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CURRICULUM VITAE
Ulf Rørbæk Pedersen



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VITEA

2009-2011 Currently in postdoctoral position at “University of California, Berkeley” under the supervision of Prof. David Chandler (chandler@cchem.berkeley.edu), exploiting a grant from “The Danish Council for Independent Research | Natural Sciences (FNU)“.

2009 Scientific Assistant at the “Danish National Research Foundation Center for Viscous Liquids Dynamics (Glass and time)”, Feb.-Apr. 2009.

2006-2009 Philosophiae doctor (Ph.D.) in physics from Roskilde University, Denmark (defended April 3rd 2009). Title of thesis: “Long-time simulations of viscous liquids - from strong correlations to crystallization”. Supervisor: Thomas B. Schrøder (tbs@ruc.dk). Thesis is available at www.urp.dk.

2003-2006 Master in physics and chemistry from Roskilde University (Denmark). Title of thesis: "Structural changes of a phospholipidmembran perturbed with n-alcohol investigated by MD-simulations and SAXS". Supervisors: Peter Westh (chemistry; pwesth@ruc.dk), Dorte Posselt (physics; dorte@ruc.dk) and Günther H. Peters (external; ghp@kemi.dtu.dk).

1999-2003 Bachelor in physics and chemistry from Roskilde University (Denmark).

1996-1999 Himmelev Gymnasium (Denmark).

SKILLS

Programming Matlab/Octave, C++, Java, Fortran and bash-shell scripting.

Simulations LAMMPS, GROMACS, NAMD, VMD and home-made codes.

Platforms Windows, Linux, Mac, and using a Unix Cluster

Language Danish (native) and English (fluent)

RESEARCH INTERESTS

My main interest is within the field of soft condense matter, and am using molecular computer simulations to investigate viscous liquids, but have also worked on phospholipid membranes. Although I have a theoretical approach, I appreciate having contact with experiments.

Strongly correlating viscous liquids. The major part of my Ph.D. research focus on a class of liquids referred to as "strongly correlating liquids", and with a special focus on viscous liquids. An important conclusion is that this class of liquids have simpler physics that in general - where some have been observed experimentally and some are predictions.

Low temperature fate of liquids: crystal or amorphous structure. In collaboration with Peter Harrowell (Sydney Uni.; p.harrowell@chem.usyd.edu.au) I am investigating metastability and crystallization of simple liquids. For a particular liquid we identified the local structure responsible for super-arrhenius slow-down, which turned out to be the same as the one forming the crystal.

Solutes in phospholipid membranes. The major constituents of biological membranes are phospholipids, however, many other constituents are important for the physical properties. Thus, understanding the role of solutes in phospholipid membranes is important. I have worked on the understanding of structure and packing of perturbed phospholipid membranes. In collaboration with Peter Westh (Roskilde Uni.; pwesth@ruc.dk) and

Günther Peters (Technical Uni. of Denmark; ghp@kemi.dtu.dk) I have investigated the changes alcohols and ions make on membranes. Moreover, connected to my work on strongly correlating simple liquids, I have reported and explained strong energy and volume correlations in the thermal fluctuations of phospholipid membranes.

PUBLICATIONS

- 2010b** *Geometry of Slow Structural Fluctuations in a Supercooled Binary Alloy*
Ulf R. Pedersen, Thomas B. Schröder, Jeppe C. Dyre, Peter Harrowell
Phys. Rev. Lett. 104, 105701 (2010)
- 2010a** *Correlated Volume Energy Fluctuations of Phospholipid Membranes: A Simulation Study*
Ulf R. Pedersen, Günther H. Peters, Thomas B. Schröder, Jeppe C. Dyre
J. Phys. Chem. B, 114 (6), 2124-2130 (2010)
- 2009d** *Pressure-energy correlations in liquids. IV. 'Isomorphs' in liquid state diagrams*
Nicoletta Gnan, Thomas B. Schröder, Ulf R. Pedersen, Nicholas P. Bailey, Jeppe C. Dyre.
J. Chem. Phys., 131, 234504 (2009).
- 2009c** *Pressure-energy correlations in liquids. III. Statistical mechanics and thermodynamics of liquids with hidden scale invariance*
Thomas B. Schröder, Nicholas P. Bailey, Ulf R. Pedersen, Nicoletta Gnan, Jeppe C. Dyre.
J. Chem. Phys., 131, 234504 (2009).
- 2009b** *Hidden scale invariance in molecular van der Waals liquids: A simulation study*
Thomas B. Schröder, Ulf R. Pedersen, Nicholas P. Bailey, Søren Toxvaerd, Jeppe C. Dyre.
Phys. Rev. E 80, 041502 (2009).
- 2009a** *Stability of supercooled binary liquid mixtures.*
Søren Toxvaerd, Ulf R. Pedersen, Thomas B. Schröder, Jeppe C. Dyre
J. Chem. Phys. 130, 224501 (2009)
- 2008g** *Termiske fluktuationer - er der noget nyt under Solen?* (in danish)
Ulf R. Pedersen, Thomas B. Schröder, Jeppe C. Dyre
Kvant: Tidskrift for fysik og astronomi 19(4):26-29
- 2008f** *Pressure-energy correlations in liquids. II. Analysis and consequences.*
Nicholas P. Bailey, Ulf R. Pedersen, Nicoletta Gnan, Thomas B. Schröder, Jeppe C. Dyre
J. Chem. Phys., 129, 184508 (2008).
- 2008e** *Pressure-energy correlations in liquids. I. Results from computer simu-*

lations.

Nicholas P. Bailey, Ulf R. Pedersen, Nicoletta Gnan, Thomas B. Schröder, Jeppe C. Dyre
J. Chem. Phys., 129, 184507 (2008)

2008d *Glass-forming liquids: one or more 'order' parameters?*

Nicholas P. Bailey, Tage Chistensen, Bo Jakobsen, Kristine Niss, Niels Boye Olsen, Ulf R. Pedersen, Thomas B. Schröder, Jeppe C. Dyre
Journal of physics-condensed matter 20, 244113

2008c *Volume-energy correlations in the slow degrees of freedom of computer-simulated phospholipid membranes*

Ulf R. Pedersen, Günther H. Peters, Thomas B. Schröder, Jeppe C. Dyre
AIP Conf. Proc. 982, 407-409

2008b *Feasibility of a single-parameter description of equilibrium viscous liquid dynamics.*

Ulf R. Pedersen, Tage Christensen, Thomas B. Schröder, Jeppe C. Dyre
Phys. Rev. E 77, 011201

2008a *Strong pressure-energy correlations in van der Waals liquids.*

Ulf R. Pedersen, Nicholas P. Bailey, Thomas B. Schröder, Jeppe C. Dyre
Phys. Rev. Lett. 100, 015701

2007b *Molecular packing in 1-hexanol-DMPC bilayers studied by molecular dynamics simulation.*

Ulf R. Pedersen, Günther H. Peters, Peter Westh
Biophysical Chemistry 125, 104-111

2007a *Single-order-parameter description of glass-forming liquids: A one-frequency test.*

Niels L. Ellegaard, Tage Christensen, Peder Voetmann Christiansen, Niels Boye Olsen, Ulf R. Pedersen, Thomas B. Schröder, Jeppe C. Dyre
J. Chem. Phys 126, 074502

2006b *The effect of calcium on the properties of charged phospholipid bilayers.*

Ulf R. Pedersen, Chad Leidy, Peter Westh and Günther H. Peters
Biochimica et Biophysica Acta (BBA) - Biomembranes 1758, 573-582

2006a *An energy landscape model for glass-forming liquids in three dimensions.*

Ulf R. Pedersen, Tina Hecksher, Jeppe C. Dyre and Thomas B. Schröder
Journal of non-crystalline solids 352, 5210-5215

ORAL- AND POSTER PRESENTATIONS

Cairns 2010 *Statistics of density fluctuations in supercooled viscous liquids* Oral presentation at the XXIV International Conference on Statistical Physics of the International Union for Pure and Applied Physics (IUPAP) [Convention Centre, Cairns, Queensland, Australia, 19-23 July, 2010]

- Sydney 2010** *From amorphous Frank-Kasper clusters to a Laves phase in a highly supercooled melt* Oral presentation at the meeting Liquid Out of Equilibrium [U. Sydney, July 12-16, 2010, Sydney, Australia]
- Nyborg Strand 2010** *A repulsive reference reproducing dynamics of a dense liquid with attractions* Oral presentation at the Annual Meeting of Danish Physical Society 2010 [Nyborg Strand Hotel, 22-23 June, 2010, Nyborg Strand, Denmark]
- Søminestationen 2010** *Statistics of density fluctuations in supercooled viscous liquids.* Oral presentation at the international workshop Viscous Liquids and the Glass Transition, VIII. [Søminestationen, May 28-30, 2010, Holbæk, Denmark]
- Berkeley 2010** *Long-lived structural fluctuations and crystallization of a binary Lennard-Jones mixture.* Poster presented at the Berkeley Mini Statistical Mechanics Meeting [University of California, Berkeley, January 8 - 10, 2010 16-18].
- Holderness 2009** *Structural Fluctuations in a Supercooled Binary Lennard-Jones Mixture: Crystal Nucleation or Glassy Relaxation.* Poster presented at The Physics and Chemistry of Liquids (Gordon Conference) [Holderness School, New Hampshir, August 2-7, 2009].
- Lyngby 2009** *Long-lived structural fluctuations and crystallization of a binary Lennard-Jones mixture.* Poster presented at the Danish Physical Society Nordic Meeting [Technical University of Denmark, June 16-18, 2009].
- Sydney 2009** *Fluctuations in Liquids: Scaling Laws, Glassy Relaxation and Crystallization* Seminar given at the School of Chemistry [University of Sydney (Australia), June 10, 2009].
- Søminestationen 2009** *Experimental prediction for strongly correlating liquids: A new look at the Prigogine-Defay ratio.* Oral presentation at Viscous Liquids and the Glass Transition (VII). [Søminestationen, Holbæk (Denmark), Friday April 24 to Sunday April 26, 2009]
- Roskilde 2009** *Stability of Super-cooled Liquids.* Oral presentation given in the series of IMFUFA seminars [Roskilde University (Denmark), April 25 2009].
- Kyoto 2008** *Density scaling as a property of strongly correlating viscous liquids and Long-lived structural fluctuations and crystallization of a binary mixture.* Two posters presented at Unifying Concepts in Glass Physics IV (UCGP2008) [Kyoto, Japan, November 25-28 2008].
- Copenhagen 2008** *Long-lived structural fluctuations and crystallization of a binary Lennard-Jones mixture.* Oral presentation at the international workshop Fragility of Viscous Liquids: Cause(s) and Consequences [Carlsberg Academy, Copenhagen, Denmark, October 8-10, 2008].
- Sitges 2008** *Equilibrium fluctuations of volume and energy of simulated phospholipid membranes.* Poster presented at the XXI Sitges Conference on

Statistical mechanics: Statistical Mechanics of Molecular Biophysics [Sitges, Barcelona, Spain, June 2-6, 2008].

Nyborg Strand 2008 *Volume-energy correlations in the slow degrees of freedom of phospholipid membranes.* Oral presentation at the Danish Physical Society Annual Meeting [Nyborg Strand Hotel, Denmark, June 17-18, 2008].

Andalo 2008 *Long-lived structural fluctuations and crystallization of a binary Lennard-Jones mixture.* Poster presented at XI International Workshop on Complex Systems [Andalo, Italy, March 17-20, 2008].

Sendai 2007 *Volume-energy correlations in the slow degrees of freedom of phospholipid membranes.* Poster presented at the 5th International Workshop on Complex Systems [Sendai International Center, Sendai, Japan, September 25-28, 2007].

Holderness 2007 *Strong pressure-energy correlations in model liquids.* Poster presented at The Physics and Chemistry of Liquids (Gordon Conference) [Holderness School, New Hampshire, July 29 - August 3, 2007].

Søminestationen 2007 *Crystallization of the Wahnström binary Lennard-Jones liquid.* Oral presentation at Viscous Liquids and the Glass Transition VI [Søminestationen, Holbæk, Denmark, June 29 - July 1, 2007].

Pisa 2006 *The dynamical Prigogine-Defay ratio: Is the glass transition controlled by one or more order-parameters?* IV Workshop on Non Equilibrium Phenomena in Supercooled Fluids, Glasses and Amorphous Materials [Pisa, Italy, September 17-22, 2006].

Søminestationen 2006 *A "tumbling" model of toluene.* Oral presentation at Viscous Liquids and the Glass Transition V [Søminestationen, Holbæk, Denmark, May 26-28, 2006].

Nyborg Strand 2006 *Molecular Dynamic Simulations of Viscous Toluene.* Poster presented at the Danish Physical Society Annual Meeting [Nyborg Strand Hotel, Denmark, June 1-2, 2006].

Lille 2005 *An energy-landscape model for viscous liquids in three dimensions.* Poster presented at International discussion meeting on relaxation in complex systems V [Lille, France, July 7-13, 2005].

Søminestationen 2005 *A simple energy landscape lattice model.* Oral presentation given with Tina Hecksher at "Viscous Liquids and the Glass Transition IV" [Søminestationen, Holbæk, Denmark, June 3-5, 2005].

TEACHING

2006-2008 Supervising student projects at Roskilde University (Denmark).

REFERENCES

Professor David Chandler

University of California, Berkeley, USA (chandler@cchem.berkeley.edu)

Professor Jeppe C. Dyre

Roskilde University, Denmark (dyre@ruc.dk)

Professor Peter Harrowell

Sydney University, Australia (p.harrowell@chem.usyd.edu.au)