# EFFECTS OF SILVER-DOPED ON BARIUM-SITE OF YBCO123 SUPERCONDUCTOR USING DENSITY FUNCTIONAL THEORY VIA FIRST PRINCIPLE STUDY

**FATIN NADIAH BINTI ABDUL JABAR**

**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

### EFFECTS OF SILVER-DOPED ON BARIUM-SITE OF YBCO123 SUPERCONDUCTOR USING DENSITY FUNCTIONAL THEORY VIA FIRST PRINCIPLE STUDY

The effect of Ag-doping on Ba-site of YBCO phase 123 has been analysed via computational simulation to determine the structural and electronic properties. The software used in this project is Material Studio, CASTEP. The structural properties that have been analysed were lattice parameter and bond length while the electronic properties were band structure, density of state, partial density of state and electron density difference. Generally, YBCO has a perovskite-orthorhombic structure where $a \neq b \neq c$. The orthorhombicity in this project remains unchanged as there were not much difference in lattice parameter for all concentrations of dopant. The bond length at concentration x=0.2500 shows a structural modification due to the changes in oxygen content at CuO chain and changes in electronic arrangement in CuO plane. From the simulation of Material Studio CASTEP software through Density Functional Theory, the optimized crystal structure has been developed. The band structure at the concentration x=0.2500 shows no energy band gaps since the conduction bands and valence bands overlap with each other. The density of states graph shows that the electron near and above Fermi level was highly concentrated which are involved in the formation of superconducting properties. Based on other studies and theory, we can assume that when the YBCO is over-doped which is more than x=0.2500, it will destroy the superconductivity properties. This is resulting in the excess of hole content which will lower the critical current density, $J_C$ and critical temperature, $T_C$.