Investigation of MgHfX3(X= S, Se) Chalcogenide Perovskites: Findings on Structural, Electronic, and Optical Properties For Photovoltaic Applications

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**Abstract**. Due to their various qualities and their potential use in optoelectronic, thermoelectric and photovoltaic systems, chalcogenide perovskites materials have received much attention [1-2]. Using a computational approach based on density functional theory (DFT), we investigate the structural, electronic and optical properties of MgHfX3(X= S, Se) chalcogenides. The optimized volume, bulk modulus and lattice parameters are calculated to estimate the stability of these compounds [3]. The electronic characteristics, which are density of states and band structure, reveal their band gap tunability and semiconducting behaviour [4]. To examine their potential in photovoltaic applications, the optical characteristics including dielectric functions, absorption coefficients, refractive index, and optical conductivity are calculated. From the analysis ​​of all these properties it is clear that these materials have high absorption coefficient and direct band gap which is very suitable for photovoltaic applications.

References:

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