# Abstract

Halide perovskites (PVSK) have come a long way in recent years, but they still face two key difficulties in terms of broad deployment: long-term stability and the usage of lead. Therefore, to reduce existence of lead from the existing compounds, we proposed silicon (Si) at the position of lead $A_2BX_6$ (here A = Cs, B = Si, X = Cl,Br, and I). The highly effective Perdew-Burke-Ernzerhof (GGA-PBE) functional are used in well-known WIEN2k software to investigate the structural, electronic, and optoelectronic properties under the working platform of density functional theory (DFT). All the selected materials were optimized with face centred cubic structure having a space group $Fm\bar{3}m$ (No. 225). The calculated parameters like lattice constant of $A_2BBr_6$, (a=b=c=21.94251 Bohr), bandgap (1.74eV), and optical properties are similar with the existing practical and theoretical outcomes. The compounds, $Cs_2SiCl_6$ and $Cs_2SiBr_6$ show band_gaps lies in the optimal range of 1.76–3.54 eV, and the conduction_band_maxima (CBM) and valence_band_maxima (VBM) are localized at the gamma symmetry line $\Gamma(0.0,0.0,0.0)$ in the first Brillouin zone, which shows that the studied compounds have direct band_gaps. The valance band formed due to the hybridization of Cs-s, Si-s,p,d, Br-s,p and in conduction band it has a contribution of Cs-s,p, Si-s,p,d, Br-s,p,d. These perovskites are useful for high-performance single and multi-junction perovskite solar cells due to their perfect bandgap, high dielectric constants, and optimum light absorption.