

## Special Issue

# Machine Learning for Materials Design

### Message from the Guest Editors

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:

- Machine learning algorithms for material discovery:
- Data-driven material design:
- Inverse design and optimization:
- Big data and materials informatics:
- Predictive modeling and simulations:
- Case studies and applications:

### Guest Editors

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### Deadline for manuscript submissions

20 September 2025



## Materials

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## About the Journal

### Message from the Editor-in-Chief

*Materials* (ISSN 1996-1944) was launched in 2008. The journal covers twenty-five comprehensive topics: biomaterials, energy materials, advanced composites, advanced materials characterization, porous materials, manufacturing processes and systems, advanced nanomaterials and nanotechnology, smart materials, thin films and interfaces, catalytic materials, carbon materials, materials chemistry, materials physics, optics and photonics, corrosion, construction and building materials, materials simulation and design, electronic materials, advanced and functional ceramics and glasses, metals and alloys, soft matter, polymeric materials, quantum materials, mechanics of materials, green materials, general. *Materials* provides a unique opportunity to contribute high quality articles and to take advantage of its large readership.

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### Editor-in-Chief

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