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Phase ransitions and magnetic susceptibility in one-dimensional Hubbard chains under electric fields

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Palavras Chave:*Perovskite-based materials, solar cells, optoelectronic properties, alloys, and power conversion efficiency.*

Highlights

Exploring the Structural Stability and Electronic Properties of Perovskite-Based Materials for the Next Generation of Solar Cells: high charge carrier density, low production cost, high absorption coefficient, tunable optoelectronic properties, and power conversion efficiency (PCE) of approximately 26%.

Abstract

Nowadays, solar cell technology is based on silicon, which has a high production cost. In contrast, perovskite materials emerge as a promising alternative for low-cost solar panels, making clean energy more accessible and accelerating the energy transition [1]. The perovskite structure consists of an octahedral inorganic framework surrounded by organic or inorganic cations, as schematically shown in Figure 1.

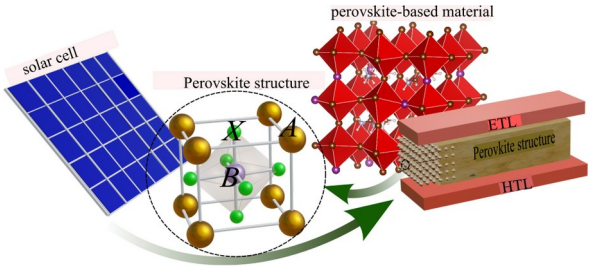

Figure 1: *Perovskite solar cell architecture: Electron transport layer (ETL); hole transport layer. A is the cation site (Cs, CH_3NH_3, etc.); B is the metal site (Pb, Sn, Ge, etc.); and X is the halide site (Cl, Br, I, etc.).*

Although halide perovskites exhibit desirable optoelectronic properties for solar cells, their scalability for industrial applications is compromised due to instability when exposed to humidity and ultraviolet light. In this context, perovskite-based alloys emerge as a strategy to enhance the structural stability of perovskites [2].

In this particular work, by means of density functional theory (DFT), we explore alloy compositions in the perovskite structure, for example, $A_xA'_{1-x}PbI_3$ [3]. Through an energetic stability analysis, we show that the $Cs_xMA_{1-x}PbX_3$ composition is more stable compared to $FA_xMA_{1-x}PbX_3$. The higher electronegativity of Cs^+ reduces octahedral distortions and improves charge distribution on the halides, contributing to increased light absorption and, consequently, improve PCE.

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