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Topic I : Nanomaterials and Functional Nanostructures

T1-P18

DFT Insights into the Optoelectronic Properties of Double Perovskite Oxides for Functional Nanostructure Applications

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Abstract

We present a density functional theory (DFT) study on the structural, electronic, and optical properties of the double perovskite oxides X_2InSbO_6 (X = Ca, Sr, Ba). Structural optimization was carried out within the local density approximation (LDA) and the generalized gradient approximation (GGA), showing good agreement with theoretical reference values. The calculated electronic band structures and density of states confirm the semiconducting nature of these compounds with tunable band gaps, while the optical response, including dielectric function, absorption coefficient, and refractive index, reveals strong interaction with visible and ultraviolet light. These results demonstrate that double perovskite oxides are promising nanomaterials with potential applications in functional nanostructures for optoelectronic devices, photocatalysis, and next-generation energy conversion systems. The insights provided here may guide the rational design of advanced oxide-based nanomaterials for emerging technologies.

Keywords: Density Functional Theory (DFT), Double Perovskite Oxides, Electronic and Optical Properties, Nanomaterials and functional nanostructures,

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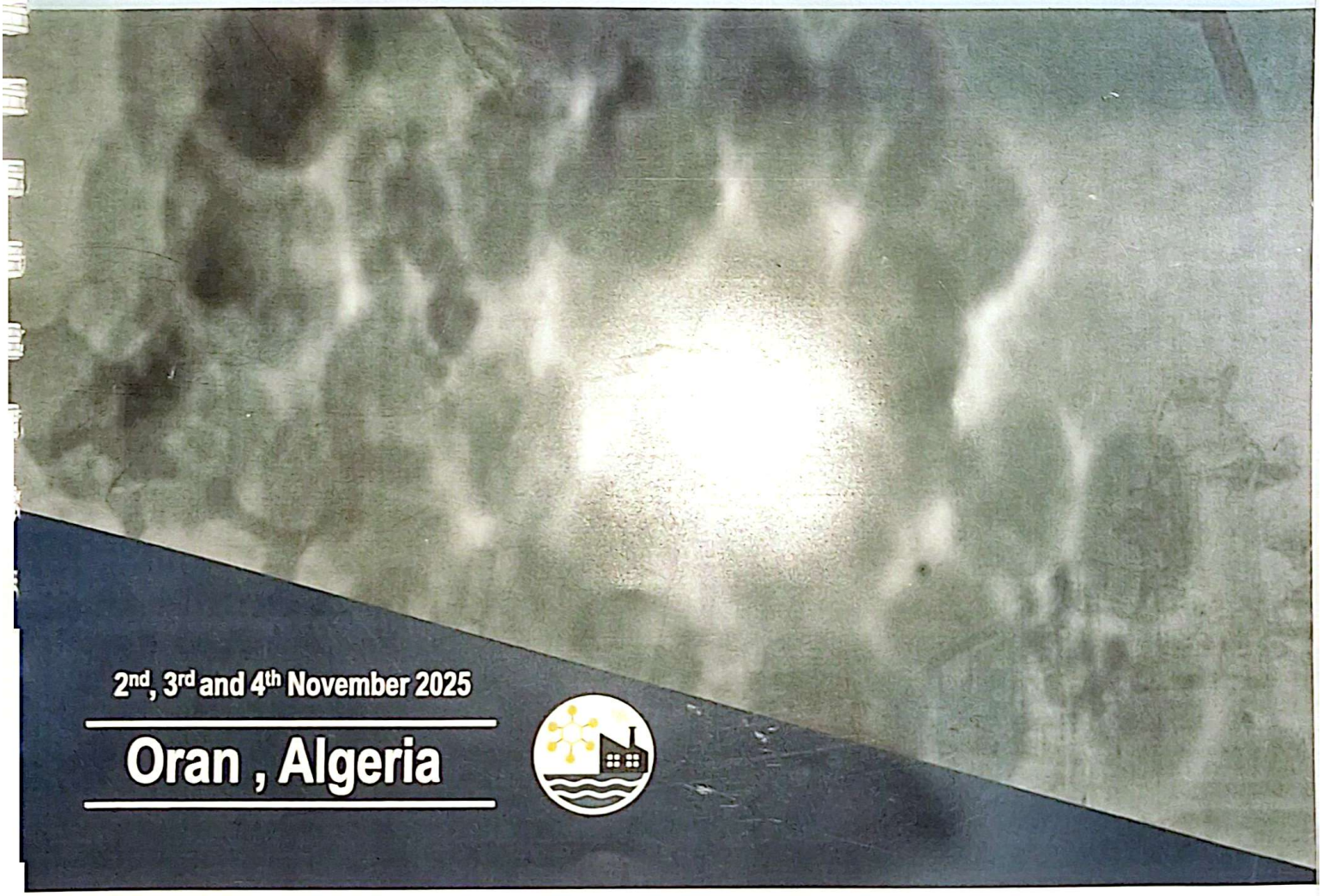
Abstract Book



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