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Aims and scope

Molecular Catalysis publishes full papers that are original, rigorous, and scholarly contributions examining the molecular and atomic aspects of catalytic activation and reaction mechanisms. The fields covered are:

1. Heterogeneous catalysis including immobilized molecular catalysts

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2. Homogeneous catalysis including organocatalysis, organometallic catalysis and biocatalysis
3. Photo- and electrochemistry
4. Theoretical aspects of catalysis analyzed by computational methods

Manuscripts submitted to *Molecular Catalysis* ideally fall into the field of chemical synthesis, i.e. the preparation of chemical compounds used as pharmaceutical building blocks, fine chemicals, commodity chemicals or as bulk chemicals (or as precursors for them). Manuscripts dealing with non-synthetic topics such as degradation reactions (e.g. photocatalysis for the degradation of dyes/pollutants), (bio)sensors or fuel cells will not be considered for publication in *Molecular Catalysis*.

Contributions that do not fall within the above aims and scope will be rejected at the editorial level.

Examples are papers that are limited to:

1. Routine preparation and characterization of catalytic materials
2. Routine synthetic organic applications of catalysis
3. Routine computational studies that merely reproduces experimental data

Since the scopes of the Elsevier journals *Molecular Catalysis*, *Applied Catalysis A: General*, *Applied Catalysis B: Environmental*, and *Catalysis Communications* are complementary, an appropriate submission to each journal could be borderline, in which case the advice of another Editor will be sought, possibly redirecting the submission to either *Applied Catalysis A: General*, *Applied Catalysis B: Environmental*, or *Catalysis Communications* (for letters) with the author(s)'s agreement.

Molecular Catalysis publishes regularly full papers; special issues on well-defined topics are published only by invitation. However, proposal from authors are welcome anytime and enquiries regarding the submission of special issues should be directed to the Editors. Any special issue should contain at least 30 articles featuring work from leading experts in the area and/or from leading institutes.

Review and Perspective articles are normally published by invitation.

Perspectives are short articles covering current areas of interest for molecular catalysis audience in the form of personal accounts. The length of a published perspective ranges from 1500 to 2000 words (excluding figures, structures, photographs, schemes, tables, etc.) with at least 20 or more references.

A new article format called "Ongoing Story" will focus on a still open molecular catalysis research showing the developments in the understanding by a specialist area. The length of a published "Ongoing story" ranges from 500 to 1000 words (excluding figures, structures, photographs, schemes, tables, etc.)

Guidelines for catalyst characterization and reporting experimental results:

Every manuscript published in Molecular Catalysis has to provide sufficient experimental detail to reproduce the experiments and calculations reported. Also, the identity of the products (especially if a new product is synthesized) has to be established together with the yield and its purity.

Catalyst characterization: To establish the identity of new catalysts a precise synthesis and purification procedure is inevitable as well as sufficient spectroscopic (e.g. UV-Vis, NMR etc.), crystallographic and chromatographic identification (ideally placed into the supporting information).

In case of enzyme catalysts, a detailed description and documentation (e.g. SDS-gels etc) of the enzyme preparation (such as expression system, induction, fermentation conditions, downstream processing and enzyme purification) has to be provided.

Catalyst activity assays have to be described in detail (including reagents, assay conditions and activity calculations).

Reaction conditions: A detailed description of the reaction conditions comprises: solvent composition (if appropriate buffer strength, pH etc.), reaction temperature, pressure, shaking- or stirring etc. Whereas possible, the concentrations of all reagents must be given in molar concentrations. This applies in particular to time courses shown in the manuscript. Authors should refrain from showing %-conversions but rather show molar concentrations of products and starting materials. To evaluate the efficiency of a catalyst, turnover numbers and turnover frequencies (together with the conditions and equations for their calculation) should be included in the manuscript text.

Statements on efficiency and/or environmental benignity: In general, authors should refrain from claims of 'efficiency' and/or environmental benignity ('greenness') unless these claims are substantiated by a quantitative comparison with a method of the state-of-the-art. Manuscripts using such terms excessively without quantitative justification will not be considered for publication.

Plagiarism: All manuscripts submitted to Molecular Catalysis are routinely screened with respect to originality of concept, content, and writing. It is not appropriate for an author to reuse wording from publicly available sources (including the authors' own publications) no matter if cited (or not). Manuscripts with a plagiarism level (similarity index) above 10%, including self-plagiarism will be automatically rejected at Editorial level.



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