system by scavenging photogenerated holes,

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they can also boost the photocatalytic efficiency.<sup>9</sup> Some of these sacrificial donors change the pH of the medium, thus introducing an additional variable to the experiment. The contribution of the sacrificial donor in the photocatalytic scheme needs to be carefully assessed and discussed in the manuscript.

**Catalyst Reproducibility and Stability.** These issues should also be addressed by including appropriate data regarding repeatability, reusability, and stability of the catalyst material. Inclusion of data showing reproducibility of the experimental procedures will alleviate concerns of “cherry picking” of the best results from a myriad of mixed results. Good practice should also include characterization (e.g., electron microscopy, X-ray diffraction) of the catalyst after use.

We hope that by asking our authors to address these issues in their papers, the photocatalyst and broader materials community will benefit by the improved standards for reporting materials and photocatalyst data.

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### Notes

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

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