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Editorial

Applications of Machine Learning to the Study of Crystalline Materials

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This Special Issue, "Applications of Machine Learning to the Study of Crystalline Materials", is a collection of seven original articles published in 2021 and 2022 and dedicated to applications of machine learning in materials research.

Machine learning (ML) is rapidly revolutionizing many fields and is starting to change landscapes for physics, chemistry, materials science, and structural research. With its ability to solve complex tasks autonomously, ML is being exploited as a radically new way to help find material correlations, understand materials chemistry, analyze crystal structures and related properties, and generally accelerate the discovery of new materials. Thus, one goal of this special issue is to demonstrate available, practical machine learning techniques that can be used to study crystalline materials today by means of the application of different ML techniques (including deep learning), as well as by the demonstration of best practices.

The focus of this Special Issue is the practical application of ML in materials research in order to inspire more materials scientists and crystallographers to use ML as a powerful tool in research and also to demonstrate the potential benefits of ML, as well as to improve communication between theoretically and more practically working scientists, in order to reduce any inhibitions that may exist. In this context, one goal may be to establish ML as a way to usefully extend existing analytical procedures and also to obtain results that cannot be obtained by experiments and standard procedures, or only at a disproportionately high cost.

The development of new ceramic gas separation membranes for the production of pure oxygen is demonstrated by Schlenz et al. [1]. For this work, mainly experimental data were used to generate training data for ML, where the training data contained information on both crystal structures and the microstructures of selected ceramic phases. The use of artificial neural networks (ANNs) for optimizing the fabrication and alloying processes of Al75O75-TiC composites is demonstrated by Alam et al. [2]. Using ANNs, the crystallite sizes and lattice strains of the composites could be predicted. An alternative approach is taken by Shu et al. [3] for the prediction of microstructures of polycrystalline phases. For this purpose, grain knowledge graphs were used, and a new heterogeneous grain graph attention model (HGGAT) is presented. The operation of HGGAT is demonstrated using the prediction of magnesium alloy microstructures as an example. Even Gómez-Peralta et al. [4] used ANNs for materials research, this time, however, in order to classify crystal structures. In this work, different halite, fluorite, ilmenite, spinel, and perovskite phases could be distinguished with an average precision of about 94%, by means of crystal-site-based features. Spinel represents the focus of the work of Lin et al. [5]. They applied ML to the development of new photocatalytic phases, based on highly entropic spinels. Predictions for this promising class of materials are demonstrated using the system $(Co, Cr, Fe, Mn, Ni)_3O_4$ as an example. As in the work of Schlenz et al. [1] and Gómez-Peralta et al. [4], perovskite is the focus of interest in the work of

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Li et al. [6]. Here, ML was used for the successful prediction of specific properties, for example, formation energies, thermodynamic stability, crystal volume, and oxygen vacancy formation energies, where the latter again provides important information for the first contribution [1]. Li et al. [6] tested different ML algorithms for this purpose and compared their results. Finally, Trampert et al. [7] used deep neural networks for image analysis. Microscopy images were analyzed with Convolutional Neural Networks (CNNs), but with a special feature: synthetic image data were generated for training the CNNs, which makes it possible to train neural networks in a meaningful way in the case of insufficient image data.

We hope that the contributions in this Special Issue will be especially helpful for further progress in materials research and for the establishment of ML methods as a standard tool, and we would also like to express our sincere thanks to all the authors who have made their contributions to this issue.

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