3D Lead-Free Halide Perovskites: Optoelectronic Properties and Potential for Photovoltaic Applications

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Abstract

Lead halide perovskites stand out for their remarkable optoelectronic properties, making them promising candidates for photovoltaic applications due to their exceptional physical performance. However, the toxicity of lead and their instability at room temperature hinder their large-scale deployment.

From a sustainable development perspective, our research aims to identify and characterize lead-free alternatives that are more environmentally friendly [1], [2] .

This work presents key results from *ab- initio* calculations based on density functional theory (DFT), applied to 3D lead-free halide perovskites. We specifically focus on their structural, electronic (band structures), optical (absorption coefficients), and selected elastic properties, in order to evaluate their potential for photovoltaic applications [3], [4]. These results contribute to a better understanding of the optoelectronic behavior of these alternative materials and pave the way for safer, more efficient, and more sustainable solar technologies.

References

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