UNIVERSITI TEKNOLOGI MARA

A STUDY ON STRUCTURAL AND ELECTRONIC PROPERTIES OF Ag AND Sb-DOPED IN Ba-SITE OF $YBa_2Cu_3O_{7-\delta}$ SUPERCONDUCTOR VIA COMPUTATIONAL METHOD

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Thesis submitted in fulfillment
of the requirements for the degree of
Doctor of Philosophy
(Physics)

Faculty of Applied Sciences

August 2022

ABSTRACT

The structural and electronic properties of $YBa_2Cu_3O_{7-\delta}$ superconductors doped with Ag and Sb have been predicted theoretically. The Ag ionic radius of 126 pm matches the Ba atom, which is 134 pm, promoting electrical conductivity. When an Sb atom with a lower ionic radius of 76 pm is doped into the Ba-site of $YBa_2Cu_3O_{7-\delta}$, it undergoes structural modifications. To further understand its interatomic behaviour, the structural and electronic properties of both elements doped at the Ba-site of $YBa_2Cu_3O_{7-\delta}$ were computationally analysed, over a wide range of dopant percentages. Focuses were made at $x = \pm 0.200$, where Ag dopant enhanced electrical conductivity, and Sb dopant provided structural alterations from prior experiments. The CASTEP computer code was applied employing various exchange-correlation functionals such as Local Density Approximation and Generalized Gradient Approximation on standard DFT (LDA CA-PZ, GGA-PBE, GGA-PBEsol, and GGA-WC) with the VCA technique and 2×2×1 supercell Hubbard U correction method, DFT+U (LDA CA-PZ+U, GGA-PBE+U, GGA-PBEsol+U, and GGA-WC+U) with U = 10.0 eV. Based on the computational calculation, the GGA-PBEsol and GGA-PBEsol+U give the best-validated results as compared to the referred experimental and theoretical studies. The lattice parameters of all samples differ by less than 5% from the previous experimental investigation. DFT via GGA-PBEsol indicated considerable bond length changes along the Cu(1)-O(1) and Cu(1)-O(4) by +0.62% and -0.38%, respectively. CuO chain behaves as the charge reservoir to the conducting CuO_2 plane. The bond length along Cu(2)-O(2), Cu(2)-O(3), and Cu(2)-O(4) changes to experimental by +0.52%, +0.36%, and -4.65%, respectively. As Ag dopant was added to the sample, the bond length on the CuO chain and CuO_2 plane decreased, indicating contraction due to impurity addition at the Ba-site. As Sb dopant was added, an increment of bond length was observed along with Cu(2)-O(2) and Cu(2)-O(3) by +2.89% and +23.95%, respectively, showing an increment of bond length upon Sb doping. The electronic band structure, total and partial density of states (DOS), and electron density show that hybridization exists between the Cu 3*d* and O 2*p* atoms, verifying the Van Hove Singularity at the Fermi level. Applying GGA-PBEsol, the bandgap of 3.30 eV for pure $YBa_2Cu_3O_{7-\delta}$ shows a 17.50% difference compared to other theoretical work. When the DFT+U method was employed via GGA-PBEsol+U, the calculated electronic bandgap for pure, Ag and Sb-doped samples was increased. The DOS on Cu(1) 3*d*, O(1) 2*p*, and O(4) 2*p* atoms along the CuO chain and Cu(2) 3*d*, O(2) 2*p*, and O(3) 2*p* atoms on the CuO_2 plane were increased when doped with Ag atom. When doped with Sb atom, the increment of Cu(1) 3*d*, O(1) 2*p*, and O(4) 2*p* atoms are +132.84%, +136.73%, and +104.33% on CuO chain and along the CuO_2 plane for Cu(2) 3*d*, O(2) 2*p*, and O(3) 2*p* atoms by +96.70%, +103.36%, and +121.01%, respectively. Impurity dopants have the highest concentration on O atoms due to their electronegativity, increasing their electron density. As Ag and Sb dopants were added to the Ba-site of $YBa_2Cu_3O_{7-\delta}$, respectively, the total charge on Cu(2) increased substantially where Cu atoms exhibit the most atomic population on orbitals. This work will help researchers understand the structural and electronic properties gained by computational methods. This approach could be used in future experiments to establish the Ag and Sb dopant percentages in $YBa_2Cu_3O_{7-\delta}$ superconductor, resulting in high-performance sample preparation.

ACKNOWLEDGEMENT

First and foremost, I would like to express my heartfelt gratitude to my supervisor, Prof. Ts. Dr. Azhan Bin Hashim@Ismail, for his unwavering support of my PhD studies, as well as his patience, enthusiasm, and vast expertise. His advice was invaluable during the research and writing of this thesis. Also, thanks to my co-supervisor, Assoc. Prof. Dr. Mohamad Fariz Bin Mohamad Taib, for his guidance and knowledge sharing during the study.

My heartfelt gratitude also goes to Dr. Nur Hafiz Bin Hussin, Dr. Mohd Hazrie Bin Samat, and everyone at iMADE, the Theoretical and Computational Lab of UiTM Shah Alam, and Postgraduate Research Lab of UiTM Cawangan Pahang, Kampus Jengka for allowing me to join their team and access to their laboratory and research facilities. This research would not be possible without their invaluable assistance.

To my dear friends, Nurbaisyatul Ermiza Binti Suhaimi, Norihan Binti Yahya, Nor Habibah Binti Mohd Rosli, Roziana Binti Bujang, and Siti Nasuha Binti Mohd Rafien, my labmates and friends who have been involved in my PhD path. You have made the road a lot easier with your encouragement and support, which I will never be able to return.

Last but not least, my heartfelt gratitude goes to my family: my parents, Saipuddin Bin Mohamad and Rustidah Binti Daud, my parents-in-law, Arifin Bin Husin, and Norziah Binti Bakar, my siblings and siblings-in-law for spiritually supporting me throughout my PhD journey and my life in general. My special thanks goes to my beloved husband, Muhd Hellemey Bin Arifin, and my beautiful children, Nur Aysha Binti Muhd Hellemey, Nur Alya Binti Muhd Hellemey, Muhammad Ammar Bin Muhd Hellemey, and Muhammad Arman Bin Muhd Hellemey, for always being present, supportive, and understanding of the difficulties I had while learning. Without your help, I would not have completed this study. I will never be able to express my gratitude sufficiently to everyone who has contributed in some way to my PhD journey. Thank you very much.

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