

PERSONALIA

Name: Daniel ('Daan') Frenkel Born, July 27, 1948, Amsterdam, NL

ADDRESS

Department of Chemistry, University of Cambridge

Lensfield Road, Cambridge CB2 1EW, UK

Tel:. +44 1223336376 E-mail: df246@cam.ac.uk

Website: http://www.ch.cam.ac.uk/person/df246

EDUCATION

1966 - 1977 University of Amsterdam, Amsterdam, NL Degrees:

Masters degree Physical Chemistry, 1972 PhD Physical Chemistry, 1977

RESEARCH INTERESTS

My research focuses on numerical simulations of many-body systems, with special emphasis on problems relating to the prediction of stability and kinetics in complex self-assembly in soft and biological materials. I develop novel algorithms when I need them.

PROFESSIONAL Experience

- 2007- 2018, Professor of Chemistry/Director of Research, University of Cambridge
 - 2007, Elected 1968 Professor of Chemistry, University of Cambridge
 - 2011-2015, Head of Department of Chemistry, University of Cambridge
 - o 2015-2018, Director of Research, University of Cambridge
- 1998 2013, Professor of Chemistry, Van 't Hoff Institute for Molecular Science, University of Amsterdam,
- 1987 2007, Professor of Chemistry, Van 't Hoff laboratory for Colloid Science, Utrecht University, Utrecht, NL
- 1987 2013, Group Leader, FOM Institute AMOLF, Amsterdam, NL
- 1981 1986, "Lecturer/Reader", Department of Physics, Utrecht University, Utrecht, NL
- 1980 1981, Research Scientist, Shell Research, Amsterdam, NL
- 1977 1980, Postdoctoral Research Fellow, Department of Chemistry, UCLA, Los Angeles, CA, USA

MEMBERSHIP OF LEARNED SOCIETIES

2016: Foreign Associate of the National Academy of Sciences (USA)

- 2013: Member of the Academia Europaea
- 2012: Associate Fellow of TWAS World Academy of Sciences
- 2008: Foreign Honorary Member of the American Academy of Arts & Sciences
- 2006: Foreign Member Royal Society (London).
- 2002: Member of the "Hollandsche Maatschappij der Wetenschappen"

(NL)

1998: Member of the Royal Dutch Academy of Sciences (NL)

HONOURS, AWARDS AND NAMED LECTURES

- 2022: Sam Edwards Medal and Prize, Institute of Physics
- 2022: Lorentz Medal of the Netherlands Academy of Sciences
- 2021: McBain Memorial Lecture, NCL, Pune (India)
- 2020: Liquid Matter Prize, European Physical Society
- 2020: Sheikh Saud lecture, Temple University, Philadelphia, USA.
- 2020: G.N. Ramachandran Memorial Lecture, S.N. Bose Center, Kolkata
- 2019: Staudinger-Durrer Prize, ETH Zürich
- 2019: Ben May Lecture, Weizmann Institute, Israel.
- 2019: NTNU Lars Onsager Medal and Visiting Professorship
- 2019: Bragg Lecture, University College London
- 2018: President's International Fellowship Initiative Award (Chinese Academy of Sciences)
- 2018: C.V. Raman Memorial Lecture 2018, IISc, Bangalore, India.
- 2018: ICTS-Infosys Chandrasekhar Lectures, Bangalore, India
- 2017: Cohen Lectures, Northwestern University, Evanston, IL, USA
- 2016: Elected Honorary Fellow of Trinity College Cambridge
- 2016: Sir Eric Rideal Lecture of the SCI/RSC.
- 2016: Boltzmann Medal (IUPAP)
- 2015: Bakhuis-Roozeboom medal Netherlands Academy of Sciences
- 2013: Hinshelwood Lectures, Oxford University
- 2012: Robert Scott Lecture, University of California at Los Angeles.
- 2012: Spiers Memorial Award of the Royal Society of Chemistry
- 2011: Joseph E Hirschfelder Prize, U. Wisconsin at Madison (USA)
- 2011: Concurrent Professor, Nanjing University (China)
- 2011: Robert S. Mulliken Memorial Lecture, U. Chicago (USA)
- 2011: Fritz London Memorial Lecture, Duke University (USA)
- 2010: Pitzer Lecturer, U.C. Berkeley (USA)
- 2010: Soft Matter & Biophysical Chemistry Award Royal Society of Chemistry
- 2010: Elected Fellow of the Royal Society of Chemistry (UK).
- 2008: Awarded ERC Advanced grant.
- 2007: Aneesur Rahman Prize for Computational Physics of the American Physical Society
- 2007: Laughlin Lecturer, Department of Chemistry, Cornell University (USA)
- 2007: Honorary Doctorate, University of Edinburgh (UK)
- 2007: Berni Alder-CECAM prize of the European Physical Society.

2007: Royal Society Wolfson Merit Award

2006: Kivelson Memorial Lecture, Dept. of Chemistry and Biochemistry,

UCLA, (USA)

2006: Wohl Memorial Lecture, Dept. of Chem. Eng, U. Delaware (USA)

2005: Honorary Professor, Beijing University of Chemical Technology

(CN)

2004: Rothschild Professor, University of Cambridge (UK)

2002: First UCLA Distinguished Lecturer in Engineering (USA)

2000: NWO Spinoza Award (NL)

1999: Bourke lecturer & medalist, Royal Society of Chemistry (UK).

1999: James Franck Institute Distinguished Lecturer. U. Chicago (USA)

1999: Eli Burstein Lecture in Materials Science, U. Pennsylvania (USA)

1998: Regents lecturer. University of California at Los Angeles (USA).

1997: ``Lennard-Jones" lecture of the Royal Society of Chemistry (UK).

1997: "Physica" lecture and Prize of the Dutch Physical Society.

1984: Visiting lecturer at the K.U. Leuven (Belgium)

1975: Shell graduate-student travel award

1969: Unilever Undergraduate Chemistry award.

RESEARCH-RELATED ACTIVITIES

Publications and Oral Presentations:

Over 500 articles in international, refereed journals (h-index: 98 (ISI) / 121 (Google Scholar)). https://orcid.org/0000-0002-6362-2021

Over 500 talks at international meetings and academic institutions, including plenary talks at the Annual meetings of the German (2x), Italian, Belgian, Spanish, Brazilian and Dutch Physical Societies.

Numerous public lectures and lectures at over 20 summer/winter schools.

Books:

Simulation of Liquids and Solids, Molecular Dynamics and Monte Carlo Methods in Statistical Mechanics. G. Ciccotti, D. Frenkel and I.R. McDonald, North-Holland, Amsterdam (1987).

Understanding Molecular Simulation. From Algorithms to Applications D. Frenkel and B. Smit, Academic Press, Boston (1996/2002). Over 10,000 copies sold – cited over 20,000 times.

SCIENCE MANAGEMENT AND PROFESSIONAL SERVICES:

Chair of the International Research Assessment Panel of Physics/Chemical

Physics/Atmospheric Science at the University of Utrecht (2022)

Member Review Panel Computational Science IIT Genova (2021)

Chair Joint Institute Portfolio Review Committee Dutch Science Foundation/Netherlands Academy of Sciences (2017-2018)

Member Advisory Board, Lund Institute for advanced Neutron and X-ray Science (LINXS) (2018-2022)

Member Scientific Advisory Board of PoreLab (Norway).

Member International Advisory Panel Chinese Academy of Sciences Institute of Physics, Condensed Matter Centre of Excellence (2017)

Chair of the International Research Assessment Panel of Physics/Chemical Physics/Atmospheric Science at the University of Utrecht (2017)

Member of the International Research Assessment Panel of Physics at the Universities of Leiden (2016)

Panel Chair, ERC panel PE3 – Advanced Grants (2015-2018).

Member Advisory Board, Department of Biomedical Engineering, Technical University Eindhoven.

Member Scientific Advisory Board, Max Planck Institute for Polymer Research (Mainz, DE).

Founding Director of the International Research Center for Soft Matter of Beijing University of Chemical Technology (2014). (now: Beijing Advanced Innovation Center for Soft Matter Science and Engineering at Beijing University of Chemical Technology)

Rapporteur for the 2014 Chemistry Institutes evaluation of the Max Planck Gesellschaft

Member Advisory Committee of the Condensed Matter Physics Center (IFIMAC) at Universidad Autónoma de Madrid

Chair of the Computational Science Board of the Lorentz Centre (Leiden) 2008-2013

Chair of the Board of the Amsterdam Centre for Multi-scale Modelling (ACMM) Member of the Scientific Council of the Max Planck Institut für Metallforschung.

Member the Advisory Board of the INFM Centre for Complexity (Roma).

Member the Board of the John von Neumann Computing Centre (Germany) Member of the External Review Panel of Physics at the University of Leeds (2006).

Chair of the International Research Assessment Panel of Physics at the Universities of Leiden and Delft (2003)

Member of the IoP International Review Panel of Physics and Astronomy in Britain (2005).

Member of the Board of the Liquids Section of the European Physical Society (Chair: 2002-2005).

Member Committee on Biophysics and Biochemistry of the Royal Dutch Academy of Sciences (Chair 2003-2007).

Chairman of the foresight panel Matter of the Royal Dutch Academy of Sciences on the Physics of Living Systems.

Dutch scientific representative on the CECAM Scientific council. 1989-2013 (Chair: 1992-1994 and 2002-2004).

Program leader of the FOM-Shell Industrial Partnership Program on Waves in Complex Media (2007)

Program leader of the FOM Programs Physical Biology I & II

Program leader of the FOM Program on Soft Materials (1998-2008)

Initiated (together with B. Smit) an international Molecular Simulation Course.

This course has been taught in Amsterdam (15+ times), Lyon, Bangalore (2x) and Kanpur.

Initiated FOM/AMOLF program to involve high-school teachers in research.

Referee for some 20+ journals (including Nature/Nature group, Science, PNAS, Physical Review Letters and Europhysics Letters).

Editor in Chief of the European Physical Journal E (2009-2014)

Current or former member of the editorial board of: PNAS and Molecular Physics. Former editorial Board Member: Soft Matter, Journal of Computational Physics, Journal of Chemical Physics, Journal of Physics C, AICHe Journal, JSTAT, Advances in Chemical Physics

TRAINING YOUNG SCIENTISTS

Mentored over 65 postdocs.

Supervised PhD students

(Most of these continued in academia. 14 are at present Full or Associate Professor).

- 1. Amarante Böttger, A light scattering study of precursor effects near phase transitions in liquid crystals. Universiteit Utrecht, 20-4-1988.
- 2. Winfried G.T. Kranendonk, Computer simulations of models for colloidal systems. Universiteit Utrecht, 12-3-1990.
- 3. Berend Smit, Simulation of phase coexistence, from atoms to surfactants. 10-12-1990, Universiteit Utrecht.
- 4. Jan A.C. Veerman, Computer simulation studies of model systems for liquid crystals. Universiteit Utrecht, 15-4-1991.
- 5. Martin A. van der Hoef, Simulation study of diffusion in lattice-gas fluids and colloids. 14 december 1992, Universiteit Utrecht.
- 6. Evert-Jan Meijer, Computer simulation of molecular solids and colloidal dispersions. Universiteit Utrecht, 10-2-1993.
- 7. Germonda C.A.M. Mooij, Novel simulation techniques for the study of polymer phase equilibria. Universiteit Utrecht, 23-11-1993.
- 8. Marjolein Dijkstra, The effect of entropy on the stability and structure of complex fluids. 12 september 1994, Universiteit Utrecht
- 9. Monica E. van Leeuwen, Molecular simulation of the phase behaviour of polar fluids. Universiteit Utrecht, 23-1-1995.
- 10. Rene van Roij, Simple theories of complex liquids. Universiteit Utrecht, 7-10-1996.
- 11. Peter G. Bolhuis, Solid-like behavior in liquids. Liquid-like behavior in solids. Universiteit Utrecht, 7-10-1996.

- 12. Ronald Blaak, Cubatic Phase in Complex Liquids. Universiteit Utrecht, 15-9-1997.
- 13. Maarten H.J. Hagen, Diffusion of confined colloidal particles. Universiteit Utrecht, 22-10-1997
- 14. Pieter Rein ten Wolde, Numerical Study of Pathways for Homogeneous Nucleation, Universiteit van Amsterdam, 23-10-1998
- 15. Stefan Auer, Quantitative Prediction of Crystal Nucleation Rates for Spherical Colloids, A Computational Study, Universiteit van Amsterdam, 27-11-2002.
- 16. Sander Pronk, Disorder in entropic solids, Universiteit van Amsterdam, 10 December 2003.
- 17. Fabrizio Capuani, Lattice-Boltzmann simulations of driven transport in colloidal systems, Universiteit van Amsterdam, 26 November 2004.
- 18. Ivan Coluzza, Writing with amino acids, Universiteit van Amsterdam, 23-6-2005.
- 19. Chantal Valeriani, Numerical studies of nucleation pathways of ordered and disordered phases, Universiteit van Amsterdam, 16-11-2007
- 20. Behnaz Bozorgui, Computational methods to study strongly-binding polymer-colloid systems, Universiteit van Amsterdam, 9-12-2008.
- 21. Jacobus ('Koos') A. van Meel, A numerical study on the enhancement and suppression of crystal nuncleation. Universiteit van Amsterdam, 20-10-2009.
- 22. Nienke Geerts, DNA-driven assembly of micron-sized colloids. Universiteit van Amsterdam, 27-11-2009.
- 23. Craig Kitchen, Investigating the Solubility of Proteins and Cucurbiturils by Computer Simulations. Cambridge University, 2013.
- 24. William ('Will') M.Jacobs, Theory of phase separation in protein solutions, Cambridge University, 2013.
- 25. Daniel Asenjo, Direct computation of the packing entropy of granular materials, Cambridge University, 2013
- 26. Tine Curk, Modeling Multivalent Interactions, Cambridge University, 2016
- 27. Lunna Li, Computational Methodology for Solubility Prediction, Cambridge University, 2016
- 28. Stefano Martiniani, On the complexity of energy landscapes: algorithms and a direct test of the Edwards conjecture, Cambridge University, 2017.
- 29. Raman Ganti, Microscopic Forces and Flows due to Temperature Gradients, Cambridge University, 2018.

- 30. Peter Wirnsberger, Simulation and prediction of thermally induced polarisation, Cambridge University, 2018.
- 31. Alex Cumberworth, Monte Carlo Simulation of DNA Origami Self-Assembly, Cambridge University, 2019.
- 32. Simon Ramirez Hinestrosa, Diffusiophoresis in complex and confined fluids, Cambridge University, 2020.