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The Application of AI and Machine Learning for Energy Material Design

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Message from the Guest Editors

Dear Colleagues,

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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Special Issue



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Message from the Editor-in-Chief

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