CHRIS LORENZ

1. PROFESSIONAL EXPERIENCE

King's College London London, UK
Reader, Theory & Simulation of Condensed Matter Group, Department of Physics
June 2016 - Present
Senior Lecturer, Theory & Simulation of Condensed Matter Group, Department of Physics
April 2013 - June 2016
Lecturer, Materials & Molecular Modelling Group, Department of Physics
Jan. 2011 – March 2013
Lecturer, Materials Research Group, Division of Engineering May 2007-Dec. 2010
Leads world-class research programmes focussed on using state-of-theart multi-scale molecular dynamics and Monte Carlo simulations to study a broad range of systems including heterogeneous lipid bilayers, nanofluids, self-assembly of complex systems, drug-delivery systems, solvation of biological molecules and nanotribology.
Assistant Director of the EPSRC Centre for Doctoral Training in Crossdisciplinary Approaches to Non-Equilibrium Systems (CANES).
Iowa State University Ames, IA, USA
Postdoctoral Research Associate, Dept. of Physics & Astronomy Jan. 2006 – April 2007
• Conducted molecular dynamics simulations of nanofluidics, stress of Langmuir monolayers and self-assembly of block polymers, which resulted in 6 papers published in peer-reviewed physical chemistry and physics journals.
Worked in collaboration with engineers and physicists on these projects.
Sandia National Laboratories Albuquerque, NM, USA
Postdoctoral Appointee,
Multi-scale Modelling & Computational Biology Group
Nov. 2001 – Dec. 2005
Generated code and algorithms for the Monte Carlo simulations code, TOWHEE, and for the massively parallel molecular dynamics code, LAMMPS.
Conducted research programmes in the fracture of epoxies and the nanotribological properties of self-assembled monolayers.
Worked on a large Department of Energy multi-disciplinary grant that was focused on using biopolymers in replacement of petroleum-based polymers.
Grant funded work at Sandia, two US universities and several corporations.
Attended planning meetings at DOE in Washington, D.C. to organize efforts of this research programme.

2. PUBLICATION LIST

Papers:
(78) "PRODAN differentially influences its local environment", Adam Suhaj, Alix Le Marois, Klaus Suhling, Christian D. Lorenz & Dylan M. Owen, Physical Chemistry Chemical Physics accepted (2018).
(77) "On the hydration structure of the pro-drug GPG-$NH_2$and its derivatives", Paul Smith, Nicola Steinke, John F. C. Turner, Sylvia E. McLain & Christian D. Lorenz, Chemical Physics Letters accepted (2018).
(76) "Proline and water stabilization of a universal two-step folding mechanism for β-turn formation in solution," Nicola Steinke, Anna Genina, Richard J. Gillams, Christian D. Lorenz & Sylvia E. McLain, Journal of the American Chemical Society doi: 10.1021/jacs.8b03643 (2018).
(75) "Glycerol solvates DPPC headgroups and localises in the interfacial regions of model pulmonary interfaces altering bilayer structure," Wachirun Terakosolphan,

Jemma L. Trick, Paul G. Royall, Sarah E. Rogers, Olimpia Lamberti, Christian D. Lorenz, Ben Forbes & Richard D Harvey, Langmuir doi: 10.1021/acs.langmuir.8b00866 (2018).
(74) "On the solvation of the phosphocholine headgroup in an aqueous propylene glycol solution," Natasha H. Rhys, Mohamed Ali Al-Badri, Robert M. Ziolek, Richard J. Gillams, Louise E. Collins, M. Jayne Lawrence, Christian D. Lorenz, & Sylvia E. McLain, Journal of Chemical Physics 148, 135102 (2018).
(73) "Towards optimised drug delivery: structure and composition of testosterone enanthate in sodium dodecyl sulfate monolayers," Yussif Saaka, Daniel T. Allen, Yuvared Luangwitchajaroen, Yanan Shao, Richard A. Campbell, Christian D. Lorenz & M. Jayne Lawrence, Soft Matter doi: 10.1039/C7SM01893B (2018).
(72) "Interaction of testosterone-based compounds with dodecyl sulphate monolayers at the air–water interface," Daniel T. Allen, Nikou Damestani, Yussif Saaka, M. Jayne Lawrence & Christian D. Lorenz, Physical Chemistry Chemical Physics 20, 8790-8801 (2018).
(71) “Driving spin-boson models from equilibrium using exact quantum dynamics, Gerard M. G. McCaul, Christian D. Lorenz & Lev Kantorovich, arXiv preprint.
(70) “Modelling a bistable system strongly coupled to a Debye bath: A quasiclassical approach based on the Generalized Langevin Equation”, Lorenzo Stella, Herve Ness, Christian D. Lorenz & Lev Kantorovich, Computational Methods in Science and Technology 23(3), 251-264 (2017).
(69) “A novel method for constructing continuous intrinsic surfaces of nanoparticles”, Daniel T. Allen & Christian D. Lorenz, Journal of Molecular Modeling 23, 219 (2017).
(68) “Nonequilibrium Generalised Langevin Equation for the calculation of heat transport properties in model 1D atomic chains coupled to two 3D thermal baths”, Herve Ness, Lorenzo Stella, Christian D. Lorenz & Lev Kantorovich, Journal of Chemical Physics, 146, 164103 (2017).
(67) “Partition-free approach to open quantum systems in harmonic environments: An exact stochastic Liouville equation,” Gerard G. McCaul, Christian D. Lorenz & Lev Kantorovich, Physical Review B 95, 125124 (2017).
(66) “On the hydration and conformation of cocaine in solution,” Richard J. Gillams, Christian D. Lorenz & Sylvia E. McLain, Chemical Physics Letters 676, 58-64 (2017).
(65) “Salt interactions in solution prevent urea from direct association with a peptide backbone,” Nicola Steinke, Anna Genina, Christian D. Lorenz & Sylvia E. McLain, Journal of Physical Chemistry B 121, 1866-1876 (2017).
(64) “Quantification of fibrous spatial point patterns from single-molecule localization microscopy (SMLM) data”, Ruby Peters, Marta Benthem Muniz, Juliette Griffie, David J. Williamson, George W. Ashdown, Christian D. Lorenz & Dylan M. Owen, Bioinformatics 33(11), 1703-1711 (2017).
(63) “Antimicrobial peptide potency is facilitated by greater conformational flexibility when binding to gram-negative bacterial inner membranes,” Sarah-Beth T. A. Amos, Louic S. Vermeer, Philip M. Ferguson, Justyna Kozlowska, Matthew Davy, Tam T. Bui, Alex F. Drake, Christian D. Lorenz & A. James Mason, Scientific Reports 6, 37639 (2016).
(62) “c-number quantum generalised Langevin equation of an open system,” Lev Kantorovitch, Herve Ness, Lorenzo Stella & Christian D. Lorenz, Physical Review B 94, 184306 (2016).
(61) “Specific effects of monovalent counter ions on the structural and interfacial properties of dodecyl sulphate monolayers,” Daniel T. Allen, Yussif Saaka, Luis Carlos Pardo, M. Jayne Lawrence & Christian D. Lorenz, Physical Chemistry Chemical Physics 18, 30394-30406 (2016).
(60) “Comparative atomic-scale hydration of the ceramide and phosphocholine head group in solution and bilayer environments,” Richard J. Gillams, Christian D. Lorenz & Sylvia E. McLain, The Journal of Chemical Physics 144, 225101 (2016).
(59) “Nonequilibrium processes from generalized Langevin equations: Realistic nanoscale

systems connected to two thermal baths," Herve Ness, Anna Genina, Lorenzo Stella, Christian D. Lorenz & Lev Kantorovich, Physical Review B 93,174303 (2016).
(58) "Molecular scale simulations of the self-assembly of amphiphilic molecules: Current state-of-the-art and future directions," Daniel T. Allen & Christian D. Lorenz, Journal of Self Assembly and Molecular Electronics, doi: 10.13052/jsame2245-4551.2015006 (2015).
(57) "Atomic scale insights into urea-peptide interactions in solution," Nicola Steinke, Richard J. Gilliams, Luis Carlos Pardo, Christian D. Lorenz & Sylvia E. McLain, Physical Chemistry Chemical Physics 18, 3862-3870 (2016).
(56) "Assembly of Influenza hemagglutinin fusion peptide trimers in phospholipid bilayer by coarse-grained simulations," Francesca Collu, Enrico Spiga, Christian D. Lorenz & Franca Fraternali, Fronteirs in Molecular Biosciences, doi: 10.3389/fmolb.2015.00066 (2015).
(55) "Atomistic description of pressure-driven flow of aqueous salt solutions through charged silica nanopores," Neil R. Haria & Christian D. Lorenz, Journal of Physical Chemistry C, 119 (22), 12298-12311 (2015).
(54) "Applications of the generalized Langevin equation: Towards a realistic description of the baths", Herve Ness, Lorenzo Stella, Christian D. Lorenz & Lev Kantorovich, Physical Review B 91, 014301 (2015).
(53) "Solvation and hydration of the ceramide headgroup in a non-polar solution," Richard James Gilliams, Jon V. Busto, Sebastian Busch, Felix M. Goni, Christian D. Lorenz & Sylvia E. McLain, Journal of Physical Chemistry B 119, 128-139 (2015).
(52) "On the short-range interactions of concentrated proline in aqueous solution," Sebastian Busch, Christian D. Lorenz, Jonathan Taylor, Luis Pardo & Sylvia McLain, Journal of Physical Chemistry B 118, 14267-14277 (2014).
(51) "Atomistic description of solubilisation of testosterone propionate in a sodium dodecyl sulphate micelle," Daniel T. Allen, Yussif Saaka, M. Jayne Lawrence, & Christian D. Lorenz, Journal of Physical Chemistry B 118, 13192-13201 (2014).
(50) "Generalized Langevin equation: An efficient approact to nonequilibrium molecular dynamics of open systems", Lorenzo Stella, Christian D. Lorenz, & Lev Kantorovich, Physical Review B 89, 134303 (2014).
(49) "Modulation of dipalmitoylphosphatidylcholine monolayers by dimethyl sulphoxide," Aleksandra P. Dabkowska, Louise E. Collins, David J. Barlow, Robert Barker, Sylvia E. McLain, M. Jayne Lawrence & Christian D. Lorenz, Langmuir 30(29), 8803-8811 (2014).
(48) "Plasticity and conformational equilibria of influenza fusion peptides in model lipid bilayers," Neil R. Haria, Luca Monticelli, Franca Fraternali, & Christian D. Lorenz, Biochimica et Biophysica Acta 1838 (4), 1169-1179 (2014).
(47) "On the structure of water and chloride ion interactions with a peptide backbone in solution," Sebastian Busch, Luis Carlos Pardo, William B. O'Dell, Chrystal D. Bruce, Christian D. Lorenz & Sylvia E. McLain, Physical Chemistry Chemical Physics 15 (48) 21023-21033 (2013).
(46) "Charge of water droplets in non-polar oils," Andreas M. Schoeler, Dimitris N. Josephides, Shariar Sajjadi, Christian D. Lorenz & Patrick Mesquida, Journal of Applied Physics 114, 144903 (2013).
(45) "Water mediation is essential to nucleation of β-turn formation in peptide folding motifs," Sebastian Busch, Chrystal D. Bruce, Christina Redfield, Christian D. Lorenz & Sylvia E. McLain, Angewandte Chemie International Edition 52(49), 13091-13095 (2013).
(44) "Traction and nonequilibrium phase behaviour of confined sheared liquids at high pressure," Chiara Gattinoni, David M. Heyes, Christian D. Lorenz, Danielle Dini & Hugh A. Spikes, Physical Review E 88, 052406 (2013).
(43) "Hybrid gelation processes in enzymatically gelled gelatin: impact on nanostructure, macroscopic properties and cellular response," Franziska Bode, Marcelo Alves da Silva, Paul Smith, Christian D. Lorenz, Seth McCullen, Molly M. Stevens, and Cecile

A. Dreiss, Soft Matter 9, 6986-6999 (2013).
(42) "Viscosity of nanoconfined water between hydroxyl basal surfaces of kaolinite: Classical simulation results," Neil R. Haria, Gary S. Grest and Christian D. Lorenz, Journal of Physical Chemistry B 117, 6096-6104 (2013).
(41) "On the nature of hydrogen bonding between the phosphatidylcholine head group and water and dimethylsulfoxide," Aleksandra P. Dabkowska, M. Jayne Lawrence, Sylvia E. McLain and Christian D. Lorenz, Chemical Physics 410, 31-36 (2013).
(40) "Pressure free sintering of silver nanoparticles to silver substrate using weakly binding ligands," Rajkumar Durairaj, Roya Ashayer, Hiren R. Kotadia, Neil Haria, Christian D. Lorenz, Omid Mokhtari and Samjid H. Mannan, IEEE Nano2012 (2012).
(39) "The delivered dose: Applying particokinetics to in vitro investigations of nanoparticle internalization by macrophages," Raha R. Ahmad Khanbeigi, Abhinav Kumar, Fethi Sadouki, Christian D. Lorenz, Ben Forbes, Lea Ann Daily and Helen L. Collins, Journal of Controlled Realease 162, 259-266 (2012).
(38) "Ion exclusion and electrokinetic effects resulting from electro-osmotic flow of salt solutions in charged silica nanopores," Neil R. Haria and Christian D. Lorenz, Physical Chemistry Chemical Physics 14, 5935-5944 (2012).
(37) "On the estimation of the curvatures and bending rigidity of membrane networks via a local maximum-entropy approach", Fernando Fraternali, Christian D. Lorenz and Gianluca Marcelli, Journal of Computational Physics 231 (2), 528-540 (2012).
(36) "On the solvation structure of dimethylsulfoxide/water around the phosphatidylcholine head group in solution," Aleksandra P. Dabkowska, Fabrizia Foglia, M. Jayne Lawrence, Christian D. Lorenz and Sylvia E. McLain, Journal of Chemical Physics 135, 225105 (2011).
(35) "Elucidating the origin of diastereoselectivity in a self-replicating system: Selfishness vs. Altruism", Arne Dieckmann, Sabrina Beniken, Christian D. Lorenz, Nikos L. Doltsinis and Gunter von Kiedrowski, Chemistry – A European Journal, 17,468 (2011).
(34) "Molecular dynamics simulations of the interfacial and structural properties of dimethyldodecylamine-N-oxide micelles", Christian D. Lorenz, Chien-Ming Hsieh, Cecile Dreiss and M. Jayne Lawrence, Langmuir 27, 546-553 (2011).
(33) "On the hydration of the phosphocholine headgroup in aqueous solution," Fabrizia Foglia, M. Jayne Lawrence, Christian D. Lorenz and Sylvia E. McLain, Journal of Chemical Physics 133, 145103 (2010).
(32) "Unravelling a fulvene based replicator: Experiment and Theory in Interplay," Arne Dieckmann, Sabrina Beniken, Christian D. Lorenz, Nikos L. Doltsinis and Gunter von Kiedrowski, Journal of Systems Chemistry, 1, 10 (2010).
(31) "Temperature control in molecular dynamic simulations of non-equilibrium processes," Dawid Toton, Christian D. Lorenz, Nikolaos Rompotis, Natalia Martsinovich and Lev Kantorovich, Journal of Physics – Condensed Matter, 22, 074205 (2010).
(30) "Nanotribology of water confined between hydrophilic alkylsilane self-assembled monolayers," Christian D. Lorenz, Michael Chandross, J. Matthew D. Lane and Gary S. Grest, Modelling and Simulation in Materials Science and Engineering, 18, 034005 (2010).
(29) "Probe-tip induced damage in compliant substrates," Michael Chandross, Christian D. Lorenz, Mark J. Stevens and Gary S. Grest, Journal of Manufacturing Science and Engineering, 132, 030916 (2010).
(28) "Large scale molecular dynamics simulations of vapor phase lubrication for MEMS," Christian D. Lorenz, Michael Chandross and Gary S. Grest, Journal of Adhesion Science and Technology, 24, 2453-2469 (2010).
(27) "Simulation study of the silicon oxide and water interface," Christian D. Lorenz, Mesfin Tsige, Susan B. Rempe, Michael Chandross, Mark J. Stevens, and Gary S. Grest, Journal of Computational and Theoretical Nanoscience, 7, 2586-2601 (2010).
(26) "Forces between functionalized silica nanoparticles in solution," J. Matthew D. Lane, Ahmed E. Ismail, Michael Chandross, Christian D. Lorenz and Gary S. Grest,

Physical Review E 79, 050501(R) (2009).
(25) “Molecular dynamics simulations of water confined between matched pairs of hydrophobic and hydrophilic self-assembled monolayers,” Christian D. Lorenz, J. Matthew D. Lane, Michael Chandross, Mark J. Stevens and Gary S. Grest, Langmuir 25 4535-4542 (2009).
(24) “Water penetration of damaged self-assembly monolayers,” J. Matthew D. Lane, Michael Chandross, Christian D. Lorenz, Mark J. Stevens, and Gary S. Grest, Langmuir 24, 5734-5739 (2008).
(23) “Molecular dynamics of ionic transport and electrokinetic effects in realistic silica channels,” Christian D. Lorenz, Paul S. Crozier, Joshua A. Anderson and Alex Travesset, Journal of Physical Chemistry C 112, 10222-10232 (2008).
(22) “Micellar crystals in solution from molecular dynamics simulations,” Joshua A. Anderson, Christian D. Lorenz and Alex Travesset, Journal of Chemical Physics 128, 184906 (2008).
(21) “General purpose molecular dynamics simulations fully implemented on graphics processing units,” Joshua A. Anderson, Christian D. Lorenz and Alex Travesset, Journal of Computational Physics 227, 5342-5359 (2008).
(20) “Hydrogen bonding and binding of polybasic residues with negatively charged mixed lipid monolayers,” Christian D. Lorenz, Jordi Faraudo and Alex Travesset, Langmuir 24, 1654-1658 (2008).
(19) “Simulations of nanotribology with realistic probe tip models,” Michael Chandross, Christian D. Lorenz, Mark J. Stevens and Gary S. Grest, Langmuir 24, 1240-1246 (2008).
(18) “Charge inversion of divalent ionic solutions in silica channels,” Christian D. Lorenz and Alex Travesset, Physical Review E 75, 061202 (2007).
(17) “Atomistic simulations of Langmuir monolayer collapse,” Christian D. Lorenz and Alex Travesset, Langmuir 22, 10016-10024 (2006).
(16) “Salt permeation and exclusion in silica and graphitic pores,” Kevin Leung, Susan B. Rempe, and Christian D. Lorenz, Physical Review Letters 96, 095504 (2006).
(15) “Tribological properties of alkylsilane self-assembled monolayers,” Christian D. Lorenz, Michael Chandross, Gary S. Grest, Mark J. Stevens, and Edmund B. Webb III, Langmuir 21, 11744-11748 (2005).
(14) “Nanotribology of anti-friction coatings in MEMS,” Michael Chandross, Christian D. Lorenz, Gary S. Grest, Mark J. Stevens and Edmund B. Webb III, The Journal of The Minerals, Metals and Materials Society 57, 55-61 (2005).
(13) “Frictional Dynamics of Perfluorinated Akylsilane Self-Assembled Monolayers,” Christian D. Lorenz, Mark J. Stevens, Ed B. Webb III, and Gary S. Grest, Tribology Letters 19, 93-98 (2005).
(12) “Frictional Dynamics of Fluorine-terminated Alkanethiol Self-Assembled Monolayers,” Byeongwon Park, Christian D. Lorenz, Michael Chandross, Mark Stevens, Gary S. Grest, and Oleg Borodin, Langmuir 20, 10007-10014 (2004).
(11) “Role of network connectivity on the mechanical properties of highly crosslinked polymers,” Mesfin Tsige, Christian D. Lorenz, and Mark J. Stevens, Macrmolecules 37, 8466-8472 (2004).
(10) “Fracture behavior of triglyceride-based adhesives,” Christian D. Lorenz, Mark J. Stevens, and Richard P. Wool, Journal of Polymer Science, Part B: Polymer Physics 42, 3333-3343 (2004).
(9) “Atomistic simulations of end-linked Poly(dimethylsiloxane) networks: Structure and relaxation,” David R. Heine, Christian D. Lorenz, Mesfin Tsige, Mark J. Stevens, and Gary S. Grest, Macromolecules 37, 3857-3864 (2004).
(8) “Fracture behavior of Lennard-Jones glasses,” Christian D. Lorenz and Mark J. Stevens, Physical Review E 68, 021802 (2003).
(7) “The effects of surface defects in a catalysis model,” Christian D. Lorenz, Ramin Haghgooie, Chavarous Kinnebrew, Wei Li, and Robert M. Ziff, Surface Science 517, 75-86 (2002).
(6) “Excess number of percolation clusters on the surface of a sphere,” Christian D.

Lorenz and Robert M. Ziff, Physica A 296, 1-8 (2001).
(5) "Precise determination of the critical percolation threshold for the three-dimensional 'Swiss cheese' model using a growth algorithm," Christian D. Lorenz and Robert M. Ziff, Journal of Chemical Physics 114, 3659-3661 (2001).
(4) "Similarity of percolation on the HCP and FCC lattices," Christian D. Lorenz, Rachelle May, and Robert M. Ziff, Journal of Statistical Physics 98, 961-970 (2000).
(3) "Shape-dependent universality in percolation," Robert M. Ziff, Christian D. Lorenz, and Peter Kleban, Physica A 266, 17-26 (1999).
(2) "Universality of the excess number of clusters and the crossing probability function in three-dimensional percolation," Christian D. Lorenz and Robert M. Ziff, J. Phys. A: Math. Gen. 31, 8147 (1998).
(1) "Precise determination of the bond percolation thresholds and finite size scaling corrections for the sc, fcc, and bcc lattices," Christian D. Lorenz and Robert M. Ziff, Phys. Rev E 57, 230 (1998).
Book chapters:
(3) Guiseppe Milano, Irene Marzuoli, Christian D. Lorenz & Franca Fraternali, "Self-Assembly at the Multi-Scale Level: Challenges and New Avenues for Inspired Synthetic Biology Modelling", In: Synthetic Biology (ed. Maxim Ryadnov, Luc Brunsveld & Hiroaki Suga), Royal Society of Chemsitry, in press, 2017.
(2) Christian D. Lorenz and Nikos L. Doltsinis, "Molecular dynamics simulations: From "Ab Initio" to "Coarse Grained"", In: Handbook of Computational Chemistry (ed. J. Leszczynski), Springer, 1-61, 2016. (doi: 10.1007/978-84-007-6169-8_7-2)
(1) Christian D. Lorenz and Nikos L. Doltsinis, "Molecular dynamics simulations: From "Ab Initio" to "Coarse Grained"", In: Handbook of Computational Chemistry (ed. J. Leszczynski), Springer, 195-238, 2012.

3. INVITED TALKS
(18) "Investigating the beginnings of fibronectin fibrillogenesis on different interfaces," at the CNR Nano Istituto Nanoscienze in Modena, Italy – June 2018.
(17) "Investigation of the hydration and structure of model lipid membranes," at the African Materials Research Society national meeting in Gaborone, Botswana --- December 2017.
(16) "Interaction of lipid head groups with their environment," in the Department of Biochemistry seminar series at the University of Oxford, Oxford, UK --- July 2017.
(15) "HPC & SASSIE modelling of detergent micelles", at the 4th Annual CCP-SAS Project Workshop, Cardiff University, Cardiff, Wales, UK --- June, 2017.
(14) "Ion transport, ion exclusion, and electrokinetic effects in silica nanopores", at the CECAM Meeting Chemical Energy at the Nanoscale: Simulation Meets Experiment, Zaragoza, Spain – April, 2016.
(13) "Molecular dynamics simulations of the structural and dynamic properties of confined water", at the 39th Annual Meeting of the Adhesion Society, San Antonio, Texas, USA – February, 2016.
(12) "Ion transport, ion exclusion, and electrokinetic effects in silica nanopores", at the Institut Lumiere Matiere, Lyon, France – November, 2015.
(11) "Multi-scale modelling of self-assembly of surfactants and polymers", at Queen's University Belfast, Belfast, Northern Ireland – October, 2015.
(10) "Multi-scale simulations of the 'jigglings and wigglings' of peptides in solution and at interfaces", at Max Planck Institute for Polymer Research, Mainz, Germany. – March, 2015.
(9) "Ion transport, ion exclusion, and electrokinetic effects in silica nanopores", at the Non-Equilibrium Simulation School at Imperial College London – Sept., 2014.
(8) "Water mediated interactions with GPG peptide" at the CNR Nano Istituto Nanoscienze in Modena, Italy – August, 2013.
(7) "Ion transport, ion exclusion, and electrokinetic effects in silica nanopores", at the University of Warwick – March, 2012.
(6) "Molecular dynamics simulations of protein-lipid and lipid-lipid interactions," at

University of Salerno, Italy – July, 2010.
(5) "Molecular dynamics simulations of confined water under shear," at the ACAMSFI SimBioMa-ESF Workshop: Molecular Friction, University College Dublin, Dec. 2009.
(4) "Structural and mechanical properties of thin films and self-assembled structures," at the Membrane Biophysics Platform Meeting, Windsor, 16 April 2009.
(3) "Molecular dynamics simulations of water confined between matched pairs of hydrophobic and hydrophilic self-assembled monolayers," at the Advances in Boundary Lubrication and Boundary Surface Films, Sevilla, Spain, 2 April 2009.
(2) "Hydrogen bonding and binding of polybasic residues with negatively charged mixed monolayers," at SoftMatter 2008: Workshop on Electrostatic Effects in Soft Matter: Bringin Experiments, Theory and Simulation Together, Universitat Autonoma de Barcelona, 2008.
(1) "Fracture behavior of triglyceride-based adhesives," talk at the Joint Meeting of the 2nd International Conference on Green and Sustainable Chemistry and the 9th Annual Green Chemistry and Engineering Conference: Taking Measure of Green Progress: Opportunites to Meet Global Challenges, 2003.

4. RESEARCH GRANTS

(12) "How do membrane active antibiotics influence microbiome dysbiosis?", Public Health England, James Mason (KCL, Institute of Pharmaceutical Science), Rachel Tribe (KCL, Women's Health), Kenneth Bruce (KCL, Institute of Pharmaceutical Science) & Christian D. Lorenz (KCL, Physics), 2017-2021, £28,000.
(11) "Lipid aggregation : connecting new and established approaches", King's Together 2017, Maria Sanz (KCL, Chemistry), Sarah Berry (KCL, Chemistry) & Christian D. Lorenz (KCL, Physics), 2017-2018, £20,000.
(10) "ICANES", King's Together 2016, Peter Sollich (KCL, Maths), Joe Bhaseen (KCL, Physics) & Christian D. Lorenz (KCL, Physics); 2016-2017, £20,000.
(9) "Ionic ferning for improved desalination of sea water", King's Together 2016, Guy Carpenter (KCL, Mucosal & salivary biology), Brian Sutton (KCL, Randall Division) & Christian D. Lorenz (KCL, Physics); 2016-2017, £20,000.
(8) "Red Cell Physical Properties in Health and Disease", EPSRC (EP/N007980/1), Peter Petrov (Exeter, Physics), Christian D. Lorenz (KCL, Physics) & Gianluca Marcelli (Kent, Engineering & Digital Arts); 2016-2019, £759,359.
(7) "EPSRC Centre for Doctoral Training of Cross-disciplinary Approaches to Non-Equilibrium Systems (CANES)", EPSRC (EP/L015854/1), Director: Peter Sollich (KCL, Maths), Co-directors: Christian D. Lorenz (KCL, Physics) & Joe Bhaseen (KCL, Physics), Assistant directors: Franca Fraternali (KCL, Randall Division) & Bruce Malamud (KCL, Geography); 2014-2022, £3,868,978.
(6) "NANOHAT: Development of a safer and more effective sleeping sickness drug," MRC DPFS/DSC (MR/K105451/1), PI: Dr. Sarah Thomas (KCL, IPS), Co-I: Christian D. Lorenz; Cecile Dreiss (KCL IPS); Prof. Santa Persaud (KCL, Division of Diabetes and Nutritional Sciences); Dr. Vanessa Yardley & Prof. Simon Croft (London School of Hygene & Tropical Medicine); Dr. Mark Christie (KCL, IPS); 2012-2015, £766,795.00.
(5) "Program Development for the Molecular Simulation of Protein-Surface Interactions," Marie Curie Fellowship, Co-PI: Prof. Robert Latour, Clemson University; Christian D. Lorenz, 2012-2013, £151,000.
(4) "Thermostatting open systems in non-equilibrium computer simulations," EPSRC (EP/J019259/1), Co-PI: Prof. Lev Kantorovich (KCL, Physics) & Christian D. Lorenz, 2012-2016, £389,669.00
(3) "Structural studies of atomic interactions in membranes: bridging the gap between physics and membrane biology," PI: Sylvia McLain, Oxford University; Co-I: Christian D. Lorenz, 2011-2016, £1,345,000.
(2) "Lipid domain formation," BBSRC PhD studentship to start Fall 2010.
(1) "Probing the internal structure of ethyl butyrate containing microemulsions using

SANS", Ref. No. RB910520 - £40,000 – Beam time proposal with Jayne Lawrence (KCL Pharmacy), 2008.

5. PAST & CURRENT MEMBERS OF RESEARCH GROUP

Postdoctoral Research Assistants:

• Jemma Trick: 2016 – 2018: Centre Manager for the EPSRC Centre for Doctoral Training in Cross-disciplinary Approaches to Non-Equilibrium Systems (CANES) at King's College London

• Hevre Ness: 2013 – 2017: PDRA at King's College London with Prof. Mark von Schilfgaarde

• Lorenzo Stella: 2012-2013: Lecturer at Queen's University Belfast

PhD Students:

• May Yee: 2017-current

• Paul Smith: 2017-current

• Rob Ziolek: 2017-current: CANES CDT student (w/ Prof. Franca Fraternali & Dr. Dave Barlow)

• Adam Suhaj: 2017-current: LIDo DTP student (w/ Dr. Dylan Owen)

• Demi Pink: 2017-current: LIDo DTP student (w/ Prof. Jayne Lawrence)

• Irene Marzuolli: 2016-current: CANES CDT student (w/ Prof. Franca Fraternali)

• Mateusz Bieniek: 2015-current: Crick/KCL studentship (w/ Dr. Willie Taylor)

• Philip Ferguson: 2015-current: Pharmaceutical Sciences (w/ Dr. James Mason)

• Gerard McCaul: 2015-current: CANES student (w/ Prof. Lev Kantorovich)

• Christian Jorgensen: 2013-current: Transferred to my group from Carmen Domene's group when she left for Bath.

• Daniel Allen: 2013-2017, Python Developer at Lambert Labs; 2017, Software Engineer, Scrape Technologies; 2017 - current : Thesis: 'Multi-scale simulations of selfassembly and drug encapsulation of colloidal and polymeric micelles'

• Neil Haria: 2009-2013, Postdoc at Warwick University; 2014-2016, Global Valuation Ltd.; 2016 – 2018, Data Scientist at IQVIA; 2018-Current : Thesis: 'Molecular dynamics simulations of nanofluidic systems: from desalination to protein adsorption'

• Yu-Lin Chen: co-supervisor, 2008-2012: Thesis: 'Modeling the behaviour of drug molecules at the blood-brain barrier'

MPhil/MSc Students

• Edward Lambert: M.Sci., 2018: Molecular dynamics simulations of the interaction between toxins and model red blood cell membranes

• Paul Smith: M.Sci., 2017: Molecular dynamics simulations of the constituents of synovial fluid

• Sarah-Beth Amos: M.Res., 2016: Molecular dynamics of the mechanisms of action of antimicrobial peptides

• Mariella De Piano: Master's thesis, 2013 (Uni. Salerno, Italy): Thesis: 'Modelling of ionic interactions with model red-blood cell lipid membranes'

• Louise Collins: M.Phil., 2012: Thesis: 'Molecular scale understanding of lipid raft formation from scattering experiments and molecular dynamics simulations'

• Rossella Giordano: Master's thesis, 2012 (Uni. Salerno, Italy): Thesis: 'Modelling of force propogation in granular materials'

Summer Research Students/Project Students

• Kieran Borchard (2018)

• Patrick Simcock (2018)

• Zelong Zhao (2017)

• Vemal Mistry (2017)

• Olimpia Lamberti (2016)

• Yongshen "Lyndon" Li (2016)

• Leyla Doroudi (2015)

• Anna Genina (2014 & 2015)

• Nikou Damestani (2015)

• Daniel West (2015)

• Holly Farler (2015)
• Thomas Bossingham (2015)
• Simone Caenazzo (2010-2012)

ADMINISTRATIVE DUTIES

• Served as Career Services Liaison for the students of the Division of Engineering (2007-2012)
• Served as Senior Tutor for the Department of Physics (2012 - 2014)
• Awarded Personal Tutor of the Year in NMS Faculty (2014)
• Alumni Liaison for the Department of Physics (2012-2016)
• Serving as Cohort Tutor for the EPSRC CDT in CANES (2014-2015 Cohort)
• Postgraduate Admissions Tutor for the Department of Physics (2015-2016)
• Assistant director of the EPSRC Centre for Doctoral Training in Cross-disciplinary Approaches to Non-Equilibrium Systems (CANES) (2014-).
• Elected by the faculty to serve as the Senior Representative of the Faculty of Natural & Mathematical Sciences to the Academic Board at King's College London (2016-).
• Assistant director of the Centre for Non-Equilibrium Science (CNES) (2017-).

TEACHING EXPERIENCE

• Engineering Maths 1B (2007-2009): A first-year second semester mathematics course in the Department of Engineering at KCL, which focussed on solving ordinary differential equations, multi-variable calculus, statistics and probability. Designed and delivered module.
• Rapid Prototyping Engineering (2007-2009): A Master's level course in the Department of Engineering at KCL, which covered the materials, computational methods and design procedures which are instrumental in the emerging technology of rapid prototyping. Designed and delivered module.
• Introduction to Financial Engineering (2009-2010): A Master's level course in the Department of Engineering at KCL, which covered various modelling approaches used in Financial Engineering ranging from Black-Scholes to Monte Carlo. Designed and delivered module.
• Sensors and Actuators (2010-2012). A Master's level course in the Department of Engineering at KCL, which covered the underlying theory and mechanisms that are used in a variety of engineering relevant sensors and actuators.
• Computational Lab (2013-2014). A second-year computational lab course in the Physics Department at KCL, which was used to introduce undergraduate students to the basics of the underlying theory and how to use and apply a variety of computational simulation techniques that are generally applied in the area of computational materials research. Designed and delivered module.
• Bio- and Nanomaterials in the Virtual Lab/Simulation Methods for Non-equilibrium systems (2014-): A Master's level course that is co-listed in the Department of Physics and within the CANES CDT. The two courses have the same root but there is some deviation of content for the two student population. Basis is to introduce them to the underlying theory and application of simulation methods for studying bio/nano/non-equilibrium problems. I have designed and delivered these modules.

6. SKILL SETS AND EXPERTISE

• Prolific computer programming in multiple languages: C/C++, Fortran 77/90, Perl, Python.
• Generating algorithms for massively parallel molecular dynamics computer code called LAMMPS (C++). Recent algorithms are aimed at allowing scientists to simulate systems that were previously unable to be simulated (i.e. reactive systems) and for phenomena that previously were not feasible (temperature-driven transport). Also contributed to the development of the GPU-based molecular dynamics code called HOOMD.
• Developing algorithms for single-processor Monte Carlo computer code called TOWHEE (Fortran-90). Algorithms are aimed at using novel methods to find minimum

energy structure of proteins and forcefield development using genetic algorithms.

PROFESSIONAL ACTIVITIES

• SCI Treasurer for the RSC/SCI Joint Colloids & Interfacial Science Committee (2016-current)

• Member of Thomas Young Centre's steering committee at King's College London. Organize local workshops and seminars highlighting the research of the global leaders in the field of computational materials modelling.

• Organized the Biological Interfaces: A Thomas Young Centre Workshop. Invited speakers, developed schedule for two-day workshop attended by over 100 scientists from across the globe.

• Organized the CECAM Workshop on "Protein assemblies at the interface of functionalised materials" (17/9/2014 – 19/9/2014), Lausanne, Switzerland, ~£30,000 budget with 30 participants.

• Referee manuscripts for several journals including Scientific Reports, Physical Review Letters, Journal of Physical Chemistry B, Langmuir, Physical Review E, Fluid Phase Equilibrium, Wear, Composites Science and Technology, PLoS-One, Journal of Chemical Physics, Journal of Physics – Condensed Matter, Macromolecules, Molecular Simulation, Computational Biology and Chemistry, Chemical Sciences, BBA-Biomembranes, Soft Matter, PCCP, Journal of Applied Physics, Langmuir, Journal of Physical Chemistry Letters, Journal of Physical Chemistry C, & Biophysical Journal.

• Academic editor for PLoS One.

• Member of the Review Editor & Editorial Board of Colloidal Materials and Interfaces, a speciality of Frontiers in Materials.

• Member of the editorial board of Scientific Reports.

• External evaluator of research proposals for the Biology & Biological Sciences Research Council in the UK, Greek Ministry of Education, Lifelong Learning and Religious Affairs and the National Science Foundation in the United States of America.

EDUCATION

University of Michigan, School of Engineering Ann Arbor, MI
Ph.D. in Chemical Engineering Jan. 1998 – Oct. 2001

University of Michigan, School of Engineering Ann Arbor, MI
Combined Bachelor of Science and Engineering & Master of Science and Engineering in Chemical Engineering
Sept. 1992 – Dec. 1997