AI-Driven Discovery and Design of Functional Materials: From Nanoscale Structure to Performance

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Submissions are invited for a Special Issue of ***Journal of Materials Science***, dedicated to recent advances at the intersection of artificial intelligence (AI), data-driven modeling, and nanoscale engineering for functional materials. This Special Issue aims to highlight the emerging methodologies and applications that leverage AI to accelerate the discovery, design, and optimization of materials with tailored structure-property-performance relationships.

The rapid evolution of machine learning, high-throughput simulations, and data-centric approaches is transforming the paradigm of materials research. These tools enable the exploration of vast chemical and structural design spaces, facilitate inverse design, and provide new insights into nanoscale mechanisms governing material behavior. Concurrently, advances in nanoscale characterization and fabrication offer unprecedented opportunities to engineer materials with precise structural control. Bridging these domains is essential for realizing next-generation functional materials across energy, electronics, environmental, and biomedical applications.

This Special Issue seeks high-quality original research articles, reviews, and perspectives addressing, but not limited to, the following topics:

- AI and machine learning for materials discovery and design
- Physics-informed and hybrid modeling approaches
- Data-driven prediction of structure-property relationships
- Virtual screening and generative models for materials design
- Nanoscale engineering and structure control (e.g., interfaces, defects, morphology)
- Multiscale modeling linking atomic, nano-, and macro-scale behavior
- Autonomous experimentation and closed-loop materials optimization
- Applications in functional materials, including energy storage/conversion, membranes, semiconductors, and quantum materials
- Integration of experimental, computational, and data-driven workflows

Contributions that demonstrate clear connections between nanoscale structure and macroscopic performance, particularly through AI-enabled methodologies, and/or advanced nanoscale engineering techniques are especially encouraged. Submissions that include experimental validation, interpretable models, or physically grounded insights will be prioritized.

Submission information

Authors should prepare their submissions following the journal's guidelines at https://link.springer.com/journal/10853/submission-guidelines. The submission link is https://www.editorialmanager.com/jmsc/default.aspx.

All manuscripts will be screened by the editors before undergoing rigorous peer review according to the standards of the journal. To ensure your manuscript(s) to be considered for the Special

issue, please specify the article type of “AI-Driven Discovery and Nanoscale Engineering of Functional Materials: From Structure to Performance” when preparing your submissions.

Submission deadline: January 31, 2027

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Detailed information regarding journal metrics, manuscript formatting guidelines, and publication policies is available on the journal’s website (https://link.springer.com/journal/10853).