

ABSTRACT

In the past few years fluoroperovskites have gained immense interest by researchers and making them hot candidates for optoelectronic applications. In this work, first time, we have computed the structural, electronic and optical properties of pure and Be/Sr-doped fluoroperovskite KMgF_3 . The structural stability is analysed by calculating optimised lattice parameters of pure and doped (1.04%, 4.22% and 7.04%) KMgF_3 . The structural results show that the phase transformation from cubic to body centre A_a tetragonal structure. The band gap of pure KMgF_3 is indirect, at G and R symmetry points, which converted to direct band gap, at G symmetry point, after doping at all doping concentrations. The anomalous behaviour of Be decreases the band gap from 6.135 to 2.469 eV and the insulating behaviour is transformed to semi-conducting nature. While in Sr case, the band gap decreases (6.153–5.446 eV) but the nature of the compound remains insulating. The optical properties like absorption, refractive index, reflection, loss function and extinction coefficient are computed from the complex dielectric function. The study of electric and optical properties will provide the basis for future applications of KMgF_3 in optoelectronic devices.