

# Contents

	Page
<i>Preface</i>	<i>i</i>
<i>Acknowledgements</i>	<i>iii</i>
<i>Contents</i>	<i>v</i>
<i>List of Figures</i>	<i>vii</i>
<i>List of Tables</i>	<i>viii</i>
<i>List of Symbols</i>	<i>xiii</i>
<i>List of Abbreviations</i>	<i>xv</i>
<b>Chapter 1: Introduction</b>	<b>1</b>
1.1 Anomalies in water	1
1.2 Hydrogen bonds in water	4
1.3 Role of water in biology	5
1.4 Supercooled water	6
1.5 Dynamical heterogeneities	8
1.6 Comparison of supercooled water and confined water near biological surfaces	10
1.7 Experiments	11
1.8 Computer Simulations	13
1.9 Objective	14
1.10 Thesis Outline	15
<b>Chapter 2: TIP3P and TIP4P/2005 water models for hydration dynamics near membranes</b>	<b>17</b>
2.1 Introduction	17
2.2 Simulation details	19
2.3 Lipid bilayer properties	20
2.4 Classification of water regimes	22
2.5 Pair correlation functions	26
2.6 Anomalous diffusion exponent	27
2.7 Velocity auto correlation function	28
2.8 Non Gaussian Parameter	29
2.9 Summary	32
<b>Chapter 3: Dynamics of chemically confined water near lipid bilayers</b>	<b>35</b>
3.1 Introduction	35
3.2 Simulation details	36
3.3 Categorization of water regimes	37
3.4 Translational mean square displacement	37
3.5 Reorientational auto-correlation function	40
3.6 Hydrogen bond dynamics	42
3.7 Hydrogen bond networks and lipid-lipid associations	46
3.8 Summary	49
<b>Chapter 4: Quantification of dynamical heterogeneities of hydration water in lipid membrane above supercooling</b>	<b>53</b>
4.1 Introduction	53
4.2 Simulation details	54
4.3 Definition of different classes of interface water	55
4.4 Translational mean square displacement	56
4.5 Non-Gaussian parameter	57
4.6 van Hove correlation function	59
4.7 Self intermediate scattering function	59
4.8 van Hove correlation functions from block analysis	67
4.9 Summary	70
<b>Chapter 5: Dynamic coupling of hydration water near a phospholipid membrane</b>	<b>73</b>
5.1 Introduction	73
5.2 Simulation details	74
5.3 Membrane dynamics	75
5.4 Translational mean square displacement	76
5.5 Translational van Hove correlation	77
5.6 Self intermediate scattering function	83
5.7 Correlations in lipid and IW dynamics	83

5.8 Summary	86
<b>References</b>	91
<b>List of publications</b>	117