Contribution ID: **86** Type: **Poster Presentation**

First-Principles Investigation of the Structural, Electronic, and Optical Properties of $CsPbI_3$ Perovskite for Solar Cell Applications

The growing global energy crisis necessitates the search for sustainable and environmentally friendly alternatives to fossil fuels. In this study, first-principles Density Functional Theory (DFT) calculations were employed to investigate the structural, electronic, optical, and mechanical properties of the all-inorganic perovskite compound $CsPbI_3$, a promising material for clean energy applications. Using the generalised gradient approximation (GGA-PBE functional) within Materials Studio, the crystal structure was optimized, and the electronic band structure, density of states (DOS), and optical absorption spectrum were analyzed. The results revealed that $CsPbI_3$ exhibits a suitable bandgap and strong optical absorption, making it a potential candidate for efficient solar cell applications. Mechanical property calculations, including elastic constants, bulk modulus, shear modulus, Young's modulus, and Poisson's ratio, confirmed the material's mechanical stability, satisfying the stability criteria for cubic systems. The material resisted shear deformation and ductile behaviour, as indicated by a bulk-to-shear modulus ratio (B/G) of 2.01 and supportive Pugh's and Poisson's ratios. Furthermore, low reflectance and high optical conductivity suggest excellent optoelectronic performance, while thermodynamic analysis confirmed its stability under operating conditions. Overall, the study provides valuable theoretical insights into the suitability of $CsPbI_3$ perovskite for solar energy harvesting and other energy-related applications, contributing to the advancement of clean and sustainable energy technologies.

Apply for student award at which level:

MSc

Consent on use of personal information: Abstract Submission

Yes, I ACCEPT

Primary authors: XOLILE, Mkhatshwa (University Of Venda); RANWAHA, Tshifhiwa (University Of Venda); Dr RUGUT, ELKANA (university of venda); MALUTA, Eric (University of Venda)

Presenter: XOLILE, Mkhatshwa (University Of Venda)

Session Classification: Poster Session

Track Classification: Track F - Applied Physics