Predicting Bandgaps in Organic Metal Halide Hybrids with ODIN: A Data-Driven Informatics Approach

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Organic metal halide hybrids (OMHHs) are a class of materials formed by combining organic precursors with inorganic metal halides. These materials have useful applications in optoelectronics and LED due to their tunable bandgaps, high brightness, and ability to efficiently move electrical charges. (Xu et al., 2020) The bandgap, the energy difference between the valence and conduction bands, determines how these materials interact with light. In turn, this influences their optical absorption and emission behaviors. This project: **O**rganic halide **D**ata-driven **I**nformatics I**n**vestigation (ODIN) included literature review, data analytics, and machine learning. By creating and using a database of OMHHs containing synthesis information and material properties gathered from scientific journals, data relating to bandgap and other properties was collected. The aim was to obtain reliable bandgap predictions prior to experimental synthesis using values known at the time. These predictions have the potential to optimize resource allocation by identifying promising materials early on, reducing the need for costly and time consuming experimental or computational screening. Additionally, observing and analyzing our databases leads to the understanding and visualization of data, helping uncover connections between properties. The model showed successful performance with a mean absolute error of 0.1988 eV and has the potential to accelerate the development of new OMHHs for optoelectronic applications. Furthermore, the insights gained through this approach, and the well-organized, comprehensive database will contribute to a deeper understanding of the properties of organic metal halide hybrids, including the ones that have an effect on bandgap as well as further analysis.

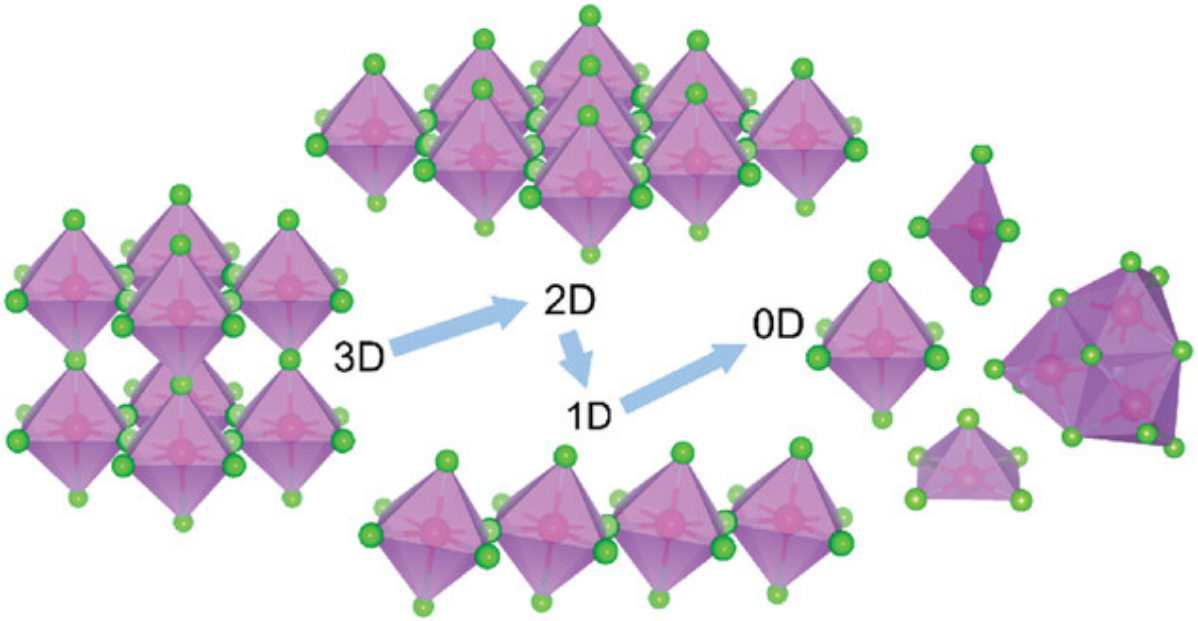

Figure 1: Structure of OMHHs with different dimensionalities (Zhou et al., 2020)

References

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