Band gap prediction & data analysis of inorganic halide perovskites using machine learning

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Machine learning is a very prominent approach towards material discovery based on data mining and big data analysis. [1] This approach has been proven extremely successful in a wide range of research fields from medicine to artificial intelligence. In the field of solid-state chemistry, machine learning can provide us with a robust method of analyzing our experimental results and making predictions on the properties and synthesis of new materials. One such class of materials is perovskites, an innovative class of semiconductor materials, which has spiked the interest of the scientific community for many years. In this project, we utilize machine learning in order to assist with the discovery of new materials combining a computational approach to identify the materials and a synthetic materials chemistry approach to attempt to verify the computational results. We ultimately seek to discover new compounds with desirable optoelectronic properties in the visible spectrum range for employment in photovoltaic research. [2] We use machine learning as an alternative method to other computational as well as test-and-trial methods, and we find that our machine learning methodology provides a higher accuracy in the prediction of photoactive perovskites. By employing machine learning on analyzing and predicting properties of perovskites, we have successfully surpassed the effectiveness hurdles of conventional theoretical methods, such as DFT.

References

[1] Lu, Materials Reports: Energy **1** (3), 100047 (2021).
[2] Stoumpos and Kanatzidis, Accounts of chemical research **48** (10), 2791-2802 (2015).

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