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

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Deadline for manuscript submissions

closed (15 December 2025)

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