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Lead-Free Perovskite based bismuth for solar cells absorbers

Ismail Benabdallah¹, Mourad Boujnah^{1,*}, Abdallah El Kenz¹, Abdelilah- Benyoussef^{1,2}, Mohamed Abatal³, Ali Bassam⁴

¹ Laboratory of Condensed Matter and Interdisciplinary Sciences (LaMCScI), Faculty of Sciences, University Mohammed V-, Rabat, Morocco

² Hassan II Academy of Science and Technology, Rabat, Morocco

³ Faculty of Engineering, Autonomous University of Carmen, 24180, del Carmen, Campeche, Mexico

⁴ Faculty of Engineering, Autonomous University of Yucatán, Av. Industrias no Contaminantes, Mérida, Yucatán, Mexico

* Corresponding authors: boujnah.mourad@gmail.com

Abstract:

Structural, electronic and optical absorption spectrum properties of lead free organometal halide perovskite CH₃NH₃BiX₃ (X =I₂Te, I₂S, I₂Se) as a new absorber for solar cells are studied in comparison to the well-known methylammonium lead iodide perovskite (CH₃NH₃PbI₃) by using first principle calculations. CH₃NH₃PbI₃ is known to be one of the major breakthrough in absorbing layers for solar cell material researches. These properties allowed this material to break records in the photoelectric conversion reaching 22% in Power Conversion Efficiency (PCE) in a short period of time, but this material have some drawbacks, putting obstacles for its commercialization. First one is the instability and the second one is the toxicity of lead. It was the reason why, the choice of Bi was the most appropriate to use in CH₃NH₃BiI₂Te, CH₃NH₃BiI₂S and CH₃NH₃BiI₂Se as it is a non-toxic element and also for the fact that it does not induce a big difference in the electronic structure, being close to lead in the periodic table. Furthermore, for its high optical absorption in the visible obtained on CH₃NH₃BiI₂Te, CH₃NH₃BiI₂S and CH₃NH₃BiI₂Se compounds. These advantages may suggest that halide perovskite CH₃NH₃BiX₃ (X =I₂Te, I₂S, I₂Se) based bismuth could be a promising alternative to CH₃NH₃PbI₃. These results may provide a basis for future applications in photovoltaic domain.

Keywords: Lead free perovskite, absorber materials, solar cells, first principle calculations.

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