
Contribution ID: **306** Type: **Oral Presentation**

# Study of inorganic lead halide perovskites properties using density functional theory for photovoltaic and optoelectronic devices

*Tuesday, 5 July 2022 15:15 (15 minutes)*

Cesium lead iodide perovskites have attracted significant interest due to their rapidly increasing efficiency when used in solar cells applications. Density functional theory was used to investigate the structural,electronic, elastic, and optical properties of CsPbI3, CsPbI2Br, CsPbBr2I and CsPbBr3 perovskite materials. The generalized gradient approximation, GGA-PBE was used to estimate the band gaps of these materials. There is gradual increase in the band gap values due to mixing composition of I and Br which may be attributed to the ionic radii differences b etween Br and I in the mixed halide compounds, and the hybridization tendency of the X-halide (I 5p and Br 4-p) state. Structural analysis shows that the calculated lattice parameters were consistent with experimental parameters reported in the literature. Also, mechanical properties including elastic constants, bulk modulus, shear modulus, Young's modulus, Poisson's ratio, and anisotropy factor were computed. The calculated electronic properties showed that the energy band gap of CsPbI3 could be tuned by substituting iodine with bromine. All four compounds were found to be semiconductors with direct energy band gaps in R symmetry point between 1.466 and 2.494 eV as predicted by the GGA-PBE. The optical properties of these perovskite compounds against the incident photon energy radiation indicate that the materials could be good candidates for solar cells applications. The elastic constants were also determined, and they revealed the ductile nature of these compounds.

## Apply to be considered for a student ; award (Yes / No)?

Yes

## Level for award;(Hons, MSc, PhD, N/A)?

PhD

**Primary author:** MALEKA, Prettier Morongoa (Yes)

**Co-authors:** Mr DIMA, Ratshilumela Steve (University of venda); Prof. MAPHANGA, Regina (CSIR); Prof. NTWAEABORWA, Martin (Wits)

**Presenter:** MALEKA, Prettier Morongoa (Yes)

**Session Classification:** Physics of Condensed Matter and Materials

**Track Classification:** Track A - Physics of Condensed Matter and Materials