

September 14, 2011

CURRICULUM VITAE  
Ulf Rørbæk Pedersen



**Name:** Ulf Rørbæk Pedersen, Ph.D.

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VITEA

**2011-** Currently, post. doc. at “Vienna University of Technology” as a part of SFB ViCoM.

**2009-2011** Post. Doc. 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 in 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”. Super-

visors: 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), English (fluent) and German (limited).

#### 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

- 2011d** *Predicting the density-scaling exponent of a glass-forming liquid from Prigogine-Defay ratio measurements*  
Ditte Gundermann, Ulf R. Pedersen, Tina Hecksher, Nicholas P. Bailey, Bo Jakobsen, Tage Christensen, Niels B. Olsen, Thomas B. Schröder, Daniel Fragiadakis, Riccardo Casalini, C. Michael Roland, Jeppe C. Dyre and Kristine Niss  
Nature Physics (in press).
- 2011c** *Pressure-energy correlations in liquids. V. Isomorphs in generalized Lennard-Jones systems*  
Thomas B. Schröder, Nicoletta Gnan, Ulf R. Pedersen, Nicholas P. Bailey, Jeppe C. Dyre  
J. Chem. Phys. 134, 164505 (2011).
- 2011b** *Crystallization of the Lewis-Wahnström ortho-terphenyl model*  
Ulf R. Pedersen, Toby S. Hudson, Peter Harrowell  
J. Chem. Phys. 134, 114501 (2011).
- 2011a** *Strongly correlating liquids and their isomorphs*  
Ulf R. Pedersen, Nicoletta Gnan, Nicholas P. Bailey, Thomas B. Schröder, Jeppe C. Dyre  
J. Non-Cryst. Solids 357, 320 (2011).
- 2010c** *A repulsive reference potential reproducing the dynamics of a liquid with attractions*  
Ulf R. Pedersen, Thomas B. Schröder, Jeppe C. Dyre  
Phys. Rev. Lett. 105, 157801 (2010).
- 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: Tidsskrift 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 simulations.*  
 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 Christensen, 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

**Vienna 2011** *Factors Contributing to the Glass Forming Ability of a Simulated Molecular Liquid.*

Poster presented at The 8<sup>th</sup> Liquid Matter Conference  
[Wien, Austria, September 6-10, 2011].

**Holderness 2011** *Transport properties of water: crossover at ambient conditions.*

Poster presented at The Physics and Chemistry of Liquids (Gordon Conference)  
[Holderness School, New Hampshire, July 24-29, 2011].

**Nyborg Strand 2011** *Glass Forming Ability of Simulated Triangular Molecules.*

Oral presentation at the Annual Meeting of Danish Physical Society 2011  
[Nyborg Strand Hotel, 21-22 June, 2011, Nyborg Strand, Denmark]

**Søminestationen 2011** *Factors contributing to the glass-forming ability of a simulated molecular liquid.*

Oral presentation at Viscous Liquids and the Glass Transition (IX)  
[Søminestationen (Holbæk, Denmark), June 16-18, 2011].

**Rutgers 2011** *Statistics of density Fluctuations in supercooled viscous liquids.*

Short-talk at 105th Statistical Mechanics Conference  
[Rutgers University, May 8-10, 2011].

**Dallas 2011** *Crystallization of the Lewis and Wahnström o-terphenyl model.*

Oral presentation at American Physical Society Meeting  
[21-25 March 2011, Dallas, Texas].

**Berkeley 2011** *Statistics of density Fluctuations in supercooled viscous liquids.*

Poster presented at the Berkeley Mini Statistical Mechanics Meeting  
[University of California, Berkeley, January 14 - 16, 2011].

- 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].
- 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 Hampshire, 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)