Machine Learning Design of Low-Dimensional Hybrid Metal Halides with Perovskite Structure Type

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The discovery of new materials with specific properties is a complex task due to the drastic effects that very slight modifications on the synthesis of materials can have on the crystal structures and the resulting properties. Machine learning can be a very useful tool in such situations and can drastically accelerate the discovery of new functional materials as well as assist us to rationalize complex mechanisms.

In this presentation, the accelerated discovery of new hybrid metal halides by machine learning will be presented. These materials have recently shown a great potential in optoelectronic applications. For this reason, many research groups are currently exploring this chemical system to discover new low dimensional hybrid metal halides of perovskite types. However, discovering such materials is challenging as the necessary structure determination by X-ray diffraction is time consuming and non-perovskite compounds are very often synthesized. In this presentation, two approaches will be introduced which guided us towards the synthesis of new hybrid metal halides of specific structures: (i) the use of deep learning to automatically identify hybrid perovskites from powder X-ray diffraction patterns,[1] and (ii) the use of molecular descriptors to identify organic amines with high probability to lead to the synthesis of hybrid perovskites.[2]

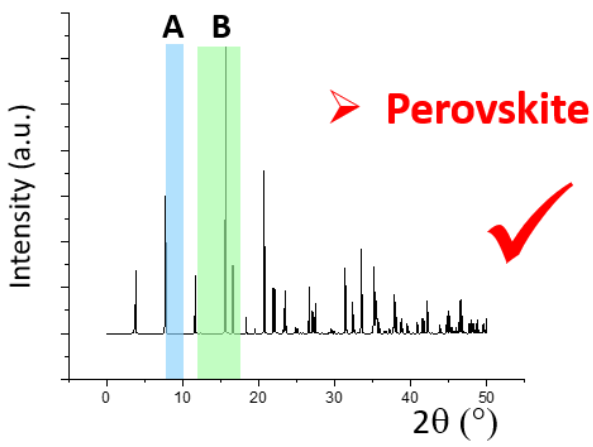

Figure 1. Deep learning assisted identification of perovskite structure type from powder X-ray diffraction.

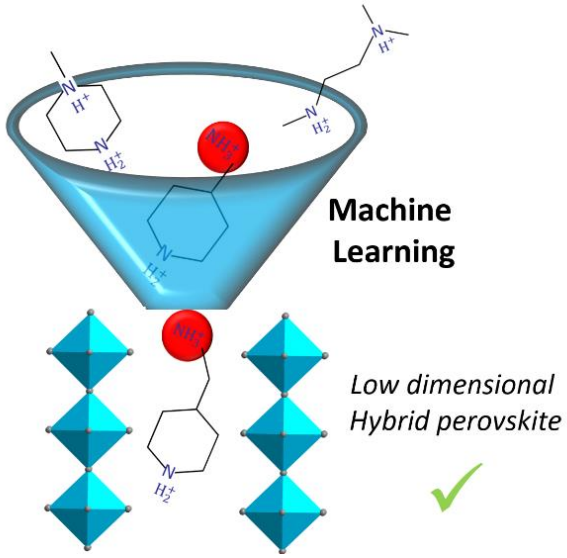

Figure 2. Identification of molecular descriptors responsible of the crystallization of hybrid metal halides in the perovskite structure type.

References

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[2] R. Laref, F. Massuyeau, R. Gautier, Small 2023, 2306481.