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Machine Learning for Materials Design

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Deadline for manuscript submissions:
20 March 2025

Message from the Guest Editors

Dear Colleagues,

The integration of machine learning with material design is revolutionizing the way new materials are discovered, characterized, and optimized. Traditional approaches to material design often involve costly and time-consuming experimental and computational methods. However, ML offers powerful tools to accelerate these processes by predicting material properties, discovering new materials, optimizing compositions, and understanding complex material behaviors. This Special Issue seeks to gather cutting-edge research that utilizes ML to address challenges and unlock new potentials in material design.

We invite submissions of original research articles, reviews, and case studies that cover, but are not limited to, the following topics:

1. Machine learning algorithms for material discovery:
2. Data-driven material design:
3. Inverse design and optimization:
4. Big data and materials informatics:
5. Predictive modeling and simulations:
6. Case studies and applications:

Prof. Dr. Wencong Lu
Dr. Minjie Li
Guest Editors

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Message from the Editor-in-Chief

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