

TABLE OF CONTENTS

COVER PAGE	i
RATIFICATION PAGE	ii
STATEMENT PAGE	iii
PREFACE	iv
TABLE OF CONTENTS	v
LIST OF FIGURES	vii
LIST OF APPENDIX	viii
ABSTRACT	ix
INTISARI	x
CHAPTER I INTRODUCTION	1
I.1 Background	1
I.2 Research Purposes	3
I.3 Research Benefits	4
CHAPTER II LITERATURE REVIEW AND HYPOTHESIS FORMULATION	5
II.1 Literature Review	5
II.1.1 Quantum mechanics/molecular mechanics (QM/MM)	5
II.1.2 2-dimensional quantum mechanics/molecular mechanics (2d-QM/MM)	6
II.1.3 Density-functional tight-binding (DFTB)	6
II.1.4 2-dimensional density-functional tight-binding/molecular mechanics (2d-DFTB/MM)	8
II.1.5 Alumina-water interface	9
II.1.6 Lennard-Jones potential	10
II.2 Hypothesis Formulation and Research Plan	11
II.2.1 Hypothesis formulation I	11
II.2.2 Hypothesis formulation II	11
II.2.3 Research planning	12
CHAPTER III RESEARCH METHOD	13
III.1 Materials and Equipment	13
III.1.1 Hardware	13
III.1.2 Software	13
III.1.3 Materials	13
III.2 Procedures	13

III.2.1	Equilibration	13
III.2.2	DFTB/MM MD	14
III.3	Data Analysis	15
III.3.1	1-dimensional radial distribution function (1d-RDF)	15
III.3.2	Vibrational stretching of OH group	15
CHAPTER IV	RESULTS AND DISCUSSION	16
IV.1	Potential Establishment and α -Al ₂ O ₃ (110) Surface Structure	16
IV.2	Molecular Adsorption at α -Al ₂ O ₃ (110)	17
IV.2.1	Molecular adsorption at single α -Al ₂ O ₃ (110) water system	18
IV.2.2	Molecular adsorption at dimer α -Al ₂ O ₃ (110) water system	19
IV.2.3	Molecular adsorption at monolayer α -Al ₂ O ₃ (110) water system	21
IV.2.4	Molecular adsorption trend at single, dimer, and monolayer water α -Al ₂ O ₃ (110)	22
IV.3	Analysis of 1-Dimensional Radial Distribution Function (1d-RDF)	23
IV.4	Analysis of Vibrational -OH Bonds	25
IV.5	Analysis of Protonation -OH Bonds	27
CHAPTER V	CONCLUSION AND SUGGESTION	29
V.1	Conclusion	29
V.2	Suggestion	29
	REFERENCES	30
	APPENDICES	34

LIST OF FIGURES

Figure I.1	Illustration of QM/MM approaches (Hofer and Tirlir, 2015)	3
Figure II.1	Visualisation of α -Al ₂ O ₃ (110) surface	10
Figure IV.1	Visualisation of unrelaxed and relaxed α -Al ₂ O ₃ (110) surface	17
Figure IV.2	Side view visualisation of single water system adsorbed to α -Al ₂ O ₃ at DFTB/MM MD level	18
Figure IV.3	Side view visualisation of dimer water system adsorbed to α -Al ₂ O ₃ at DFTB/MM MD level	20
Figure IV.4	Top view visualisation of dimer water system adsorbed to α -Al ₂ O ₃ at DFTB/MM MD level	20
Figure IV.5	Side view visualisation of monolayer water system adsorbed to α -Al ₂ O ₃ at DFTB/MM MD level	21
Figure IV.6	The elaborated visualisation for 1-dimensional radial distribution function applied to the monolayer water system	23
Figure IV.7	Analysis of 1-d radial distribution function of water molecules	24
Figure IV.8	Vibrational spectra of H ₂ O	26
Figure IV.9	Analysis of protonation states at α -Al ₂ O ₃ (110)	28

LIST OF APPENDIX

APPENDIX 1	Input File for Monolayer Water System at Equilibrium	34
APPENDIX 2	Output File for Monolayer Water System at Equilibrium	35
APPENDIX 3	Output File for α -Al ₂ O ₃ (110) Relaxed Structure	41
APPENDIX 4	DFTB Parameter for Al ₂ O ₃	46