Nanoscale physics

Study of structural, mechanical and electronic properties of 3R-$CuGa_{1-x}Fe_xO2$ super lattice from first principle calculations.

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Abstract

We calculated the structural parameters and mechanical and electronic properties of 3R- $CuGa_{1-x}Fe_xO2$ super lattice with ($0 \leq x \leq 0.05$) using the first-principles density-functional theory (DFT) as implemented in CASTEP code[1]. The obtained results were compared with other previous ones[2]. The change in lattice constants and band gap is investigated by increasing the concentration of iron. Also, the mechanical stability of this phase is studied by calculating elastic constants.

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2. J. Barry. Haycock, M. Kylee Rice, P. James. Lewis, High-throughput calculations of alloyed delafossite materials: Application to $CuGa_{1-x}Fe_xO_2$. Computational Materials Science -2014.-86, -P.155-164.