Special Issue

Explainable AI (XAI) for Industrial Catalysis: Interpretable Machine Learning for Catalyst Design, Optimization, and Process Efficiency

Message from the Guest Editor

This Special Issue aims to highlight the growing impact of XAI in industrial catalytic systems, from heterogeneous and homogeneous catalysts to electrocatalysts and process-integrated systems. We invite original research articles, reviews, and case studies that showcase how XAI contributes to the understanding, design, screening, performance prediction, and optimization of catalysts and catalytic processes. Topics of Interest include (but are not limited to):

- XAI-guided design and optimization of industrial catalysts;
- Interpretable ML models for process intensification and scale-up;
- SHAP, LIME, and other XAI tools in catalyst performance analysis;
- XAI applications in petrochemical, refinery, fine chemical, or environmental catalysis;
- Integration of XAI with process simulation, DFT, or kinetic modeling;
- Case studies of XAI for catalyst lifetime prediction, deactivation analysis, or regeneration;
- Human-in-the-loop AI for catalyst development and deployment;
- Visualization and interpretation of AI-derived structure–activity relationships.

Guest Editor

Prof. Dr. Nagireddy Gari Subba Reddy

Virtual Materials Laboratory, School of Materials Science and Engineering, Engineering Research Institute, Gyeongsang National University, Jinju 52828, Republic of Korea

Deadline for manuscript submissions

15 December 2025

Catalysts

Catalysts

an Open Access Journal by MDPI

**Impact Factor 4.0
CiteScore 7.6**

About the Journal

Message from the Editor-in-Chief

Editor-in-Chief

Prof. Dr. Keith Hohn
Carl R. Ice College of Engineering, Kansas State University, Manhattan, KS, USA

Author Benefits

High Visibility:
indexed within Scopus, SCIE (Web of Science), Inspec, Ei Compendex, CAPlus / SciFinder, CAB Abstracts, and other databases.

Journal Rank:
JCR - Q2 (Chemistry, Physical) / CiteScore - Q1 (General Environmental Science)

Rapid Publication:
manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.6 days after submission; acceptance to publication is undertaken in 2.7 days (median values for papers published in this journal in the first half of 2025).

MDPI