

STUDIES ON CORRELATION BETWEEN
ELECTRONIC STRUCTURE AND ELECTRONIC
CONDUCTIVITY IN MoX_2 ($X = \text{S}, \text{Se}$ and Te)

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Thesis submitted in fulfillment of the requirements
for the award of the degree of
Bachelor of Applied Science (Honor) Material Technology

Faculty of Industrial Sciences & Technology
UNIVERSITI MALAYSIA PAHANG

DECEMBER 2016

SUPERVISORS' DECLARATION

I hereby declare that I have checked the thesis and in my opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Bachelor of Applied Science (Honor) Material Technology.

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STUDENT'S DECLARATION

I hereby declare that the work in this thesis is my own except for quotations and summaries which have been duly acknowledged. The thesis has not been accepted for any degree and is not concurrently submitted for award of other degree.

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DEDICATION

Special Dedication to my supervisor, my family members,
my friends and all faculty members
for all your care, support and believe in me.

ACKNOWLEDGEMENTS

I would like to express the deepest appreciation to my supervisor, Dr Saifful Kamaluddin Bin Muzakir for his great ideas, invaluable guidance, continuous encouragement and constant support in making this final year project research possible. I am truly grateful to have a supervisor like him. The way he guide me not really stressful and forcing but more to independent work. It make me manage to schedule my lab work and other work properly and perfectly. I sincerely thanks for the time spent proofreading and correcting my many mistakes.

In addition, my sincere thanks go to all my lab mates and members of the material technology classes, who helped me in many ways to solve some problems and also giving some good opinion ideas about my research project. Their support during my weak time never ending and always continuous.

I acknowledge my sincere indebtedness and gratitude to my parents for their love, dream, support, and sacrifice throughout my life. They act as my backbone to finish this research with patiently. Their prayers really meaningful to make me success. The positive aura from them really make me be a person with full responsibilities like who I am today.

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LIST OF SYMBOLS

\sim	-	approximately
%	-	percent
λ	-	wavelength
a_0	-	Exciton Bohr radius
\AA	-	angstrom (10^{-10})
\AA^3	-	volume
$t_{\text{-ML}}$	-	monolayer thickness
$t_{\text{-Offset}}$	-	thickness offset
$E_{g\text{-ML}}$	-	monolayer bandgap
$E_{g\text{-Offset}}$	-	bandgap offset
σ	-	conductivity

LIST OF ABBREVIATIONS

EC	-	electrochemical capacitor
PC	-	pseudocapacitor
EDLC	-	electrochemical double layer capacitance
SSC	-	symmetric supercapacitor
ASC	-	asymmetric supercapacitor
AC	-	activated carbon
GPS	-	global positioning system
HF	-	Hartree-Fock
B3LYP	-	Becke, 3-parameter, Lee-Yang-Parr.
DFT	-	Density Functional Theory
CIF	-	Crystallographic information file
PBC	-	Periodic Boundary Conditions
HOMO	-	highest occupied molecular orbital
LUMO	-	lowest unoccupied molecular orbital