Chem Catalysis checklists

Revision 1.0, Last updated: June 21, 2021

» *Chem Catalysis* has compiled these checklists to foster improved rigor and reproducibility in research and increased clarity and transparency in data reporting.
» Authors are encouraged to include the completed checklists as supplemental information at the time of submission. The checklists will be included in the supplemental information of published articles.
» Rather than check off all items on the list, authors should mark only those items that apply to their article.

The following checklists are relevant for this manuscript:

- ☒ **Homogeneous catalysis checklist**
- ☐ **Heterogeneous catalysis checklist**
- ☐ **Biocatalysis checklist**
- ☐ **Electrochemistry checklist**
- ☐ **Photocatalysis checklist**

Homogeneous catalysis checklist

Revision 1.0, Last updated: June 29, 2021

Catalyst synthesis

- [ ] Novel methods are provided in full detail
- [ ] Comprehensive literature references are included to allow reproducibility

Catalyst characterization

- [ ] Elemental analysis
- [ ] NMR spectroscopy
- [ ] High-resolution mass spectrometry (HRMS)
- [ ] Infrared spectroscopy
- [ ] Crystallography
- [ ] Other
- [ ] The data are available in a repository

Catalyzed reaction

- [ ] Reaction conditions and complete experimental procedure
- [ ] Type of reactor (e.g., batch, semi-batch, continuous)
- [ ] Reactor size
- [ ] Operating temperature
- [ ] Operating pressure
- [ ] Solvent
- [ ] Atmosphere
- [ ] Mass balance
- [ ] Catalyst loading (mass and/or concentration and reaction volume)
- [ ] Reactant concentration at the beginning of the reaction
- [ ] Mass and/or heat transfer and mixing effects

Catalytic analysis

Activity

- [ ] Reaction kinetics
- [ ] Turnover frequency
- [ ] Turnover number
- [ ] Product selectivity
- [ ] Space-time yield
- [ ] Kinetics of deactivation

Reaction intermediates

- [ ] Isolated
- [ ] Detected *in situ*

Product or compound characterization

Identity

- [ ] ^{1}H and ^{13}C NMR spectroscopy
- [ ] Multiplicity and coupling constants (required for ^{1}H; as needed for heteronuclear spectra)
- [ ] Spectra of all compounds are provided with integration of all resonances
- [ ] Other NMR experiments (heteronuclear: ^{11}B, ^{19}F, ^{31}P, etc.; 2D correlation spectroscopy: COSY, NOESY, HSQC, HMBC, etc.)
- [ ] HRMS, infrared (IR) absorption spectroscopy, and/or UV-vis spectroscopy
- [ ] Chiral gas chromatography (GC) and/or high-performance liquid chromatography (HPLC)
- [ ] X-ray diffraction (powder and/or single crystal)

Purity

- [ ] Isolated yields
- [ ] High-field ^{1}H NMR spectra
- [ ] 1D proton-decoupled ^{13}C NMR spectra
- [ ] Combustion elemental analysis
- [ ] Quantitative GC or HPLC analytical data
- [ ] Electrophoretic analytical data

Biomacromolecules

- [ ] Sequence
- [ ] Mass spectral data

Polymers

- [ ] Dispersity
- [ ] Transition temperatures
- [ ] Modulus

Comparing catalysts

- [ ] Benchmarking table or figure (either other catalysts investigated in this study or previous literature reports with references)

Control experiments

- [ ] Reaction without catalyst

Quantification and statistical analysis

- [ ] The paper reports statistical analysis
- [ ] There is a statement of where the statistical parameters (e.g., exact value of *n* samples, standard error of the mean, standard deviation) are reported in the paper

- [ ] There is a statement of whether any methods were used to determine whether the data met the assumptions of the statistical approach

If calculations were conducted

- [x] Software details, including version number
- [x] The program package (with revision number) used
- [x] Details of all basis sets and exchange-correlation functionals or wave function methods
- [ ] Pseudopotential
- [ ] Force-field parameters
- [ ] Ensemble
- [ ] Temperature and/or pressure (if different from standard conditions)
- [ ] Simulation cell details (if periodic calculations) or details if using molecular dynamics or Monte Carlo
- [ ] Description of all enthalpic and entropic corrections to electronic energies
- [ ] Table of Cartesian coordinates (angstrom), calculated energies (Hartree), and lowest frequency of all stationary points
- [x] Data (including dynamic movie and coordinates) and code are available in a repository

Sustainability remarks

- [ ] "Principles of green chemistry" have been considered in designing and conducting the research

  For more information, please see https://www.acs.org/content/acs/en/greenchemistry/principles/12-principles-of-green-chemistry.html.

I verify that, to the best of my knowledge, this form is completed accurately in agreement with all co-authors [x]

Submitting author name: **Modesto Orozco**

For general queries or feedback regarding this form, please email catalysis@cell.com

Heterogeneous catalysis checklist

Revision 1.0, Last updated: June 29, 2021

Catalyst synthesis

- [ ] Novel methods are provided in full detail
- [ ] Comprehensive literature references are included to allow reproducibility

Characterization of new materials

- [ ] Chemical composition of the catalyst
- [ ] Phase and crystallinity
- [ ] Morphology
- [ ] Thickness analysis for two-dimensional materials (e.g., using atomic-force microscopy)
- [ ] Particle size and size distribution (both high-res and low-res transmission electron microscopy [TEM])
- [ ] Characterization and analysis of pore size
- [ ] Exposed facets and orientation
- [ ] Defect structure
- [ ] Analysis of edge or vertex sites
- [ ] Analysis of valence state

Catalyzed reaction

- [ ] Reaction conditions and complete experimental procedure
- [ ] Type of reactor (e.g., flow type, batch type)
- [ ] Reactor size
- [ ] Operating temperature, operating pressure, solvent, atmosphere
- [ ] Mass balance
- [ ] Catalyst loading (mass and/or concentration and reaction volume)
- [ ] Reactant concentration at the beginning of the reaction
- [ ] Mass and/or heat transfer and mixing effects

Catalytic analysis

Activity

- [ ] Reaction kinetics
- [ ] Turnover frequency
- [ ] Turnover number
- [ ] Product selectivity
- [ ] Space-time yield
- [ ] Reactant concentration at the beginning of the reaction

- [ ] Kinetics of deactivation

Reaction intermediates

- [ ] Isolated
- [ ] Detected *in situ*

Product or compound characterization

Identity

- [ ] ^{1}H and ^{13}C NMR spectroscopy
- [ ] Multiplicity and coupling constants (required for ^{1}H; as needed for heteronuclear spectra)
- [ ] Spectra of all compounds are provided with integration of all resonances
- [ ] Other NMR experiments (heteronuclear: ^{11}B, ^{19}F, ^{31}P, etc.; 2D correlation spectroscopy: COSY, NOESY, HSQC, HMBC, etc.)
- [ ] HRMS, infrared (IR) absorption spectroscopy, and/or UV-vis spectroscopy
- [ ] Chiral gas chromatography (GC) and/or high-performance liquid chromatography (HPLC)
- [ ] X-ray diffraction (powder and/or single crystal)

Purity

- [ ] Isolated yields
- [ ] High-field ^{1}H NMR spectra
- [ ] 1D proton-decoupled ^{13}C NMR spectra
- [ ] Combustion elemental analysis
- [ ] Quantitative GC or HPLC analytical data
- [ ] Electrophoretic analytical data

Biomacromolecules

- [ ] Sequence
- [ ] Mass spectral data

Polymers

- [ ] Dispersity
- [ ] Transition temperatures
- [ ] Modulus

Study of the catalyst after reaction

Have the following analyses been performed?

- [ ] Hot filtration
- [ ] Scanning electron microscopy, TEM, XRD, inductively coupled plasma spectrometry, loading of catalyst after reaction

Catalyst stability assessment

Does the paper report any of the following?

- [ ] Long-term stability test, including test conditions

- [ ] Recyclability test

Comparing catalysts

- [ ] Benchmarking table or figure (other catalysts investigated in this study and/or previous literature reports with references)

Control experiments

- [ ] Reaction without catalyst

Quantification and statistical analysis

- [ ] The paper reports statistical analysis
- [ ] There is a statement of where the statistical parameters (e.g., exact value of *n* samples, standard error of the mean, standard deviation) are reported in the paper
- [ ] There is a statement of whether any methods were used to determine whether the data met the assumptions of the statistical approach

If calculations were conducted

- [ ] Software details, including version number
- [ ] Details of all basis sets and exchange-correlation functionals or wave function methods
- [ ] k-point and supercell size (if doing periodic plane wave calculations)
- [ ] Convergence criteria of the force and energy
- [ ] Description of all enthalpic and entropic corrections to electronic energies
- [ ] Definitions of computed physical quantities
- [ ] Pseudopotential (if applicable)
- [ ] Data and code are available in a repository

If molecular dynamics calculations were conducted

- [ ] All basis sets and functionals
- [ ] Pseudopotential
- [ ] Force-field parameters
- [ ] Ensemble
- [ ] Temperature and/or pressure (if different from standard conditions)
- [ ] Data (including dynamic movie and coordinates) and code are available in a repository

Sustainability remarks

- [ ] "Principles of green chemistry" have been considered in designing and conducting the research

  For more information, please see https://www.acs.org/content/acs/en/greenchemistry/principles/12-principles-of-green-chemistry.html.

I verify that, to the best of my knowledge, this form is completed accurately in agreement with all co-authors ☐

Submitting author name: _____

For general queries or feedback regarding this form, please email catalysis@cell.com

Biocatalysis checklist

Revision 1.0, Last updated: June 29, 2021

Catalyst identity

- [ ] The name from the IUBMB Enzyme List to identify the enzyme
- [ ] The NCBI Taxonomy ID
- [ ] A naturally occurring variant
- [ ] The localization within the cell
- [ ] Any post-translational modification
- [ ] The full protein sequence and the appropriate NCBI GenBank or UniProt accession code

Preparation

- [ ] Novel methods are provided in full
- [ ] Comprehensive literature references are included to allow reproducibility
- [ ] Artificial modification
- [ ] Enzyme or protein purity
- [ ] Metalloenzyme

Storage conditions

- [ ] Storage temperature
- [ ] Atmosphere if not air
- [ ] pH (if stored in solution)
- [ ] Buffer and concentrations (including counter-ion)
- [ ] Metal salt(s) and concentrations
- [ ] Enzyme or protein concentration
- [ ] Statement about observed loss of activity under the above conditions
- [ ] Statement about the thawing procedure

Assay conditions

- [ ] Substrate purity
- [ ] Measured reaction as a stoichiometrically balanced equation
- [ ] Assay temperature
- [ ] Assay pressure
- [ ] Atmosphere if not air
- [ ] Assay pH
- [ ] Buffer and concentrations
- [ ] Metal salt(s) and concentrations

- [ ] Coupled assay components
- [ ] Substrate and concentration ranges
- [ ] Enzyme or protein concentration
- [ ] Total ionic strength of assay mixture

Activity

- [ ] Measurements of initial rates of the reaction
- [ ] Proportionality between initial velocity and enzyme concentration
- [ ] Enzyme activity expressed as k_{cat} (in s^{-1} or min^{-1}) or international unit (1 IU = 1 µmol min^{-1}); katal (mol/s) may alternatively be used as a unit of activity (conversion factor 1 unit = 16.67 nkat)
- [ ] Turnover number

Methodology

- [ ] Assay method
- [ ] Type of assay
- [ ] Reaction-stopping procedure
- [ ] Direction of the assay
- [ ] Reactant determined
- [ ] Concentrations of free metal cations
- [ ] Reaction equilibrium constant

Kinetic parameters

- [ ] k_{cat} (in s^{-1} or min^{-1})
- [ ] V_{max}
- [ ] K_m units or concentration necessary (e.g., mM)
- [ ] k_{cat}/K_m as concentration per time (e.g., mM^{-1} s^{-1})
- [ ] $S_{0.5}$ as concentration (e.g., mM)
- [ ] Hill coefficient, saturation ratio (RS), or other coefficients of cooperativity
- [ ] Model used to determine the parameters
- [ ] High-substrate inhibition, if observed, with K_i value

Inhibition or activation data

- [ ] Time dependence and reversibility
- [ ] Inhibition (K_i units necessary)

Comparing catalysts

- [ ] Benchmarking table or figure (other catalysts investigated for this study and/or previous literature reports with references)

Control experiments

- [ ] Reaction without catalyst

Quantification and statistical analysis

- [ ] The article reports a statistical analysis
- [ ] There is a statement of where the statistical parameters (e.g., exact value of n samples, standard error of the mean, standard deviation) are reported in the paper
- [ ] There is a statement of whether any methods were used to determine whether the data met the assumptions of the statistical approach

Sustainability remarks

- [ ] "Principles of green chemistry" have been considered in designing and conducting the research

  For more information, please see https://www.acs.org/content/acs/en/greenchemistry/principles/12-principles-of-green-chemistry.html.

I verify that, to the best of my knowledge, this form is completed accurately in agreement with all co-authors ☐

Submitting author name: _____

For general queries or feedback regarding this form, please email catalysis@cell.com

Electrochemistry checklist

Revision 1.0, Last updated: June 29, 2021

Reaction conditions

- [ ] Cell type (H-cell, gas-diffusion type, etc.)
- [ ] Cell, electrode, and membrane material
- [ ] Currents
- [ ] Electrode geometric area (cm^2)
- [ ] Reactants
- [ ] Electrolyte
- [ ] Scan rate for cyclic voltammograms
- [ ] Dependence of current on scan or stir rate
- [ ] Mass transfer conditions (rotation rate for rotating disc electrode, stir bar, flow rate in flow cells)
- [ ] pH for aqueous solutions (start, during reaction, end)
- [ ] Treatment or polishing of the electrode
- [ ] Three-electrode or two-electrode configuration (half-cell or full cell, respectively)
- [ ] Bias potential and, for three-cell configuration, the reference electrode used

Reporting data

- [ ] Polarization plot (cell voltage versus current or current density)
- [ ] Electrochemical impedance spectroscopy (EIS)
- [ ] Normalized electrochemical surface area activity
- [ ] Mass activity
- [ ] Specific activity
- [ ] Mass balance
- [ ] Faradic efficiency
- [ ] Overpotential (including clear information about how the thermodynamic potential was determined, estimated, or calculated)
- [ ] Electrochemically active surface area (ECSA, A/cm^2_{ECSA})
- [ ] Stability test conditions
- [ ] Current densities
- [ ] Vendor information, photographs, and/or schemes of any custom apparatus

If calculations were conducted

- [ ] The program package (with revision number) used
- [ ] All basis sets and functionals

- [ ] Description of all corrections
- [ ] Table of Cartesian coordinates (angstrom), calculated energies (Hartree), and lowest frequency of all stationary points
- [ ] Data (including simulation, scripts, and raw data) and code are available in a repository

I verify that, to the best of my knowledge, this form is completed accurately in agreement with all co-authors ☐

Submitting author name:

For general queries or feedback regarding this form, please email catalysis@cell.com

Photocatalysis checklist

Revision 1.0, Last updated: June 29, 2021

Reaction conditions

- [ ] Photocatalyst loading
- [ ] Substrate concentration
- [ ] Sacrificial donor
- [ ] Hole or electron scavengers
- [ ] Other additives
- [ ] Reaction vessel size, material, and thickness of glassware
- [ ] Reaction setup
- [ ] Pictures or schemes
- [ ] Source and wavelength of light used for illumination
- [ ] Wavelength distribution of light
- [ ] Quantum yields
- [ ] Apparent quantum yields or photonic efficiencies
- [ ] Photocatalytic efficiencies
- [ ] Optical irradiance at the sample ($mW \cdot cm^{-2}$)
- [ ] Total optical power impinging on the sample if liquid ($mW \cdot mL^{-1}$)

Comparing catalysts

- [ ] Benchmarking table or figure (other catalysts investigated for this study and/or previous literature reports with references)

Control experiments

- [ ] Reaction without catalyst
- [ ] Reaction without light (on/off test and reaction conducted completely in the dark)

I verify that, to the best of my knowledge, this form is completed accurately in agreement with all co-authors ☐

Submitting author name: _____

For general queries or feedback regarding this form, please email catalysis@cell.com