Special Issue

Artificial Intelligence for Catalysis

Message from the Guest Editors

Applying artificial intelligence (AI) to catalyst design is transforming the industry by making it possible to construct catalysts more quickly, precisely, and creatively. Artificial intelligence (AI)-driven approaches are gradually replacing and supplementing traditional methodologies, which mostly depend on empirical investigation. This Special Issue examines various important areas where AI and catalyst design meet and focuses on these breakthroughs. This capacity expedites the optimization process by enabling researchers to forecast how catalyst composition or structure modifications can affect their activity and selectivity. AI-driven models can also propose new catalyst formulas that are more sustainable and effective, which frequently results in the identification of materials with improved performance. Key topics covered in this Special Issue include:

- Machine Learning in Catalyst Design;
- Data-Driven Discovery of Catalysts;
- AI-Enhanced Understanding of Catalytic Mechanisms;
- Sustainability and Green Chemistry;
- Integration of AI with High-Throughput Experimentation.

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