

University of Groningen

Multiscale Membrane Models

Liu, Yang

DOI:
[10.33612/diss.136221782](https://doi.org/10.33612/diss.136221782)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2020

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):
Liu, Y. (2020). *Multiscale Membrane Models*. [Thesis fully internal (DIV), University of Groningen]. University of Groningen. <https://doi.org/10.33612/diss.136221782>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Multiscale Membrane Models

Yang Liu

University of Groningen



This study was carried out in the molecular dynamics research group at the Faculty of Science and Engineering of the University of Groningen and was funded by the China Scholarship Council (CSC) scholarship.

Copyright © 2020 Yang Liu

liu2874@foxmail.com



university of
 groningen

Multiscale membrane models

PhD thesis

to obtain the degree of PhD at the
 University of Groningen
 on the authority of the
 Rector Magnificus Prof. C. Wijmenga
 and in accordance with
 the decision by the College of Deans.

This thesis will be defended in public on
 Tuesday 3 November 2020 at 12.45 hours

by

Yang Liu

born on 15 April 1991
 in Xinjiang, China

Supervisor

Prof. S.J. Marrink

Co-supervisor

Prof. A.H. de Vries

Assessment Committee

Prof. E. van der Giessen

Prof. S.S. Faraji

Prof. L.V. Schaefer

CONTENT

CHAPTER 1	1
INTRODUCTION	2
CELL MEMBRANE.....	2
COMPUTATIONAL MICROSCOPY	6
AIM AND OUTLINE OF THIS THESIS	14
CHAPTER 2	16
GANGLIOSIDES DESTABILIZE LIPID PHASE SEPARATION IN MULTICOMPONENT MEMBRANES	17
ABSTRACT	17
INTRODUCTION	17
METHOD.....	20
RESULTS.....	24
DISCUSSION	30
CONCLUSION.....	32
SUPPLEMENTAL INFORMATION	34
CHAPTER 3	49
COUPLING COARSE-GRAINED TO FINE-GRAINED MODELS VIA HAMILTONIAN REPLICA EXCHANGE	50
ABSTRACT	50
INTRODUCTION	50
METHOD.....	52
RESULTS.....	58
DISCUSSION	67
SUPPLEMENTAL INFORMATION	70
CHAPTER 4	76

DUAL RESOLUTION MEMBRANE SIMULATIONS USING VIRTUAL SITES.....	77
ABSTRACT.....	77
INTRODUCTION.....	77
METHODS.....	80
RESULTS.....	87
DISCUSSION.....	95
CONCLUSION.....	97
SUPPLEMENTAL INFORMATION	98
<u>CHAPTER 5.....</u>	<u>105</u>
APPLYING THE VIRTUAL SITE HYBRID SCHEME TO ACCELERATE PHASE SEPARATION IN TERNARY MEMBRANES	
.....	106
ABSTRACT.....	106
METHOD.....	106
RESULTS.....	108
SUPPLEMENTAL INFORMATION	117
<u>CHAPTER 6.....</u>	<u>118</u>
APPLYING THE VIRTUAL SITE HYBRID SCHEME TO INVESTIGATE LIPID RELAXATION DYNAMICS IN VESICLES	119
ABSTRACT.....	119
METHOD.....	119
RESULTS.....	122
SUPPLEMENTAL INFORMATION	128
<u>SUMMARY AND OUTLOOK.....</u>	<u>129</u>
<u>SAMENVATTING EN VOORUITZICHT</u>	<u>132</u>
<u>BIBLIOGRAPHY.....</u>	<u>135</u>
<u>ACKNOWLEDGEMENT.....</u>	<u>149</u>