

A Density Functional Theory–Based Study of Perovskite Structures Aimed at Photovoltaic Applications

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Abstract:

Perovskite materials have emerged as promising candidates for next-generation photovoltaic devices due to their remarkable optoelectronic properties and low fabrication costs. In this work, a density functional theory (DFT)–based study is conducted to investigate the structural, electronic, and optical properties of selected perovskite structures for photovoltaic applications. Geometry optimizations are performed to determine the structural stability, followed by electronic band structure and density of states calculations to analyze the nature of the band gap and charge carrier behavior. The optical response, including absorption spectra and dielectric functions, is also evaluated to assess the light-harvesting potential of the studied materials. The results provide insight into the relationship between composition, structural parameters, and optoelectronic performance, highlighting key factors that govern photovoltaic efficiency. This study offers theoretical guidance for the design and optimization of high-performance perovskite-based solar absorbers.

Keywords:

Perovskite materials, DFT, DOS, optoelectronic properties, photovoltaic, optimization.