A Perovskite Crystal Structure Prediction and Screening System Using Complex Machine Learning Methods

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Due to a decrease in traditional energy sources, the demand for solar energy has started to rise through the use of silicon solar cells. However, its high production costs prevent its mass usage. Thus, an alternative was explored: perovskites. Perovskites are thin-film solar cells which replace silicon with man-made materials to significantly cut costs, widen its field of application, and create a higher absorption coefficient relative to silicon. Using man-made materials creates a multitude of combinatorial structures, some of which are unstable, inefficient, and unfit for commercialization. A brute force screening of these ABX3 structures is cost-ineffective and time consuming. Therefore, the need exists to develop an automated and accurate system capable of identifying promising perovskite structures. Our solution is a transfer learning based machine learning algorithm, capable of predicting the formation energy, absolute energy, band gap, tolerance factor, and stability of perovskite crystal structures, thus accelerating the screening of perovskite structures. Using convolutional neural networks and data preprocessing techniques, our M1 model predicts formation energy based on structural features. This model is transferred to train M2 that uses a similar feature prediction analysis, but with an enlarged training dataset derived from M1, and a classification component. The purpose of M2 is to predict absolute energy, band gap, and compute the tolerance factor of the structure. Overall, our system is able to accurately identify stable and efficient perovskites which are suitable for device production and allows for the evaluation of new compositions to be further explored in the lab.

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