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AB INITIO STUDY OF ELECTRONIC PROPERTIES OF LEAD HALIDE PEROVSKITES FOR OPTICAL PERFOMANCE OF SOLAR CELL

ABSTRACT
The ever increasing demand of energy has necessitated the need of coming up with measures of seeking alternative energy sources. Solar energy is one of the most important alternative sources of energy. However,the use of the first and second generations solar cells made of silicon in making solar panels has notable shortcomings such as unaffordability and lack of longevity of the electric power generated. In this regard, therefore, we report the initial electronic structure results of lead halide perovskite (APbX3) where (X = I/Br/Cl and A=CH3NH3/CH(NH2)2+/Cs+) for application in solar cells. The density functional theory investigations was done using Pwscf code from Quantum espresso and calculation of the electronic properties of lead halide perovskites done to predict its suitability in photo voltaic applications. The current calculated results of lattice parameter and band gap of this material is in agreement with other reported calculations from experimental and theoretical studies. Mechanical properties are also reported and compared with other studies.
Key words; Electronic properties, optical properties, solar cells

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