

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

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TABLE OF CONTENTS

	Page
ACKNOWLEDGEMENTS	iii
TABLE OF CONTENTS	iv
LIST OF TABLES	vi
LIST OF FIGURES	vii
LIST OF ABBREVIATIONS	ix
ABSTRACT	x
ABSTRAK	xi
CHAPTER 1 INTRODUCTION	1
1.1 Background of the study and problem statements	1
1.2 Significant of study	3
1.3 Objectives of study	3
CHAPTER 2 LITERATURE REVIEW	5
2.1 Superconductors	5
2.2 YBCO (Yttrium Barium Copper Oxide)	5
2.3 Critical Temperature (T_c)	7
2.4 Critical Current Density (J_c)	7
2.5 Doping	8
2.6 Fermi Level and Energy Band Gap	9
2.7 Density of States (DOS)	10
2.8 Computational Method	11
CHAPTER 3 METHODOLOGY	14
3.1 Apparatus	14
3.2 Finding the crystal structure	14
3.3 Model Refinement	15
3.4 Calculation and analysis of the structure	16
CHAPTER 4 RESULTS AND DISCUSSION	19
4.1 Crystal structure	19
4.1.1 Optimization of Crystal Structure	20
4.1.2 Lattice Parameter	21
4.1.3 Structural Formula	23

4.2	Band Structure	24
4.3	Density of States	27
4.4	Electron Density Distribution	35
CHAPTER 5 CONCLUSION AND RECOMMENDATIONS		39
5.1	Summary	39
5.2	Future research	40
CITED REFERENCES		41
APPENDICES		44
CURRICULUM VITAE		45

LIST OF FIGURES

Figure	Caption	Page
2.1	Comparison crystal structure between Y-123 (left) and Y-247 as mentioned by H. Schwer, E.Kaldis (1993)	6
2.2	The gap found in the 2223 system (left) and in the 2212 system (right) by Republic (1994)	10
2.3	The DOS of each element in YBCO to study the concentration of electron relating to the CuO chain (Schwingenschlögl & Schuster, 2007)	11
2.4	The latest DFT formula revised by Kohn and Sham (1965) to calculate electron energies	12
3.2.1	Brief process on how the undoped and doped Y-247 structure built and analyzed	14
3.3.1	Step 1 - The Geometry Optimization in the CASTEP calculation	15
3.4.1	Step 2 - CASTEP Setup for Energy calculations	16
3.4.2	Step 3 - CASTEP selection to calculate Band Structure, Density of States and Electron Density Differences	17
3.4.3	Step 4 - CASTEP Analysis for Band Structure	17
3.4.4	Step 5 - CASTEP Analysis for Density of States	18
3.4.5	Step 6 – CASTEP Analysis for electron density	18
4.1	The crystal structure of Y-247 obtained from the website according to Bordet (1988)	19
4.2	Y-247 Crystal Structure optimized with its Brillouin Zone	20
4.3	Energy Band Gap of pure Y-247	24
4.4	Energy Band Gap of Y-247 Fe doped at Y-site	25

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 (T_c) and critical current density (J_c) 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 CuO₂ planes. The bond length among CuO chain and CuO₂ plane at Cu-site decreases as the Fe concentrations increases.