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The need to obtain new sources of non-fossil energy, renewable and eco-friendly energy source, has prompted the research and development of new materials for photovoltaic cells with high efficiency and performance to harvest solar energy. In the last years, the study of all-inorganic perovskite compounds like $CsPbA_3$ (A = Cl, Br, I) has increased as these are very good candidates with high efficiency for photovoltaic applications. However, these materials have the drawback of containing lead (Pb), which makes them highly toxic, both for the manufacturing process and for recycling or disposal processes.

To obtain new perovskite-based materials with low concentration of Pb or Pb-free, compounds based on: $CsGe_xPb_{1-x}A_3$ and $CsSn_xPb_{1-x}A_3$ (A = Cl, Br, I; $0 \leq x \leq 1$) are a great alternative. For this reason, it is necessary to study some of their properties, such as energetic stability of the compound, photovoltaic efficiency, in-use lifetime, manufacturing cost, among others.

This work focuses on the theoretical-computational studies of different physical properties for $CsGe_xPb_{1-x}A_3$ and $CsSn_xPb_{1-x}A_3$ (A = Cl, Br, I; $0 \leq x \leq 1$) compounds, such as formation energy, electronic structure, electronic band-gap and optical absorption spectra. For this purpose, we have performed a set of ab-initio calculations based on quantum mechanics in the framework of the Density Functional Theory, together with machine learning techniques. The results obtained allowed us to understand their physical processes to promote synthesis and characterization of new high-performance materials for solar cells, seeking to be a more “eco-friendly” alternative by using less Pb in them, or even compounds without Pb.

Keywords: Perovskites, solar cells, Density Functional Theory, band-gap, machine learning.