STRUCTURE AND ELECTRONIC PROPERTIES OF CALCIUM DOPED YBCO-247 SUPERCONDUCTOR VIA DENSITY FUNCTIONAL THEORY

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ABSTRACT

The effect of doping calcium to Y-247 superconductor was studied via Density Functional Theory through the electron density of a material at ground state due to Hohenberg-Kohn and Kohn-Sham theorem respectively. Calcium was used as a dopant to substitute Cu^{2+} and Y^{3+} that possibly increases the hole concentration. It was found that direct substitution into the Cu-site of cuprate superconductors will directly affect its properties. Density Functional Theory (DFT) calculation was used as the simulation platform to calculate the energy band gap, density of states and the electron density of the Y-247 phase. The structure retains it orthorhombicity when doped at both side but decreases the lattice parameter *c*. An increase in energy band gap above the Fermi level can be seen as the concentration increase from x=0.02, x=0.04, x=0.06, x= 0.08 to x=0.10 for Ca-doping into Y-site of the system. Ca-doping into Cu-site shows a decrease in the energy band gap when the value of dopant increases. Doping Ca into Y-site shows an increase in the density of state with value x=0.02 and x=0.04 but started to decrease at x=0.06. In Cu-site, doping concentration of x=0.04 shows the highest at partial density of state of oxygen 2*p* orbital. The electron density distribution show a steady distribution along CuO chain and CuO_2 plane which shows high probability of electron existence which proves the superconducting properties at the CuO_2 plane and CuO chains respectively as the charge carriers.

CHAPTER 1

INTRODUCTION

1.1 Background and problem statement of study

Since the discovery of high T_c superconductors, these type of superconductors have been extensively studied by researchers. Superconductors are materials that transport electrons into another atom without resistance. This phenomena was obtained by cooling the material to a certain critical temperature, *Tc*. In 1911, this phenomena was discovered by Heike Kamerlingh Onnes by studying the superconductivity in mercury. The studies of superconductors are very important due to its zero resistance properties. This shows that there are no energy loss when the material becomes a superconductor. High T_c superconductor was identified by observing material that exhibit basic properties such as zero resistance, Meissner effect and pairing of quasi-particle with charge 2e (Singh & Kumar, 2018).

Superconductor were classified into two categories which is Low Temperature Superconductor (Type-I Superconductor) and High Temperature Superconductor(Type-II Superconductor). Early discovery of high T_c superconductors such as $(LaBa)_2CuO_4$ with T_c of 40K and $YBa_2Cu_3O_7$ with T_c of 95K have encourage researchers to study other oxide superconductor with