Contribution ID: **17** Type: **Abstract for Research Paper**

Ab Initio Study of Mechanical Properties of Lead Halide Perovskite For Photovoltaic Application.

The ever increasing demand for 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. 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, we report the mechanical properties results of lead halide perovskite (ABX3) where (X = I/Br/Cl , A=CH3NH3/CH(NH2)2+/Cs+ and B can be divalent metal ion for example (Pb2+, Ge2+, or Sn2+).Calculations were done using density functional theory within generalized gradient (GGA) approximations, using norm-conserving pseudopotentials generated from the Troullier-Martins scheme. Elastic constants calculated in this work include as bulk modulus B, Young's modulus E, shear modulus G and Poisson's ratio ν were calculated using the Voigt–Reuss–Hill averaging scheme. The Poisson's ratio ν obtained was 0.25 which is close to the experimental value of 0.28, this value confirms that CH3NH3PbI3 is a ductile material. The result from the elastic constants done compares well with previously done work. A ductile material can be moulded to different shapes and size, therefore CH3NH3PbI3 is suitable to be used as a photovoltaic material.

Primary author: Ms KIPKWARKWAR, Truphena .J. (Kabarak University)

Co-authors: Dr NYAWERE , Phillip .O. (Kabarak University); Dr MAGHANGA , Christopher .M. (Kabarak University)