Special Issue

Artificial Intelligence: An Innovative Solution to the Optimization and Discovery of Functional Materials

Message from the Guest Editors

Driven by the advances in artificial intelligence (AI), the discovery and optimization of functional materials have reached an unprecedented rate and scale. In recent years, AI has demonstrated success in accelerating the discovery and design of various functional materials ranging from polymers to crystals and nanomaterials. AI plays a critical role in the development of computer-aided robotics, machine learning force-fields, Bayesian optimization, generative models and data-driven approaches. Innovation of next-generation functional materials highly relies on AI-driven methods. This Special Issue "Artificial Intelligence: An Innovative Solution to the Optimization and Discovery of Functional Materials" welcomes articles that report novel development or applications of AI techniques for the optimization and discovery of functional materials with improved properties. Rooted in the field of functional materials, to the following topics are included in this Special Issue:

- Machine learning accelerated simulations;
- AI for elucidating experimental data;
- Inverse materials design;
- Automated synthesis.

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Deadline for manuscript submissions

10 February 2026

Processes

an Open Access Journal by MDPI

Impact Factor 2.8
CiteScore 5.5

mdpi.com/si/220162

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Editor-in-Chief

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