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# AI Chemistry

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# Message from the Editor-in-Chief

The integration of artificial intelligence, machine learning, data-driven methods, and chemical theory is accelerating discovery and reshaping chemistry research and applications. As artificial intelligence continues to transform the chemical sciences, we are delighted to introduce *AI Chemistry* as a platform for sharing impactful research in this field. *AI Chemistry* is dedicated to publishing high-quality, interdisciplinary research that integrates AI and chemistry. We are committed to a rigorous and efficient peer-review process and to supporting impactful, reproducible research. On behalf of the Editorial Board and Office, we warmly invite researchers and practitioners to contribute and help shape the future of AI-driven chemistry.

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## Editor-in-Chief

Prof. Dr. Matthew Oehlschlaeger

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## Aims

*AI Chemistry* (ISSN 3042-6723) is an international, open access journal dedicated to advancing the integration of artificial intelligence with chemistry. The journal aims to serve as a leading platform for disseminating high-quality, cutting-edge research that explores the innovative applications of artificial intelligence in the chemical sciences. We seek to shape the emerging field of AI-driven chemistry by promoting interdisciplinary work that combines artificial intelligence, machine learning, data science, and chemical theory with experimental and industrial practice.

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## Scope

*AI Chemistry* welcomes original research, reviews, and perspectives on the development and application of artificial intelligence in all areas of fundamental and applied chemical sciences. Topics of interest include, but are not limited to, the following:

- AI-based chemical data analysis, prediction, and discovery
- AI-enabled chemical reaction prediction, synthesis planning, and retrosynthesis
- AI-assisted drug and biomolecule design
- AI in materials discovery and design
- AI in biological sciences
- AI-enhanced chemical process optimization and control
- AI in complex, multiscale chemical systems
- AI-driven chemical sensing and environmental monitoring
- Digital twins and simulation of chemical processes
- Autonomous chemical laboratories and experiments
- Physics-informed and hybrid chemical modeling approaches
- Interpretable and explainable AI for chemistry
- AI-powered chemical education and pedagogy
- Ethics, society, and reproducibility considerations in AI chemistry

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### Thorough Peer-Review

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