

Title: First-principles study of the structural, mechanical, electronic, optical, and elastic properties of non-toxic XGeBr₃ (X=K, Rb, and Cs) perovskite for optoelectronic and radiation sensing applications

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Abstract: In this study, a comprehensive analysis of the structural, electronic, optical, and elastic properties of cubic perovskite structure was carried out using GGA-PBE functional based density functional theory in CASTEP code. The simulated values of the lattice parameter were increased with the changing of X from K to Cs ($a = 5.51 \text{ \AA}$, $5.54 \text{ \AA}$, and $5.59 \text{ \AA}$ respectively). All the compounds possessed direct band gaps and acquired values for the structures, and were 0.525 eV, 0.599 eV, and 0.708 eV, respectively. Furthermore, the atomic orbital's contribution to the formation of band structure was clarified thoroughly. The thermodynamic, as well as the mechanical stability, has been accomplished with the assurance of negative formation energy and Born-Huang approximation. In addition, a larger shearing modulus attained by manifests its strength. Moreover, all structures bear the proof of having ductility and existing central force inside the structures. Finally, the calculated anisotropic index notifies that all structures exhibit anisotropy with the trend of $\alpha < \beta < \gamma$. This is also authenticated through the 3D anisotropy contour plot generated by utilizing ELATE software, which is for the first time in regard to the comparative scenario among them. With the investigation of the optical characteristics of the compounds, intriguing features such as broad absorption spectrum, high dielectric function and refractive index at zero photon's energy, and high conductivity have been affirmed accompanying the marginal value of loss function as well as reflectivity that elevates the probability of being employed in optoelectronic applications along with different absorber layers of tandem solar cells. In addition, these compounds could be used as radiation detectors since they have broad absorption at extreme ultraviolet rays.

Keywords: Cubic perovskite, Density Functional Theory (DFT), GGA-PBE functional, CASTEP, Structural properties, Electronic properties, Optical properties, Elastic properties

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