The Electronic Properties of the Cubic $KMgF_3$ Perovskite under Pressure Effect

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Materials with perovskite crystal structure have a great potential for applications in catalysis, optoelectronics, semiconducting devices, and nonvolatile data-storage applications [1]. Fluoroperovskite KMgF3 finds applications as a vacuum-ultraviolet-transparent material for lenses in optical lithography steppers and in electrooptical applications [2, 3]. When doped appropriately, it is very promising for scintillators and radiation dosimeters [4].

The present work deals with the behaviour of electronic properties, namely, the energy band gaps, and the valence bandwidth of KMgF3 subject of hydrostatic pressures up to 30 GPa. The electronic energy bands have been evaluated here within the GGA and GWA approaches. The GWA results found here for the first time. All the calculations were carried out by means of the ABINIT code [5].

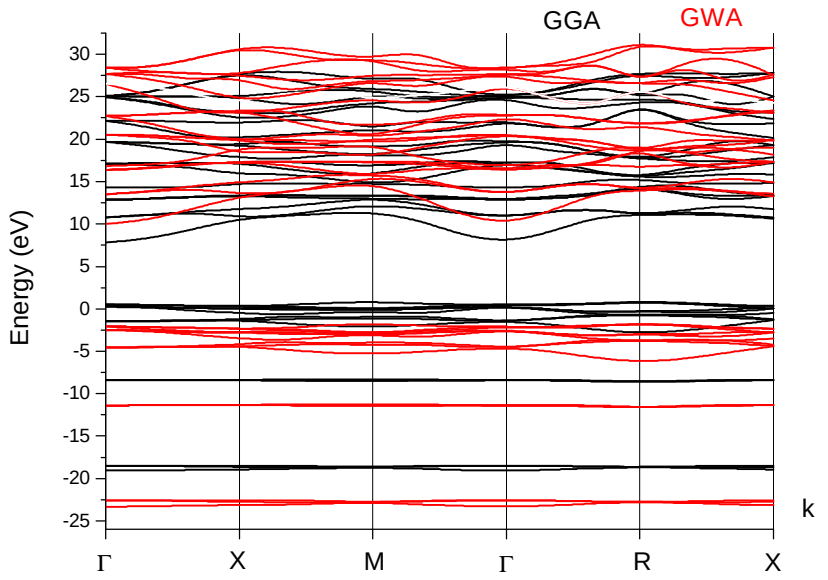

Figure 1. The electronic energy bands in $KMgF_3$ cubic crystal at ambient pressure.

We found that $KMgF_3$ has an indirect fundamental band gap Γ–R. The minimum optical gap Γ– Γ equals to 7.31 eV (GGA) and 12.04 eV (GWA). The fundamental gap equals to 6.99 eV (GGA) and 11.72 eV (GWA). The obtained here GGA band gaps are well compared with previous calculations. The measured absorption edge is 10.8 eV. So the GGA band gaps show a significant underestimation. The difference between GWA fundamental band gap and measured absorption edge equals to 0.92 eV and is found to be an exciton binding energy.

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