Abstract
A reasonable development has been made in past few years in halide perovskite compounds. Cubic perovskite have enhanced a potential interest to the researchers due to their extensive applications in the optical devices. For last decades, peroveskte specially based on lead gives outstanding impact in photovoltaic applications. Although it consider to be a good material in optical devices, but two foremost challenges yet it has. One of them is its long term stability and other is excessive use of lead. It is detected that lead create toxicity in environment and it's also very tough to excrete from body. So it's compulsory to find such elements which are environment friendly along with decent stability.
Therefore, we make a replacement of lead and use Silicon in our studied compound. ABX_3 is general formula of perovskite where, (A = Li, B = Si, X = Cl, Br, I). To investigate the structural, electronic, and optical properties we use (PBE – GGA) approximations which are implemented by WIEN2K software which is used in the frame work of Density functional theory (DFT). Our studied compounds successfully optimized through Birch Murunghan's equation having space group (at No.225). The calculated parameters like lattice constant of ABX_3 (a = b = c = 12.5353 Bohr).our studied compound $LiSiCl_3$, $LiSiBr_3$ and $LiSiI_3$ has shown band gap of 1.41 eV, 1.35eV and 0.95 eV respectively. The nature of band gap is found direct band gap which precisely shown in band gap structure as conduction band minima (CBM) and valence band maxima (VBM) lies on the same symmetry points R (0,0,0,0,0,0) in the first Brillioun zone. An ideal band gap, good dielectric constant value, and high absorption coefficient value of Halides perovskite make him appropriate for high performance perovskite solar cell. Fm3m