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AI Materials

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Message from the Editor-in-Chief

AI Materials is a new open-access journal, dedicated to exploring the dual trajectory of AI and materials science—how AI revolutionizes materials research, and, equally importantly, how advanced materials enable the next generation of AI technologies. AI Materials covers a wide range of topics, including, but not limited to, material screening, material informatics, high-performance computing, cutting-edge materials for enhancing AI applications, etc. We welcome researchers from all career stages and geographic regions to join us in shaping this exciting new chapter in materials research.

Honorary Editor-in-Chief
Prof. Dr. Xin-Gao Gong

Editor-in-Chief
Prof. Dr. Zhimei Sun

Aims

AI Materials (ISSN 3042-6715) is an international, peer-reviewed, open access journal dedicated to advancing the interdisciplinary frontier of applications between artificial intelligence (AI) and materials science. It publishes reviews, regular research papers (articles), and short communications, but other article types will also be considered. We aim to establish a platform for disseminating high-impact outcomes on the integration of AI methodologies with materials science, with key focus areas including AI-driven material screening, predictive property optimization, autonomous experimental systems, and large language models.

Scope

- AI-enhanced theory & simulation;
- generative design & discovery;
- autonomous experimentation;
- AI for characterization;
- large language models & agents;
- data infrastructure;
- open science & tools.

We welcome research on all classes of materials, including inorganic, organic, polymers, biomaterials, and hybrids. We encourage the publication of high-quality negative datasets valuable for model training.

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