Special Issue

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

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.

Guest Editors

Dr. Riccardo Dettori
Department of Physics, University of Cagliari, 09123 Cagliari, Italy

Dr. Antonio Rossi
Center for Nanotechnology Innovation, Istituto Italiano di Tecnologia, 56127 Pisa, Italy

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Crystals
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
crystals@mdpi.com

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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.

Editor-in-Chief

Prof. Dr. Alessandra Toncelli
Department of Physics, University of Pisa, 56126 Pisa, PI, Italy

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