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Editorial

Expectations for Manuscripts on Catalysis in *ACS Sustainable Chemistry & Engineering*

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ACS Sustainable Chemistry & Engineering (*ACS SCE*) reports and promotes innovation and advances in sustainable chemistry and engineering. The disciplines of sustainable chemistry and engineering are rapidly evolving, and consequently, so are our expectations for manuscripts to be published in *ACS SCE*. To help and guide authors in understanding these changes, this Editorial seeks to define the scope and standard for manuscripts reporting advances in catalysis and catalytic processes that promote resource-efficient conversion of various types of feedstocks to desired products. At the core of sustainable chemistry and engineering is the development of catalytic processes that conserve material and energy resources, minimize adverse environmental footprints, including greenhouse gas emissions, and avoid the reliance on toxic and hazardous compounds. This involves manipulating the structure and composition of catalysts, possibly with atomic precision, leading to enhanced efficiency in their functions.

Global chemical industry sales exceeded US$5 trillion in 2017 and is projected to double by 2030.[1] A majority of this growth will occur in developing nations such as China, India, and regions such as South America. The economies of these populous regions are expanding, driven by the increased affordability of everyday items, such as shampoos, diapers, synthetic clothing, and plastic containers. Meeting this growing demand will require new chemical manufacturing facilities. Future ecological burdens will worsen if today's energy-intensive chemical technologies continue to be deployed, especially if fossil-based resources are required for feedstock and energy. Such inefficiencies also pervade the specialty chemicals and pharmaceuticals industries, although their environmental footprint is much smaller relative to the commodity chemical sector because of lower production volumes. Nonetheless, all chemical industry sectors have embraced sustainability as being key to a successful business strategy.[2] In order to promote sustainability and a circular economy, new catalysts and catalytic processes are on demand to produce chemicals from not only conventional but also emerging feedstocks such as renewable biomass and CO_2, as well as waste streams such as those containing plastics and precious metals that must be recovered and recycled. New chemistries and chemical pathways are often needed for converting these often complex and recalcitrant feedstocks to make either drop-in replacements for petrochemical products or new products with unique functional properties, such as bioprivileged molecules.[3] Catalysis is playing a major role in addressing these challenges. New catalysts and alternate bench-scale technology concepts are being reported for making many commodity chemicals such as ammonia and plastic precursors with reduced environmental impact. *ACS SCE* will continue to publish advances in both fundamental as well as engineering aspects of such sustainable chemical processes. In this Editorial, we specifically outline guidelines and expectations for manuscripts submitted to *ACS SCE* in these rapidly developing areas.

ACS SCE welcomes manuscripts in catalysis that address grand challenges of sustainability in the chemical industry. Manuscripts that report (a) new or improved catalytic processes with a clear sustainability merit, characterized by significant enhancements in rates and yields compared to conventional processes, and (b) new catalysts and/or chemical routes for transforming emerging feedstocks such as biomass, CO_2, and waste streams to valuable chemicals or chemical precursors are particularly welcome. In such examples, clear rationale justifying that the feedstocks are indeed sustainable, preferably using metrics or quantitative arguments, are expected. Homogeneous and heterogeneous catalysts and their associated processes, including metal-based organo-catalysts or biocatalysts, fall within the journal's scope. Catalysts that harness the unique properties of nanostructured materials, two-dimensional materials, and ordered porous materials to promote selective conversions are highly encouraged. Activity and selectivity measures should be reported and compared to benchmarks. Catalyst characterization should be provided to establish preservation of the physical structure (such as pore volume, surface area, pore size, and enzyme/whole cell structure), elemental composition, and structure of the active site in order to demonstrate catalyst stability. The evaluation of catalyst activity and stability should be demonstrated by kinetic (time-resolved) studies and tolerance to feed impurities, not merely by isolated yields obtained by repeated runs.[4] Catalyst recycle runs to show stability are preferably performed at finite conversions, complemented by rigorous measurements of end product purity and effects of feed impurity levels in the case of biocatalysts. In all cases, considerations for the sourcing of the

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catalysts, in particular, the reliance on rare, toxic, and/or expensive starting materials, should be addressed. Biocatalyst attributes such as cofactor regeneration and downstream processing for recycling excess substrate and/or cosubstrate should also be considered.

Engineering approaches that promote sustainability such as multifunctional catalytic reactors that combine reaction and separation, novel reactor designs for process intensification, such as microreactors and mechanochemical reactors, and modular reactors for handling distributed feedstocks are also within scope and welcomed. Novel refinery schemes to handle complex feedstocks, such as biomass and waste streams, that demonstrate holistic approaches that fully utilize the feedstocks are welcome. Both chemocatalysis and biocatalysis approaches, or appropriate combinations thereof, complemented by mass and energy balances are encouraged. Authors are also encouraged to use quantitative metrics, such as technoeconomic analysis and life cycle analysis, to characterize improvements in sustainability made possible by their research. While we realize that the use of quantitative metrics is not possible or necessary in all cases, we continue to encourage authors to make these assessments to strengthen their manuscripts.[5] We also recognize that in certain emerging catalytic processes with new materials (such as photo/electrocatalytic CO_2 reduction on nanostructures), benchmarking or comparison with established processes may not be possible.

We also welcome Features and Perspectives that report significant advances and opportunities in emerging or rapidly evolving topics in sustainable catalysis and catalytic technologies. Rather than merely reporting research advances, such manuscripts should clearly discuss potential sustainability advantages of the reviewed topic, as well as the fundamental and practical challenges that must be addressed for timely implementation.

We discourage manuscripts that (a) report incremental improvements in catalyst performance compared to existing literature and processes, (b) present results without clear evidence that the intrinsic catalyst activity data were obtained under kinetically controlled conditions eliminating mass transfer limitations, (c) do not clearly discuss the sustainability attributes, either qualitatively or quantitatively, for both the catalyst synthesis itself and the catalytic process studied, and (d) report only computational chemistry work (such as quantum chemical calculations of electronic structures of molecules and chemical dynamics) without validation from complementary experiments, either within the work or other publications. Such manuscripts will not be sent out for review. As described in a previous Editorial,[6] catalysis that deals with remediation of either aqueous or air-borne pollutants is deemed out of scope. Multistep catalytic synthesis with poor overall yield also will not be considered for publication either, even if benign materials are used. In a similar vein, and while we acknowledge the need for research on Earth-abundant catalytic materials, only contributions reporting appreciable activity without expensive and/or unsustainable ligands are of interest. Finally, when using model compounds during catalyst development, clear justification and discussion should be provided regarding their suitability as a proxy for real feedstocks.

Future Editorials will address the evolving scope and expectations for manuscripts in other topical areas covered by *ACS SCE*. Our intention is that the topically specific discussions of scope will help *ACS Sustainable Chemistry & Engineering* authors and reviewers understand the types of research contributions that are most likely to be sent for external review and accepted in the journal.

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Notes

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