

## Special Issue

# Artificial Intelligence and Machine Learning for Material Design, Discovery, and Optimization

### Message from the Guest Editors

This Special Issue focuses on recent advancements in the use of artificial intelligence (AI) and machine learning (ML) techniques in the broad field of material science. The rapid advancement of AI/ML and their subsequent adoption by the scientific community has seen an explosion in research in this field. We welcome contributions focusing on the use of AI/ML techniques for computational, experimental, and/or theoretical purposes. We seek manuscripts that focus on the successful deployment of technologies in application topics including, but not limited to, material discovery, high throughput experimentation and data analysis, the optimization of material processing, multiscale modeling and simulation, optimal experimental design, etc. Special interest will be given to those manuscripts which leverage AI/ML techniques beyond pure data-driven techniques and which create “black-box” discoveries. For example, the successful combination of AI/ML for the discovery of fundamental physical laws will be of particular interest.

### Guest Editors

Dr. Craig Hamel

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### Deadline for manuscript submissions

20 November 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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