ELECTRICAL PROPERTIES & STRUCTURE PROPERTIES OF IRON DOPED YBCO-247 VIA FIRST PRINCIPLE THEORY

MUHAMMAD ASHRAFF BIN HAMDAN

Final Year Project Report Submitted in
Partial Fulfilment of the Requirements for the
Degree of Bachelor of Science (Hons.) Physics
in the Faculty of Applied Sciences
Universiti Teknologi MARA

JANUARY 2020

TABLE OF CONTENTS

LIST OF FIGURES

ABSTRACT

ELECTRICAL PROPERTIES & STRUCTURE PROPERTIES OF IRON DOPED Y-247 VIA FIRST PRINCIPLE THEORY

YBCO is one of the high temperature superconductors that are widely studied by the researchers to enhance its superconducting properties. By improving the critical temperature (*Tc*) and critical current density (*Jc*) of the superconductor, it can be used in various applications to withstand the high temperature. Y-123 phase is one of the YBCO family that is commonly used to study the doping effect to the structure. The Y-123 phase has critical temperature about 90 K. Other phase such as Y-247 is not commonly studied due to high oxygen pressure requirements to build it. Common studies use solid-state method or sol-gel method to make the pure and doped YBCO. Computational method was used to study the electrical and structural properties of Y-247. The structure was doped with different amount of Fe at Y-site and Cu-site. Using the first principle theory it can calculate the band structure, density of states and analyze the electron distribution. For both Y-site and Cu-site, same pattern of band structure were shown. The valence band and conduction band are overlapped with each other and showing the conducting properties. Copper *3d* orbital state and oxygen *2p* state plays important role to maintain the superconducting properties with electron-hole migration concept. Energy band gap at Y-site increasing in number but decrease when x=0.08 and x=0.10 were doped to the structure. For Cu-site, the energy band gap decrease as the concentration of Fe increase. The Partial Density of States shown that the optimum concentration of Fe at Y-site is x=0.02 and at Cu-site is x=0.08. The electron distribution shows a high concentration can be found in the CuO chain and CuO_2 planes. The bond length among CuO chain and CuO_2 plane at Cu-site decreases as the Fe concentrations increases.