



UvA-DARE (Digital Academic Repository)

Dynamics of water interacting with biomolecules

Groot, C.C.M.

Publication date

2017

Document Version

Other version

License

Other

[Link to publication](#)

Citation for published version (APA):

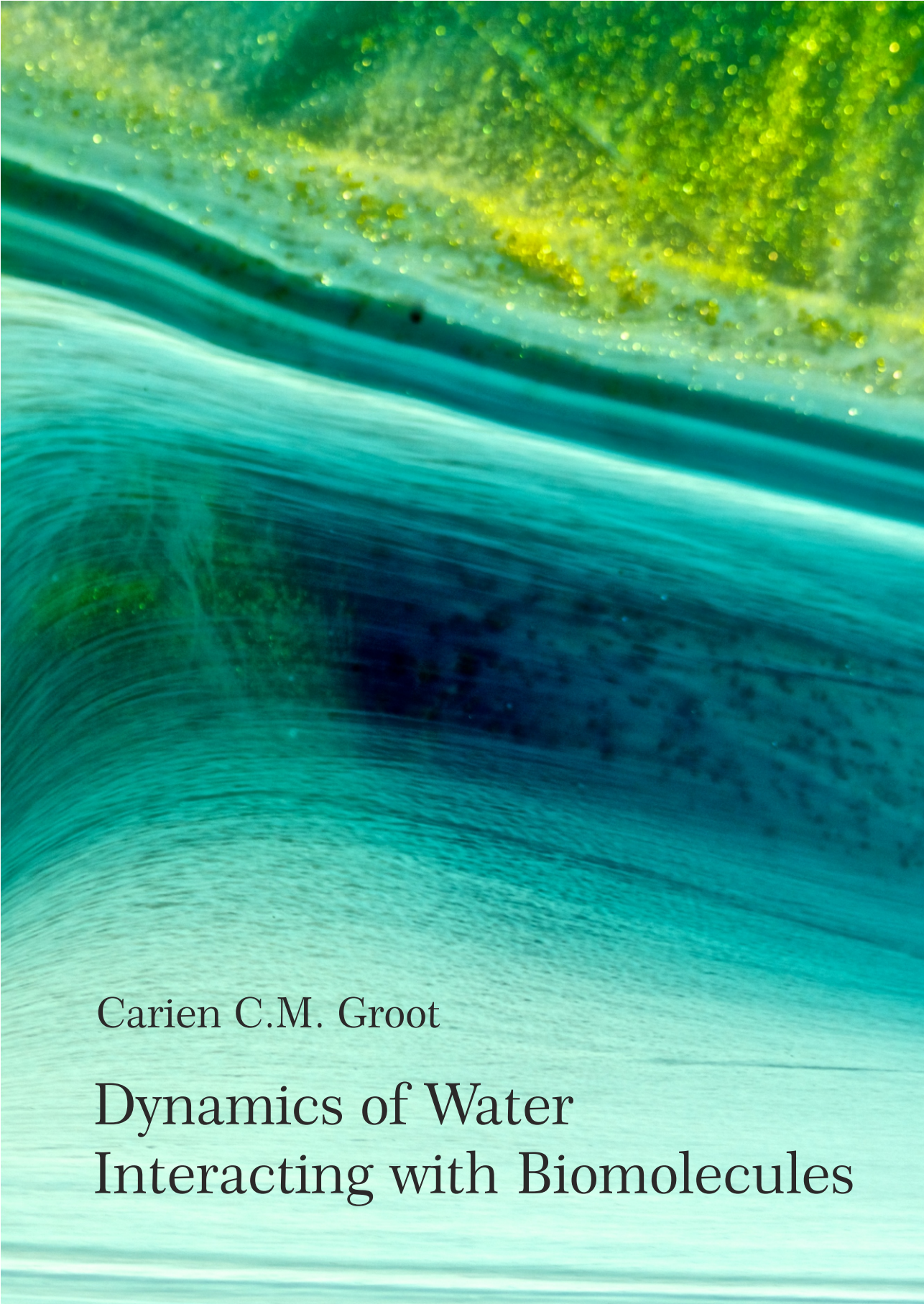
Groot, C. C. M. (2017). *Dynamics of water interacting with biomolecules*. [Thesis, externally prepared, Universiteit van Amsterdam].

General rights

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), other than for strictly personal, individual use, unless the work is under an open content license (like Creative Commons).

Disclaimer/Complaints regulations

If you believe that digital publication of certain material infringes any of your rights or (privacy) interests, please let the Library know, stating your reasons. In case of a legitimate complaint, the Library will make the material inaccessible and/or remove it from the website. Please Ask the Library: <https://uba.uva.nl/en/contact>, or a letter to: Library of the University of Amsterdam, Secretariat, Singel 425, 1012 WP Amsterdam, The Netherlands. You will be contacted as soon as possible.



Carien C.M. Groot

Dynamics of Water
Interacting with Biomolecules

**Dynamics of Water
Interacting with Biomolecules**

ISBN 978-94-92323-11-8

© 2016, C.C.M. Groot. All rights reserved.

Cover art: "Cool blues" by Pery Burge (chronoscapes.com)

Dynamics of Water Interacting with Biomolecules

ACADEMISCH PROEFSCHRIFT

ter verkrijging van de graad van doctor
aan de Universiteit van Amsterdam
op gezag van de Rector Magnificus
prof. dr. ir. K. I. J. Maex
ten overstaan van een door het College voor Promoties
ingestelde commissie,
in het openbaar te verdedigen in de Agnietenkapel
op vrijdag 13 januari 2017, te 10:00 uur

door

Catharina Cecile Maria Groot

geboren te Nijmegen

PROMOTIECOMMISSIE

Promotor:	prof. dr. H. J. Bakker	Universiteit van Amsterdam
Overige leden:	prof. dr. P. G. Bolhuis	Universiteit van Amsterdam
	prof. dr. A. M. Brouwer	Universiteit van Amsterdam
	prof. dr. M. Havenith	Ruhr-Universität Bochum
	prof. dr. J. L. Herek	Universiteit Twente
	prof. dr. J. Oomens	Universiteit van Amsterdam
	prof. dr. K. P. Velikov	Universiteit Utrecht

Faculteit der Natuurwetenschappen, Wiskunde en Informatica

This thesis is part of NanoNextNL, a micro and nanotechnology innovation consortium of the Government of the Netherlands and 130 partners from academia and industry.

The work described in this thesis was performed at the FOM Institute AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands. This work is part of the research programme of the Foundation for Fundamental Research on Matter (FOM), which is financially supported by the Netherlands Organisation for Scientific Research (NWO).

PUBLICATIONS COVERED IN THIS THESIS

- C. C. M. Groot and H. J. Bakker. Hydration dynamics of aqueous glucose probed with polarization-resolved fs-IR spectroscopy. *J. Chem. Phys.* *140*, 234503, 2014. - *chapter 5*
- C. C. M. Groot and H. J. Bakker. A femtosecond mid-infrared study of the dynamics of water in aqueous sugar solutions. *Phys. Chem. Chem. Phys.* *17*, 8449, 2015. - *chapter 5*
- C. C. M. Groot and H. J. Bakker. Proteins take up water before unfolding. *J. Phys. Chem. Lett.* *7*, 1800-1804, 2016. - *chapter 6*
- C. C. M. Groot, K. P. Velikov and H. J. Bakker. Structure and dynamics of water confined in triglyceride oils. *Phys. Chem. Chem. Phys.* *18*, 29361-29368, 2016. - *chapter 8*
- C. C. M. Groot, K. Meister, A. L. DeVries and H. J. Bakker. Dynamics of the hydration water of antifreeze glycoproteins. *J. Phys. Chem. Lett.* *7*, 4836-4840, 2016. - *chapter 7*

OTHER PUBLICATIONS

- S. Lotze, C. C. M. Groot, C. Vennehaug and H. J. Bakker. Femtosecond mid-infrared study of the dynamics of water molecules in water-acetone and water-dimethyl sulfoxide mixtures. *J. Phys. Chem. B* *119*, 5228-5239 (2015).
- Z. F. Brotzakis, C. C. M. Groot, W. H. Brandeburgo, H. J. Bakker and P. G. Bolhuis. Dynamics of hydration water around native and misfolded α -lactalbumin. *J. Phys. Chem. B* *120*, 4756-4766 (2016).

CONTENTS

1	Introduction	11
1.1	Water	11
1.2	Water and biomolecules	12
1.3	Spectroscopy of water	14
1.4	Outlook	15
2	Vibrational spectroscopy	17
2.1	Vibrations and the harmonic oscillator	17
2.2	The quantum harmonic oscillator	18
2.3	Linear spectroscopy	22
2.3.1	Absorption cross section	22
2.3.2	Absorption lineshape	23
2.4	Pump-probe spectroscopy	24
2.5	Frequency-resolved pump-probe spectroscopy: 2DIR	26
2.5.1	2D lineshape	27
2.5.2	Cross peaks	28
2.6	Polarization-resolved pump-probe spectroscopy	30
3	Experimental methods	35
3.1	Optical frequency conversion	35
3.2	Single-color infrared pump-probe setup	38
3.3	Dual-color (2D) infrared pump-probe setup	39
3.4	Sample cell	41
4	Data modelling	43
4.1	Isotropic transient spectrum	43
4.1.1	Relaxation models	43
4.1.2	Least-squares fit	45
4.2	Anisotropy dynamics	45
5	Water dynamics in aqueous sugar solutions	47
5.1	Introduction	48
5.2	Experimental	48
5.3	Results	49
5.3.1	Linear spectra	49
5.3.2	Isotropic and anisotropic signals	50
5.3.3	Reference measurements in DMSO	52
5.3.4	Spectral decomposition model	53

5.3.5	Modeling water reorientation of sugar hydration shells . . .	54
5.4	Discussion	56
5.4.1	Solute dynamics	56
5.4.2	Water dynamics	57
5.5	Conclusions	60
5.6	Appendix: Hydration shell model	60
6	Water dynamics in aqueous protein solutions	65
6.1	Introduction	66
6.2	Experimental	66
6.3	Results and discussion	67
6.3.1	Vibrational relaxation	67
6.3.2	Native proteins	69
6.3.3	Heat-denatured proteins	72
6.3.4	Urea-denatured proteins	74
6.4	Conclusions	77
7	Hydration of antifreeze glycoproteins	79
7.1	Introduction	80
7.2	Experimental	81
7.3	Results	82
7.3.1	Vibrational relaxation	82
7.3.2	Hydration dynamics of AFGPs	83
7.3.3	The effect of borate	85
7.4	Discussion	87
7.5	Conclusions	88
8	Structure and dynamics of water in triglyceride oils	89
8.1	Introduction	90
8.2	Experimental	90
8.3	Results	91
8.3.1	Linear spectra	91
8.3.2	2DIR spectra	96
8.4	Discussion	101
8.5	Conclusions	102
9	Water in triglyceride oils: the C=O stretch vibration	103
9.1	Introduction	104
9.2	Experimental	104
9.3	Results	105
9.3.1	Linear spectra	105
9.3.2	Time-resolved spectra	106
9.3.3	Anisotropic response	109
9.4	Discussion	110
9.5	Conclusions	111

Bibliography	113
Appendix: The value of science	129
Summary	133
Samenvatting	137
Acknowledgements	141