Perovskite or Not Perovskite? A Deep-Learning Approach to Automatically Identify New Hybrid Perovskites from X-ray Diffraction Patterns

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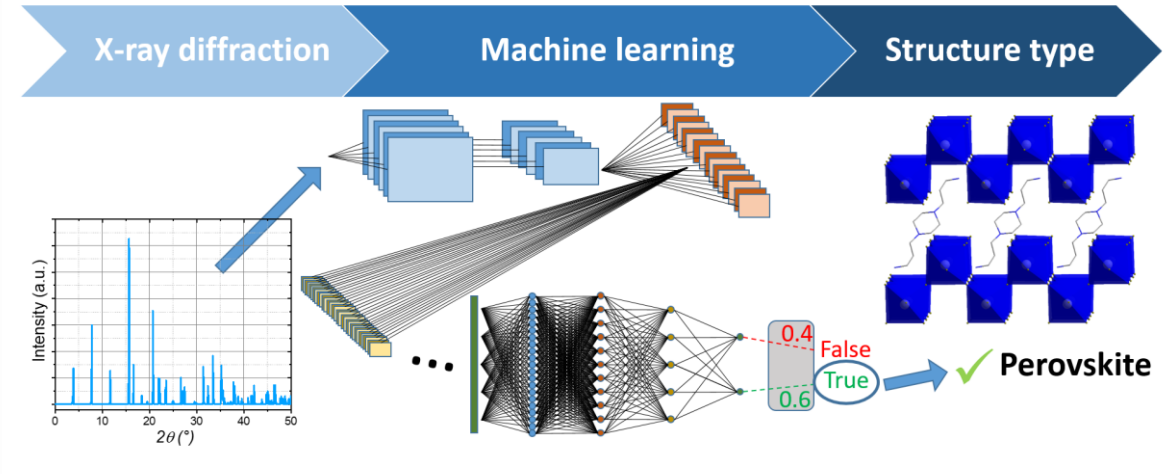
Abstract :
Determining the crystal structure is a critical step in the discovery of new functional materials. This process is time consuming and requires extensive human expertise in crystallography. Here, a machine-learning-based approach is developed, which allows it to be determined automatically if an unknown material is of perovskite type from powder X-ray diffraction. After training a deep-learning model on a dataset of known compounds, the structure types of new unknown compounds can be predicted using their experimental powder X-ray diffraction patterns. This strategy is used to distinguish perovskite-type materials in a series of new hybrid lead halides. After validation, this approach is shown to accurately identify perovskites (accuracy of 92% with convolutional neural network). From the identification of the key features of the patterns used to discriminate perovskites versus nonperovskites, crystallographers can learn how to quickly identify low-dimensional perovskites from X-ray diffraction patterns.



Left : Simulated X-ray diffraction pattern. Middle : Part of the Convolutional Neural Network used to identify the structure type. Right : Labelling of the structure.