EFFECTS OF ANTIMONY-DOPED ON YTTRIUM-SITE OF YBCO-123 USING DENSITY FUNCTIONAL THEORY VIA FIRST PRINCIPLE STUDY

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ABSTRACT

EFFECTS OF ANTIMONY-DOPANT ON YTTRIUM SITE OF YBCO-123 USING DENSITY FUNCTIONAL THEORY VIA FIRST PRINCIPLE STUDY

Antimony-doped on Yttrium site of $YBa_2Cu_3O_\delta$ was examined using Density Functional Theory via First Principle Study. The effect of Sb doping on YBCO-123 has been studied via computational simulation to determine the structural properties and electronic properties. From the simulation of Material Studio CASTEP software through Density Functional Theory, the optimized crystal structure has been developed. Generally, the lattice parameters results shows that the doped samples did not differ much from the standard sample for x = 0.0625 until x = 0.1875 except for Sb doped of x = 0.2500 until x = 0.5000 that displayed shortening of a-parameter and b-parameter while elongating c-parameter. The sample has a crystal structure of orthorhombic as they have different lattice parameter where $a \neq b \neq c$. For the electronic band structure, the addition of Sb (III) have a negligible effect on the main crystalline structure of the YBCO-123 specially at low concentration from doping x = 0.0625 to x = 0.2500 but start to be unstable specially at high concentration from doping x = 0.3125 to x = 0.5000 The results were analysed that the states of existing holes in $Y_{1-x}Sb_xBa_2Cu_3O_\delta$ are obtained by investigating the states above the Fermi level, not below it. The density of states graph showed that the electron near and below Fermi level was highly concentrated which are involved in the formation of superconducting properties. The charge density for one electron per unit cell above Fermi level shows that holes exist mainly in the $Cu\text{-}O_2$ plane. The energy shifts observed via total and partial density of state at Cu 3*d* and O 2*p* orbital towards the Fermi level with different concentration of dopant confirms the superconducting ability and its electronic behaviour.