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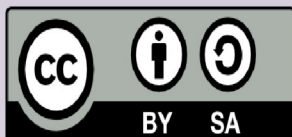
Publicaciones Científicas

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Electronic structure of all-inorganic perovskites.
Towards the design and modeling of solar cells

2021

*Evento: III Simposio Internacional de
Nanociencia y Nanotecnología NANO 2021.
Universidad Nacional de Trujillo (UNT), Perú*



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Nacional Arturo Jauretche

Cita recomendada:

Saltos, H.B., Limousin, L., Olivera, L.M., Cappelletti, M.A. y Gil Rebaza, A.V. (10-12 de noviembre de 2021).
Electronic structure of all-inorganic perovskites. Towards the design and modeling of solar cells [Resumen de
Ponencia]. III Simposio Internacional de Nanociencia y Nanotecnología NANO 2021, Universidad Nacional de
Trujillo, Perú. <https://rid.unaj.edu.ar/handle/123456789/2862>

Este documento es resultado del financiamiento otorgado por el Estado Nacional, por lo tanto, queda sujeto al cumplimiento de la
Ley N° 26.899

Secretaría de Políticas Universitarias del Ministerio de Educación de la Nación. Universidad, Cultura y Territorio 2021. Argentina.
Fortalecimiento de trayectos formativos para la educación y el trabajo. Experiencias de articulación con actores de la economía
popular y social de Florencio Varela.

Electronic structure of all-inorganic perovskites. Towards the design and modeling of solar cells

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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 ($A = \text{Cl, Br, I}$) 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: $\text{CsGe}_x\text{Pb}_{1-x}\text{A}_3$ and $\text{CsSn}_x\text{Pb}_{1-x}\text{A}_3$ ($A = \text{Cl, Br, I}$; $0 \leq x \leq 1$) 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 $\text{CsGe}_x\text{Pb}_{1-x}\text{A}_3$ and $\text{CsSn}_x\text{Pb}_{1-x}\text{A}_3$ ($A = \text{Cl, Br, I}$; $0 \leq x \leq 1$) 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.