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Advances in Machine Learning for Atomistic Simulations: Paving the Way for Next-Generation Material Design

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Message from the Guest Editors

This Special Issue highlights recent advances in integrating machine learning (ML) with atomistic simulations to improve, accelerate, and increase the accuracy of computational materials science techniques. In emphasizing ML role in enhancing simulation efficiency, it aims at showcasing machine-learned interatomic potentials (MLIPs) that significantly reduce computational costs while maintaining ab initio high accuracy. Another crucial advancement involves the fusion of ML with high-throughput computational screening to accelerate material discovery, enabling the prediction of new compounds through ML algorithms trained on extensive datasets. Additionally, ML can guide material scientists in interpreting complex simulation data through dimensionality reduction, making outcomes more understandable and uncovering hidden patterns. The goal of this issue is to survey ML applications and techniques' impact on material science and predict future innovations in material design.

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Message from the Editor-in-Chief

Welcome to *Crystals*, the journal dedicated to the fascinating world of crystallographic research! Crystals are more than mere decorative elements; they hold the key to understanding the fundamental structure of matter. Our mission is to explore the crucial significance of this research across various fields. From medicine to technology, chemistry to geology, crystals play a vital role. Their structure provides insights into new advanced materials, innovative drugs, and groundbreaking technologies. Through *Crystals*, we delve into the microscopic world to discover solutions that will shape the future. Join us on a journey through the *Crystals*, where science merges with beauty and innovation.

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