

## **Shift of band gap from direct to indirect and optical response of LiF under pressure**

### **Abstract**

We hereby are reporting the transition pressure at which lithium fluoride (LiF) compound transforms from direct band gap to indirect band gap insulator on the basis of FP-LAPW calculations. The fundamental band gap of LiF compound suffers direct to indirect transition at a pressure of 70 GPa. The study of the pressure effect on the optical properties e.g. dielectric function, reflectivity, refractive index and optical conductivity of LiF in the pressure between 0-100 GPa, shows that this pressure range is very critical for LiF compound as there are significant changes in the optical properties of this compound.

**Keywords** — Band structure, DFT, hydrostatic pressure, Lithium fluoride, optical properties