Special Issue

Advances of Machine Learning in Nanoscale Materials Science

Message from the Guest Editor

Cutting-edge machine learning (ML) techniques—such as gradient boosting models (e.g., XGBoost), graph neural networks (e.g., CGCNN, SchNet, ALIGNN), ML interatomic potentials (e.g., BPNN, GAP, M3Gnet, NequIP, MACE, NEP), and deep learning DFT Hamiltonians (e.g., DeepH, HamGNN, DeePTB)—are transforming materials science by enabling rapid property prediction, high-throughput materials discovery, large-scale accurate simulations, and mechanistic insights across scales. This Special Issue focuses on the application of ML, ML-based interatomic potentials, and data-driven methods in materials science. Topics include ML-assisted property prediction, inverse design, automated experimentation, uncertainty quantification, interpretable AI models, electronic structure prediction, and materials database development. Contributions on novel methodologies, benchmarks, and applications in energy materials, ferroelectrics, functional ceramics, catalysts, polymers, and two-dimensional materials are welcome. We invite experts and emerging researchers to share recent findings and perspectives to provide an authoritative overview of advances and future directions at the ML-materials science interface.

Guest Editor

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Message from the Editor-in-Chief

Nanoscience and nanotechnology are exciting fields of research and development, with wide applications to electronic, optical, and magnetic devices, biology, medicine, energy, and defense. At the heart of these fields are the synthesis, characterization, modeling, and applications of new materials with lower nanometer-scale dimensions, which we call “nanomaterials”. These materials can exhibit unusual mesoscopic properties and include nanoparticles, coatings and thin films, metal–organic frameworks, membranes, nano-alloys, quantum dots, self-assemblies, 2D materials such as graphene, and nanotubes. Our journal, *Nanomaterials*, has the goal of publishing the highest quality papers on all aspects of nanomaterial science to an interdisciplinary scientific audience. All of our articles are published with rigorous refereeing and open access.

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