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

NURHAFIZHAH BINTI MOHD RAZALI

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ABSTRACT

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

The effect of Antimony,Sb doped on Barium,Ba site of $YBa_{2-x}Sb_xCu_3O_\delta$ superconductor have been studied using density functional theory via first principle study. The superconducting properties were investigated in computer simulation. The computer simulation used to determine the crystalline structure, band structure, density of states, the electron density and bond length between the Cu-O chain and CuO_2 plane. Generally, the $YBa_{2-x}Sb_xCu_3O_\delta$ has orthorhombic crystal structure since the value of a, b and c are not same. From the band structure, the largest band gap is when $x = 0.5000$ where the band gap is slowly increasing between conduction band and valence band. Next, in the density of states, the electrons are more concentrated towards Fermi level. In the electron density differences and bond length, the effect of electron contribution by Cu and O were observed. From all result above, the obvious modification happened when the concentration of Sb is $x = 0.5000$. From the observation when the concentration is $x = 0.5000$, the $YBa_{2-x}Sb_xCu_3O_\delta$ is over-doped with Antimony.