Special Issue

The Application of AI and Machine Learning for Energy Material Design

Message from the Guest Editors

The development of a high-performance methodology for functional energy material (EM) discovery has become increasingly important against the background of the global energy crisis. Recently, the occurrence of novel AI and Machine Learning technologies has largely facilitated material designs that have crystal structures; and the obtained computational insights could be further instructive for experimental work. To accelerate functional energy material (EM) discovery, various kinds of deep learning architectures have been utilized for crystal structure predictions and optimization, like Graph Convolutional Network (GCN), Convolution Neural Network (CNN), etc. The aim of this issue is to collect AI and Machine Learning-based computational papers focusing on energy 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.

Editor-in-Chief

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